

**Search for boosted Higgs boson
and other resonances decaying
into b -quark pairs using the ATLAS detector
and studies of
CMOS pixel sensors for the HL-LHC**

THÈSE

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**«Search for Boosted Higgs Boson
and other Resonances Decaying
into b -quark Pairs Using the ATLAS Detector
and Studies of
CMOS Pixel Sensors for the HL-LHC»**

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The Large Hadron Collider (LHC) at CERN is the largest particle collider ever built and enables experimental study of the fundamental constituents of matter at the highest centre-of-mass energy ($\sqrt{s}$) ever achieved. Between 2015 and 2018, the LHC provided proton-proton collisions at a record energy of $\sqrt{s} = 13$ TeV.

In this thesis, two novel analyses looking for jets stemming from the hadronization of b -quarks (b -jets) are presented together with a detailed description of the tools and the related recent improvements for identifying the jets produced by beauty quarks (b -tagging). The first analysis is an inclusive search for boosted Higgs bosons decaying into a pairs of b -quarks using 80.5 fb^{-1} . This search has long been considered impossible due to the overwhelming QCD background. However, recent developments in the reconstruction of boosted environments made it possible to search inclusively for $H \rightarrow b\bar{b}$. In the signature used in the analysis the Higgs boson acquires high transverse momentum by recoiling against an initial jet. When the transverse momentum of the Higgs boson becomes larger than twice its mass, the subsequent decay products tend to merge and are effectively better identified by constructing a single jet with a large radius parameter of 1.0. An evidence of $W/Z+jets$ processes is also presented. This represents the first measurement performed by the ATLAS experiment of vector bosons in the boosted regime with heavy-quarks in the final state. In addition, exclusions limits are placed on resonant dark matter mediator models. The second analysis is a search for heavy resonances with masses above 1.1 TeV decaying to one or two b -quarks, producing two isolated jets in a back-to-back topology. The analysis was performed with the full dataset collected at 13 TeV which corresponds to 139 fb^{-1} . For both analyses it is crucial to identify jets initiated by heavy quarks with high accuracy. The performance of the algorithm which discriminates between jets initiated by b -quarks against jets initiated by c - or light-flavored quarks or gluons is discussed. The addition of novel b -tagging techniques which significantly improve the performance at high transverse momentum

are also presented.

Looking to the future, the physics programme at the LHC will be expanded by the High-Luminosity LHC (HL-LHC) project foreseen to start in 2024. The integrated luminosity will be increased to 3000 fb^{-1} . Such a high luminosity poses unique challenges in terms of radiation-hardness of the detectors. A novel technology of pixels detectors based on the commercially available CMOS manufacturing processes was studied during this thesis. Results of test-beam measurements show high detection efficiency under unprecedented radiation conditions.

Le collisionneur de hadrons (LHC) du CERN est le plus grand collisionneur de particules jamais construit qui permet l'étude expérimentale des constituants fondamentaux de la matière au plus haut niveau d'énergie du centre de masse ($\sqrt{s}$) jamais atteint. Entre le 2015 et le 2018, le LHC a fourni collisions proton-proton à une énergie record de $\sqrt{s} = 13$ TeV. Dans cette thèse, deux nouvelles analyses à la recherche de jets issus de l'hadronisation des b -quarks (b -jets) sont présentés. La première analyse est une recherche inclusive de la désintégration des bosons de Higgs en paires de b -quarks en utilisant 80.5 fb^{-1} . Cette recherche a longtemps été considérée impossible en raison de l'haute niveau de bruits de fonds. Cependant, les récents développements dans la reconstitution d'environnements boostés ont permis de rechercher de manière inclusive $H \rightarrow b\bar{b}$. Dans la signature utilisée dans l'analyse, les bosons de Higgs acquièrent une haute énergie en reculant contre un jet. Lorsque le moment transversal du boson de Higgs devient plus grand que deux fois sa masse, les produits de cette désintégration sont effectivement mieux identifiés en construisant un seul jet avec un rayon de paramètre 1.0. Une évidence des processus $W/Z + jets$ est présentée pour la première fois par l'expérience ATLAS dans le régime boostés avec des quarks lourds dans l'état final. De plus, des limites d'exclusions sont placés sur des modèles résonants de matière noire. La deuxième analyse est une recherche de résonances lourde de masses supérieures à 1.1 TeV qui se décomposent en un ou deux b -quarks, produisant deux jets isolés. L'analyse a été réalisée avec toutes les données recueillies à 13 TeV, qui correspondent à 139 fb^{-1} . Pour les deux analyses c'est crucial d'identifier les jets initiés par des quarks lourds avec une grande précision. De nouvelles b -tagging techniques, qui améliorent considérablement la performance à haut moment transversal, sont également présentées.

À l'avenir, le programme de physique du LHC sera élargi par le projet à haute luminosité (HL-LHC) qui démarrera en 2024. La luminosité intégrée sera augmentée à 3000 fb^{-1} . Une luminosité aussi élevée pose des défis uniques en termes d'irradiation

des détecteurs. Une nouvelle technologie de détecteurs des pixel basée sur la procédure de fabrication CMOS a été étudiée au cours de cette thèse. Les résultats des mesures du faisceau de test montrent une grande efficacité de détection sous conditions de radiation sans précédent.

Personal contributions

The ATLAS collaboration consists of about 3000 scientists working together to ensure stable detector operation, data-processing and calibrations to name but a few. The most significant contributions of the author are listed below:

- *b*-tagging characterization (Chapter 4): The author characterized the performance of the *b*-tagging algorithms for the analysis of the full data-set collected with $\sqrt{s}=13$ TeV (referred to as Run2). In particular, a new training strategy to optimize the performance at high- p_T was implemented. Novel taggers such as a recurrent neural network and a soft-muon tagger were integrated, characterized and validated to improve the *b*-tagging performance. The improvements in light-jet rejection at 77 % *b*-jet efficiency are a factor of ~ 3 better than the previous *b*-tagging configuration for a jet- p_T of ~ 600 GeV. The *b*-tagging performance on MC simulations needs to be corrected to match the performance in collision data. To do this, dedicated calibration analyses are employed. These calibrations adjust the efficiency of pre-defined *b*-efficiency values, the so-called working points. The author defined the *b*-tagging working points used by the ATLAS collaboration in Run2. The results of this work are documented in [1, 2].
- Search for heavy resonances decaying into one or two *b*-quarks (Chapter 5): The author coordinated and validated the QCD background estimate for the high-mass resonance search with one or two *b*-quarks in the final state. It is particularly interesting to address the impact of the improved *b*-tagging performance at high p_T given that the analysis probes the highest energy regime provided by the LHC. A factor of ~ 2.5 improvement in the exclusions limits was observed with the updated *b*-tagging configuration. The results of the analysis are documented in [3].

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- A new algorithm for b -tagging very energetic jets (Chapter 5): A new approach for b -tagging very high-energy jets was studied. The idea of this new algorithm is to exploit the fact that at very high transverse momentum the lifetime of the b -hadron increases together with the collimation of its decay products. Using the high spatial resolution of the inner detector, a small cone, used to count the number of pixel hits around the jet-axis can be defined. Such an algorithm was studied and integrated with the other track-based b -tagging algorithms. It was shown that this trackless approach is able to exploit complementary information compared to the other b -taggers. This work triggered an on-going effort to further develop this algorithm for the next data-taking period starting in 2021.
 - Search for boosted Higgs bosons and other resonances (Chapter 6): The author was one of the main analyzers of a new analysis searching for boosted Higgs bosons and other new resonant particles decaying into b -quark pairs. The author mainly contributed to trigger selections, QCD multi-jet background and $t\bar{t}$ background estimates and the statistical interpretation of the results. The analysis also provided the first evidence of the event yields of W/Z in $b\bar{b}$ final states in a boosted regime. The results of the analysis are documented in [4].
 - Characterization of HV-CMOS pixel sensors (Chapter 8): The author took part in an R&D effort to demonstrate the feasibility of using HV-CMOS pixel sensors at a high-rate and a high-radiation environment. The author contributed to the characterization of a Telescope for test-beam analysis developed at the University of Geneva, to the characterization of CMOS pixel prototypes using TCAD simulations and laboratory measurements and was a main analyzer of the test-beam data collected at the CERN SPS and the Fermilab facilities. He was co-author of *proteus* [5], a C++ software for test-beam reconstruction which is now used by different teams of the ATLAS silicon test-beam group. The results of this work are documented in [6–9].

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Introduction

The current knowledge of elementary particles and their interactions is given by the Standard Model (SM) of particle physics. SM predictions have shown an astonishing compatibility with measurements performed by a large variety of experiments over more than fifty years. Despite this very solid theoretical framework, many questions remain unanswered. For example, the SM does not provide a source for the matter-antimatter asymmetry and it does not explain the origin of dark matter. Over the years, many theories which expand and complement the SM have been proposed. However, there is still no experimentally verified theory describing "new physics" beyond the SM. From an experimental perspective, it becomes progressively more important to improve the analysis techniques employed in searches for possible deviations from the SM. Among those, the ability to identify jets originating from heavy-flavor quarks is key to many aspects of the physics programme pursued by general-purpose experiments at a hadron collider, such as the ATLAS experiment at the Large Hadron Collider (LHC).

This thesis presents the results of the search for boosted Higgs bosons and the search for heavy resonances, both in b -quark final states. In addition, the algorithms used to identify b -jets, and their related performance, are presented with emphasis on novel tagging techniques which significantly improve the performance at high transverse momentum. The search for heavy resonances was performed using the full 139 fb^{-1} dataset collected in Run2. Exclusion limits are set on a number of benchmark models with a mass larger than 1.1 TeV . This analysis is used as a demonstrator to study the benefits of the improvements in the performance of b -jet identification. An improvement in the analysis sensitivity of a factor of ~ 2.5 was observed compared to the previous b -tagging configuration.

The search for boosted Higgs bosons decaying to pairs of b -quarks is also presented. The analysis, performed for the first time by the ATLAS experiment, is based on the

data collected in 2015, 2016 and 2017 corresponding to a cumulative luminosity of 80.5 fb^{-1} . The aim of the analysis is to probe the Yukawa coupling between the Higgs boson and the b -quark at very high energy. In addition, the yield of the $W/Z+jets$ process with heavy-quarks in the final state was also observed with a significance of 5σ . The latter measurement is particularly relevant to validate the QCD multi-jet background estimation procedure and the challenging reconstruction techniques employed in the analysis. In addition, exclusion limits on dark matter mediator models with masses between 100 and 200 GeV are also set, complementing the mass reach of the other analysis presented in this thesis.

The LHC is routinely upgraded during dedicated development periods, alternating with the time allocated to collisions. In order to enlarge the physics reach of the LHC, a major upgrade of the machine, called the High-Luminosity LHC (HL-LHC) is foreseen to start in 2024. The HL-LHC aims to increase the total integrated luminosity to 3000 fb^{-1} . This poses unique challenges in terms of the required radiation hardness of the detectors. In particular, the inner tracking detector will be fully replaced with a full-silicon tracker, the ITk. A characterization of a novel technology of pixel sensors based on the CMOS manufacturing process is discussed in this thesis. An extensive test-beam campaign was conducted to study the performance of several sensor prototypes at different irradiation levels. In particular, a high detection efficiency above 99 % was obtained for prototypes irradiated at $1 \cdot 10^{15} \text{ n}_{eq}/\text{cm}^2$, which corresponds to the irradiation level expected for an outer pixel layer of the ITk. With these promising results obtained for small prototypes, a full-size demonstrator was also produced and characterized.

This thesis is organized as follows. The SM is introduced in Chapter 1, including a more detailed discussion on boosted Higgs boson and dark matter mediators. In Chapter 2 the LHC accelerator and the ATLAS detector are presented. A brief description of jet reconstruction at the LHC is given in Chapter 3. The techniques employed for the identification of heavy-flavored jets are introduced in Chapter 4. Chapter 5 is devoted to the search for heavy resonances decaying to pairs of b -quark, where the improvements in the analysis results due to the upgraded b -tagging techniques are discussed. This Chapter also presents results of an innovative approach to identify b -jets at very high transverse momentum. In Chapter 6 the result of the search for boosted Higgs bosons and other narrow resonances in the $b\bar{b}$ final state is discussed. Chapter 7 describes the main properties of silicon detectors and in Chapter 8 the results of the characterization of the CMOS pixel detector are presented. Concluding remarks can be found in Chapter 9.

CHAPTER 1

The theory framework

The theory describing the dynamics of elementary constituents of matter is called the Standard Model of particle physics (SM). The SM has successfully described the electromagnetic, weak and strong interactions throughout a glorious period for particle physics with alternating theoretical predictions and experimental measurements. More recently, the only missing piece towards the completion of the SM, the Higgs boson, was discovered by the ATLAS and CMS collaborations.

Although there are no formal limitations of the SM predictions before the *Planck* scale $\sim 10^{19}$ GeV, where the effects of gravitational force are expected to become apparent, the SM leaves many unanswered questions. Among those, astrophysical measurements give evidence for an elusive form of matter, called Dark Matter (DM). From astrophysical and cosmological measurements it is inferred that DM is massive, weakly interacting, stable and makes up around 85 % of the composition of matter in the universe. The models describing DM usually predict new resonances produced in LHC collisions which decay either to SM particles or to other DM particles producing different signature in the detectors. A different approach to search for extensions of the SM is to postulate a scale of new physics Λ high enough such that it will manifest itself through deviations of known observable, usually at high energies.

The work conducted for this thesis explores both methodologies: searches for DM particles will be discussed and a search for Higgs bosons at high transverse momentum will be presented.

In this chapter, a concise description of the SM will be presented, from the gauge principle to the description of the spontaneous symmetry breaking mechanism and the

Higgs boson discovery by the ATLAS and CMS collaborations. Finally, a discussion on new physics mechanisms manifesting as deviations from the expected high-energy cross section of the Higgs boson and a description of dark-matter searches at the LHC will be given.

1.1 The gauge principle in quantum field theory

The mathematical framework of the SM is based on a quantum field theory description of the particles and their interactions. Quantum field theory is a synthesis of quantum mechanics and special relativity. To introduce the theory, it is instructive to start from the Lagrangian formalism developed in classical mechanics, extend this formalism to classical field theory and finally to quantum field theory.

The starting point is the Lagrangian which is defined as the difference between the kinetic and the potential energy of the system:

$$L(q, \dot{q}) = (m/2)(\dot{q})^2 - V(q) \quad (1.1)$$

a second fundamental quantity, the *action*, is then defined as $S = \int dt L(q, \dot{q})$. Using a variational approach it can be shown that for any possible variation of the path of the particle, δq , the equation of motion of the system is the one that minimizes the *action*. The resulting equations are called the *Euler-Lagrange* equations:

$$\frac{\partial L}{\partial q} - \frac{\partial}{\partial t} \frac{\partial L}{\partial \dot{q}} = 0 \quad (1.2)$$

With the dynamics of a particle defined, it is possible to extend the formalism developed in classical mechanics to field theory. The first step is to generalize the path of a particle which is only a function of time $q(t)$, into a function which depends on space-time coordinates $\phi(x)$. One of the main differences arising from this extension is that the representations of the field can acquire, not only a scalar representation, but also vectorial or tensorial form thanks to the Lorentz invariance properties of the space-time. Of particular interest for particle physics is a sub-set of the vectorial representations called spinors. Spinors are dimension two representations and are divided into left-handed and right-handed, depending on their chirality: ψ_L and ψ_R . A convenient representation to describe the dynamics of relativistic particle is the *Dirac* spinor $\Psi = (\psi_L, \psi_R)$ which is at the same time a representation for Lorentz and parity transformations.

The dynamics of a free spinor field are described by the following Lagrangian which is invariant under Lorentz transformation of the fields:

$$\mathcal{L}_D = \bar{\Psi}(i\gamma^\mu \partial_\mu - m)\Psi \quad (1.3)$$

where γ , also called Dirac matrices, are built as an extension of the Pauli matrices into a four dimensional space-time. In addition, QFT describes local phenomena, it is thus more appropriate to use the Lagrangian density, $L = \int \mathcal{L}(\phi, \partial_\mu \phi)$. It can be shown that the *Euler-Lagrange* equations, initially derived for classical mechanics, are also satisfied in classical field theory.

The second fundamental point towards the building of a quantum field theory is a theorem relating symmetries of the system to conserved quantities; this is Noether's theorem. Through this theorem, symmetries become a fundamental building block of the physical theory. A particular set of transformations, called gauge transformations, which by construction leave invariant the Lagrangian of the SM constitute a building principle of the SM itself. Gauge invariance will be introduced more formally using classical electrodynamics as an example in the following.

Let us consider a transformation of the form:

$$\Psi \rightarrow e^{i\theta} \Psi \quad (1.4)$$

in the terminology of group theory, this is an example of a global $U(1)$ transformation. It can be easily shown that $\mathcal{L}_D$ is invariant under such a transformation and that the related conserved current is $\bar{\Psi} \gamma^\mu \Psi$. It is however more interesting to promote this global symmetry into a local symmetry: $\theta \rightarrow \theta(x)$ meaning that gauge invariance is required in each point of the space-time. The Lagrangian is no longer invariant under this transformation due to the covariant derivative which leads to unbalanced term of the form $\partial_\mu \theta$. To make the Lagrangian explicitly invariant, the inclusion of an additional field, which mediates the forces, is needed. In electromagnetism this is the photon whose dynamics are given by Maxwell's equation. The action of Maxwell's equations is expressed in a covariant form as: $-\frac{1}{4} F_{\mu\nu} F^{\mu\nu}$ where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ with A_μ being the four-vector of the electrostatic and magnetic potential: $(V, \vec{A})$. Maxwell's equation are a set of 8 equations with only 6 unknowns, this gives the freedom to choose a *gauge* of the theory, in fact the action of free electromagnetic field is invariant under $A_\mu \rightarrow A_\mu - \partial_\mu \theta$. To ensure local gauge invariance it is possible to define a *covariant* derivative of the form: $D_\mu \Psi = (\partial_\mu + iqA_\mu) \Psi$. Replacing ∂_μ by D_μ in $\mathcal{L}_D$ one finds:

$$\mathcal{L}_D = \bar{\Psi} (i\gamma^\mu \partial_\mu - m) \Psi - qA_\mu \bar{\Psi} \gamma^\mu \Psi \quad (1.5)$$

the electrodynamics of a particle represented by a spinor Ψ is thus obtained by coupling the field A_μ with the current $\bar{\Psi} \gamma^\mu \Psi$. This formalism can be generalized to any group theory beyond the abelian $U(1)$ group.

The procedure described above was derived in the context of classical field theory. Quantization of the theory can be introduced in different ways [10]. In the canonical quantization procedure, one considers the Heisenberg picture of quantum mechanics

where the fields are promoted to operators that are functions of the space-time. Fields are then described, in the energy-momentum space, by a set of creation and annihilation operators which obey commutation relations postulated by quantum mechanics. This is the so-called second¹ quantization of the theory. In particular, the charge q of the previous equation becomes, after quantization, the electric charge in units of e and the corresponding symmetry group which generates the interaction is called $U(1)_{em}$.

The SM is a gauge theory which, analogously to what was described in this section, is invariant under $SU(3)_c \otimes SU(2)_L \otimes U(1)_Y$. The $SU(2)_L \otimes U(1)_Y$ terms describe the electro-weak sector while $SU(3)_c$ described the strong force. A more detailed discussions follows.

1.1.1 The electro-weak sector

The electroweak interaction is a fundamental piece of the SM. Initially, the weak and the electromagnetic interactions were described by two different theories. The latter was described by the QED formalism while the former was described based on an effective field theory at low energies, the Fermi theory. According to this theory, charged current interactions are approximated by a point-like interaction with a coupling called G_F [10]. The theory breaks at energies $\mathcal{O}(100 \text{ GeV})$ where the real propagator of the interaction, the $W^\pm$ boson, is revealed. From low energy experiments analyzing neutrino scattering and experiments studying β decays, it became clear that only the left-handed chirality were coupled to charged currents. A natural choice of the symmetry group needed to define the weak interactions is therefore $SU(2)_L$ where L stands for left-handed. An $SU(2)_L$ left-handed doublet can be arranged as follows:

$$\chi_L = \begin{pmatrix} \nu_l \\ l \end{pmatrix}_L \quad l_R \quad (1.6)$$

where $l = (e, \mu, \tau)$, and a right-handed neutrino singlet is not introduced since there is still no observation of such a particle. A similar representation is given for quarks where both up (u, s, t) and down-types (d, c, b) have a right-handed component, singlet under $SU(2)_L$. This picture of the weak currents is still unsatisfying since it was experimentally observed that neutral currents involving Z bosons were coupled with right-handed particles as well. A solution to this problem was proposed by Glashow, Weinberg and Salam [11]. They proposed to combine the $SU(2)_L$ with $U(1)_{em}$ into a single, larger, symmetry group: $SU(2)_L \otimes U(1)_Y$. This gives rise to a total of 4 generators which corresponds to 4 gauge bosons. Following the prescription of gauge invariance explained in the previous section, the gauge transformation can be written as:

¹This term is used to differentiate the quantization in QFT theory w.r.t. the quantization of classical mechanics which does not respect Lorentz invariance.

$$\chi'_L \rightarrow e^{i\beta y} e^{i\sigma^i \alpha_i} \chi_L \quad (1.7)$$

In order to make $\mathcal{L}_D$ invariant under local gauge transformation, i.e. $\beta \rightarrow \beta(x)$; $\alpha^i \rightarrow \alpha^i(x)$, the following kinetic term of the gauge boson needs to be defined:

$$B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu \quad (1.8)$$

$$\tilde{W}_{\mu\nu} = \partial_\mu \tilde{W}_\nu - \partial_\nu \tilde{W}_\mu - ig[\tilde{W}_\nu, \tilde{W}_\mu] \quad (1.9)$$

where the first equation is equivalent to the QED described in the previous section since $B_{\mu\nu}$ corresponds to $SU(2)_L$ singlet while the second equation accounts for the fact that the generators of $SU(2)_L$ are non-abelian. The quantum number related to the $SU(2)_L$ symmetry group is called *weak isospin*. It is now convenient to define $W_{12} = \frac{1}{\sqrt{2}}(\tilde{W}_\mu^1 \pm i\tilde{W}_\mu^2)$, where W_{12} corresponds to the charged $W^\pm$ bosons as we shall see in the next section. To characterize the interactions of the vector bosons, the gauge-invariant kinetic term of the fields is constructed in analogy to the QED case:

$$\mathcal{L}_{\text{kin}} = -\frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{4}W_{\mu\nu}^a W^{a\mu\nu} \quad (1.10)$$

where the index a runs over the three gauge bosons. Expanding the previous equation one finds cubic and quartic self-interaction terms among the gauge bosons which defines vertices of the type $WW \rightarrow WW$ and similar four-point interactions. These vertices are of great interest since it can be shown that their cross-sections un-naturally increases as a function of the center-of-mass energy of the system until unitarity, dictated by conservation of probability, is violated. If a real scalar field is introduced into the theory, this feature is eliminated due to cancellations via quantum interference. This is one of the main motivations for the inclusion of the Higgs boson into the theory. The second is that gauge symmetry forbids to write a mass term for the gauge bosons as well as for fermionic masses since they would communicate the left- and right-handed fields, which have different transformation properties under $SU(2)_L$, and therefore it would produce an explicit breaking of the gauge symmetry.

1.1.2 The Higgs sector

The mechanism which allows one to write in a gauge invariant way a mass term for the gauge bosons is the BEHHGK² mechanism. This mechanism, also called Sponta-

²The names come from the different authors contributing to the evolution of the spontaneous symmetry breaking : Englert and Brout [12], Higgs [13] and Guralnik, Hagen and Kibble [14]. Sometimes it takes the name of BEH mechanism.

neous Symmetry Breaking (SSB), postulates a complex field which is invariant under $SU(2)_L \times U(1)_Y$:

$$\phi(x) = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \quad (1.11)$$

a potential $V(\phi)$ is then introduced of the form:

$$V(\phi) = \frac{1}{2}\lambda^2(\phi^\dagger\phi - \eta^2)^2 \quad (1.12)$$

A schematic representation of the potential is shown in Figure 1.1. After a perturbation of the theory, the initial state placed at the center of the potential converges to one of the vacuum states thus breaking the symmetry of the system. When moving across the different minima of the potential, the field is not subject to any excitation of the potential, leading to the creation of massless particles, the so-called Goldstone bosons.

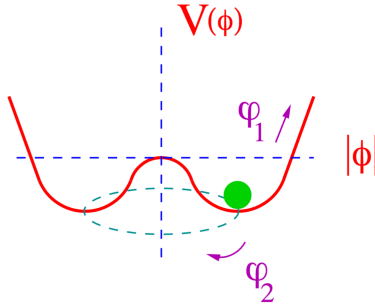


Figure 1.1 – Schematic representation of the Higgs potential. It can be seen that there are an infinite number of degenerate states of minimum energy that can be parametrized as $\phi_0(x) = \frac{v}{\sqrt{2}}e^{i\theta(x)}e^{i\frac{\sigma_i}{2}}$.

After breaking of the symmetry the field can be parametrized as:

$$\phi(x) = e^{i\theta_i(x)\frac{\sigma_i}{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + H(x) \end{pmatrix} \quad (1.13)$$

The three fields appearing in the exponent of the previous equation are precisely the massless Goldstone bosons associated with the breaking of the symmetry. Due to the gauge invariance of the $SU(2)_L \otimes U(1)_Y$ group, the Goldstone bosons represent unphysical states of the system. In fact, by choosing a particular solution, $\theta_i = 0$ for

example, as the ground state, the symmetry is spontaneously broken. The Goldstone bosons are removed from the theory to give mass to the three vector bosons. This can be seen by:

$$\mathcal{L}_\phi = (D_\mu \phi)^\dagger (D^\mu \phi) - V(\phi) \quad (1.14)$$

$$D_\mu = i\partial_\mu - ig\sigma_i \tilde{W}_{i\mu} - ig'y B_\mu \quad (1.15)$$

where the first equation describes the dynamics and the potential of the field ϕ and the latter defines the covariant derivative demanded by gauge invariance. By expanding these equations one finds:

$$\mathcal{L}_\phi = \left[\frac{1}{2}(\partial_\mu H)^2 - \lambda v^2 H^2 \right] + \frac{1}{8}g^2 v^2 (W_\mu^1 W^{1\mu} + W_\mu^2 W^{2\mu}) \quad (1.16)$$

$$+ \frac{1}{8}(gW_\mu^3 - g'B_\mu)(gW_\mu^3 - g'B_\mu) - \lambda v H^3 - \frac{\lambda}{4}H^4 \quad (1.17)$$

where the first term of the equation describes the mass and kinematics of a new real scalar field, the Higgs boson. The second term can be identified as a mass term of the two charged vector bosons: $m_W = gv$. The last two terms represent the trilinear and quartic self-interactions of the Higgs boson. To recover a massless and a massive field corresponding to the photon and the Z boson, a last step is necessary. A linear combination of the third component of the field $W_{3\mu}$ and B_μ is taken of the form:

$$\begin{pmatrix} W_{3\mu} \\ B_\mu \end{pmatrix} = \begin{pmatrix} \cos\theta_W & \sin\theta_W \\ -\sin\theta_W & \cos\theta_W \end{pmatrix} \begin{pmatrix} Z_\mu \\ A_\mu \end{pmatrix} \quad (1.18)$$

where the Z_μ and A_μ are the field of the Z boson and the photon and θ_W is the Weinberg angle, one of the fundamental parameters of electroweak interactions. Rearranging equation 1.17 and imposing $\cos\theta_W = \frac{g}{\sqrt{g^2 + g'^2}}$ and $\sin\theta_W = \frac{g'}{\sqrt{g^2 + g'^2}}$, it is clear that a mass term for the Z boson can be identified: $m_Z = \frac{1}{\sqrt{2}}\sqrt{g^2 + g'^2}v$ while the photon remains massless. The weak *hypercharge* Y is thus defined as:

$$Y = 2Q - 2T_3 \quad (1.19)$$

where Q is the electric charge and T_3 is the third component of the weak isospin. A summary of quantum charges for the electron family is shown in the Table 1.1.

Table 1.1 – Quantum numbers of the $SU(2)_L \otimes U(1)_Y$ group for the electron family.

	T	T_3	Q	Y
ν_L	1/2	1/2	0	-1
e_L	1/2	1/2	-1	-1
e_R	0	0	-1	-2

Fermions also acquire mass through a dynamical interaction with the Higgs field. In fact a mass term of the form: $m_l \bar{l}l$ explicitly breaks gauge invariance. A fermion-scalar interaction needs to be postulated into the SM Lagrangian and it is called the Yukawa coupling:

$$\mathcal{L}_{Yukawa} = c_1 (\bar{u}, \bar{d})_L \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \begin{pmatrix} d_R \\ u_R \end{pmatrix} + c_2 (\bar{u}, \bar{d})_L \begin{pmatrix} \phi^{0*} \\ -\phi^- \end{pmatrix} \begin{pmatrix} u_R \\ d_R \end{pmatrix} + \dots \quad (1.20)$$

After spontaneous symmetry breaking, this Yukawa-type Lagrangian takes the simpler form:

$$\mathcal{L}_{Yukawa} = (H + v)(c_1 \bar{d}d + c_2 \bar{u}u \dots) \quad (1.21)$$

The term proportional to H defines the tree-level interaction between the Higgs boson and the fermions. The coupling $H f \bar{f}$ is proportional to the mass of the fermion and it is a fundamental and unique property of the Higgs boson interaction. Fermionic mass terms are easily identified as:

$$m_u = -\frac{c_1 v}{\sqrt{2}}, \quad m_d = -\frac{c_2 v}{\sqrt{2}}, \quad \text{etc...} \quad (1.22)$$

a priori the masses of the particles are not predicted and instead need to be measured.

1.1.2.1 Renormalization

The quantum field theory treatment suffers from divergences in higher order diagrams occurring at very low and very high energy. One of the main examples is the unbounded integral over the particle momentum in loop-level diagrams. To cure these divergences in such a way that the theory becomes finite and calculable, a systematical procedure called *renormalization* is employed. The parameters postulated in the SM Lagrangian are considered un-physical and only represent *bare* quantities [10]. The *renormalizability* of spontaneously-broken gauge theories was demonstrated by

't Hooft and Veltman [15] and ensures the predictive power to the SM. Important examples of the effects of renormalization are the running of the coupling constant where screening and anti-screening effects of virtual particles produced by the polarization of the vacuum alter the coupling constant, becoming a function of the energy scale probed by the interaction. Another great example is the mass of the Higgs boson. Due to the nature of the Yukawa coupling, which favors coupling to the heaviest fermion, top-loops induce a significant dependence on the mass of the Higgs boson:

$$m_H^2 = m_0^2 + \Delta m_H \quad (1.23)$$

where m_0 is the Higgs boson's *bare* mass and Δm_H are the quantum corrections which can be expanded to [16]:

$$\Delta m_H = -\frac{\lambda_f^2}{16\pi^2} (2\Lambda^2 + \mathcal{O}(m_f^2) \ln(\frac{\Lambda}{m_f})) \quad (1.24)$$

as the new physics scale Λ potentially reaches the Planck scale, a careful fine-tuning of the bare mass is needed to keep the mass of the Higgs boson close to its measured value of 125 GeV. One could object that this argument is not general and it depends on the renormalization schemes. However, the crucial point is that the mass of the Higgs boson is not protected by any symmetry. In the case of fermion masses, chiral symmetry would become an exact symmetry of the model if all the masses of the fermions were equal, nonetheless the masses of the fermions are still protected at any order of perturbation theory due to the broken chiral symmetry. In the Higgs sector, no such symmetry exists leaving the mass of the Higgs boson potentially unbounded. Since new physics is expected at the planck scale, the quantum corrections on the mass of the Higgs boson will be $\Delta m_H \sim M^2$ where M is the characteristic mass of new physics resonances. Two options exist to solve these *un-natural* differences between mass scales: the first is a meticulous ad-hoc cancellation of each term contributing to the increase of the Higgs boson mass, while the second is to build a theory which naturally restores the mass of the Higgs boson. The most common example of the latter is Supersymmetry where the additional symmetry postulated by the model leads to natural cancellations in the loop corrections due to fermion and boson loops, both contributing to the mass of the Higgs boson but with opposite signs.

From an experimental perspective, measuring the fundamental properties of the Higgs boson not only offer a way to test the consistency of the SM predictions, but also represent a unique opportunity to study new physics beyond the standard model as will be further discussed in Section 1.3.0.2.

1.1.3 Quantum Chromodynamics

Quantum Chromodynamics, QCD, is the theory of the strong interactions. It is a gauge theory based on $SU(3)_c$, the unit of charge is conventionally called the *colour* charge. A total number of 8 generators and hence bosons mediating the force are formed, the gluons. $SU(3)_c$ is non abelian which, similarly to what was shown for $SU(2)_L$, leads to self-interacting gauge bosons carrying color charge themselves. In contrast to the weak boson, gluons are massless.

The QCD Lagrangian can be written as:

$$\mathcal{L}_{QCD} = i \sum_q \bar{\psi}_q^k \gamma^\mu (D_\mu)_{jk} \psi_q^k - \sum_q m_q \bar{\psi}_q^j \psi_q^j - \frac{1}{4} G_{\mu\nu} G^{\mu\nu} \quad (1.25)$$

where the covariant derivative is defined as:

$$(D_\mu)_{jk} = \delta_{jk} \partial_\mu - i g_s (T_a)_{jk} G_\mu^a \quad (1.26)$$

with the index a representing the 8 $SU(3)_c$ generators, the indices i, j representing the three color charges (red, green and blue) and the index q the flavors of the quarks. T_a is the generator of the group, also called the Gell-Mann matrices. The $\frac{1}{4} G_{\mu\nu} G^{\mu\nu}$ is the kinetic term of the gluons. By expanding the previous equations it can be shown that self- and quartic-interactions among the gauge fields arise from the non-abelian nature of the symmetry group.

One of the most remarkable properties of QCD is the so-called *asymptotic freedom*. As mentioned in the previous chapter, screening effects of virtual particles lead the coupling constants to be a function of the transferred momentum in the interaction Q^2 . In QCD, quarks behave as free particles for high transverse momentum while the coupling constant α_s becomes large at low-energies. The complete dependency is defined as:

$$\alpha_s(Q^2) = \frac{33 - 2n_f}{12\pi} \ln\left(\frac{Q^2}{\Lambda_{QCD}^2}\right) \quad (1.27)$$

where n_f is the number of quark flavors and Λ_{QCD}^2 is the QCD scale parameter commonly chosen such that $\alpha_s(Q^2)$ depends only on one variable. Λ_{QCD} is measured to be ~ 200 MeV. It sets the scale between different regimes of the theory: for $Q^2 \gg \Lambda_{QCD}^2$ the theory is asymptotically free and strong interactions are described by perturbative expansions in α_s . If instead $Q^2 \ll \Lambda_{QCD}^2$ the coupling constant increases and results in the *confinement* of quarks and gluons into bound states. Therefore quarks cannot be observed as free particles but instead form colorless hadrons that can be classified as either mesons ($q\bar{q}$) or baryons (qqq or $\bar{q}\bar{q}\bar{q}$).

1.2 The search for the Higgs Boson

The concept of SSB was brought into the context of particle physics in 1964. A coherent description of electro-weak symmetry breaking, which included the Higgs boson, was incorporated in 1971. After that, a series of experimental successes such as the discovery of charm quark, the Z^0 and the $W^\pm$ bosons and finally the discovery of the top quark validated the SM predictions [17]. The main missing piece that remained to be seen was the Higgs boson together with the determination of its mass and couplings. To understand the situation of the search for Higgs boson at that time, it is useful to cite a remarkable quote written by Ellis et al. [17]:

"We should perhaps finish our paper with an apology and a caution. We apologize to experimentalists for having no idea what is the mass of the Higgs boson, ..., and for not being sure of its couplings to other particles, except that they are probably all very small."

The situation improved with the analysis of data from LEP1 and its upgrade LEP2. The direct production of Higgs bosons through s-channel processes at e^-e^+ colliders is disfavored due to the low mass of the electrons and positrons. The main channel contributing to the early studies of the Higgs boson was the Higgs boson production in association with a Z boson $e^-e^+ \rightarrow ZH$ which enabled the exclusion of Higgs boson masses below ~ 110 GeV. The second big step forward came with the discovery of the top quark. The estimation of m_t allowed for a global fit of electro-weak data from different facilities including LEP, Tevatron and SLC. The quantum corrections induced by the Higgs boson in characteristic electroweak processes made it possible to indirectly estimate the mass of the Higgs boson $m_H \sim 100 \pm 30$ GeV [18]. Tevatron experiments also excluded the high mass region of the Higgs boson to be below ~ 130 GeV at 95 % CL. With the mass range cornered up, the first results coming from LHC experiments at 7 TeV further extended the exclusion region. A summary of the search of the Higgs boson at that time is summarized in Figure 1.2, where only a tiny region in mass was left for the Higgs boson discovery. Finally in 2012, both ATLAS and CMS observed a resonance with mass around 125 GeV. A combination of the analyses of the two experiments at a c.o.m. energy of 7 and 8 TeV led to an estimation of the mass of the Higgs boson of $125.09 \pm 0.21(stat) \pm 0.11(syst.)$ GeV [19]. Since then the properties of the Higgs boson have been measured showing good compatibility with the SM expectations of a spin 0 and a positive parity. Last summer, in 2018, the first evidence for the direct Yukawa coupling between the Higgs boson and the bottom quark was announced by both ATLAS and CMS collaborations in the VH production mechanism; the top-Higgs interaction was also announced in the $t\bar{t}H$ production mode. Current effort is ongoing to measure with as high accuracy as possible the Higgs boson properties. Additionally, efforts are also ongoing to expand the kinematic phase-space probed by the analyses searching for Higgs bosons such as the search presented in this thesis for the Higgs boson in the boosted regime.

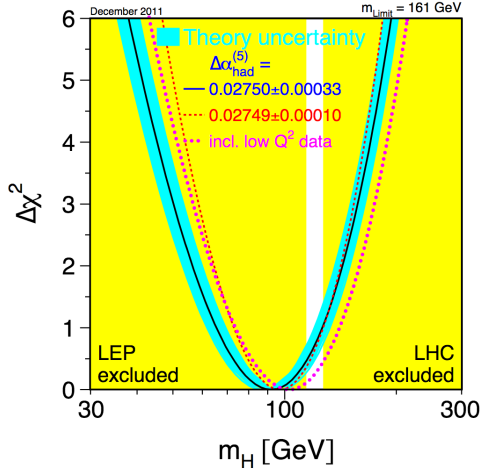


Figure 1.2 – A compilation of information about the possible mass of the Higgs boson. The yellow-shaded regions have been excluded by searches at LEP, the Tevatron collider and the LHC [17].

1.2.1 Higgs boson at the LHC

The main production mechanisms of the Higgs boson in a pp machine, such as the LHC, are shown in Figure 1.3. The primary production mechanism occurs via a quantum loop in the gluon-gluon-fusion process. The second leading mechanism is via associated production with a vector boson. This channel has the great advantage of using the leptons from the V decays to trigger the event and reduce the QCD background. As mentioned already, in 2018 the interaction of the Higgs boson to the bottom quark was observed in this channel, providing one of the first measurement of the Yukawa coupling of the Higgs boson to quarks.

The branching ratios of the Higgs boson are shown in Figure 1.4. The Higgs boson was initially discovered in the so-called golden channels: $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ^* \rightarrow 4l$ as despite their low cross-sections, they present a very low yield of the background events. It is remarkable to note that the highest BR of around 60 % is into $b\bar{b}$ pairs. However, an inclusive search for $H \rightarrow b\bar{b}$ was for a long time considered to be impossible due to the overwhelming background from di- b production: $\sigma_{H_{b\bar{b}}}/\sigma_{\text{QCD}} \sim 10^{-7}$. With the development of experimental techniques which enable the reconstruction of very boosted objects, it was noted that the QCD background is reduced due to the boosted topology making it possible to search for Higgs boson in an inclusive way [21, 22]. This is particularly interesting since it probes the loop diagram of the ggF production mechanism. At low energies, the loop is treated as point-like given the high mass of the

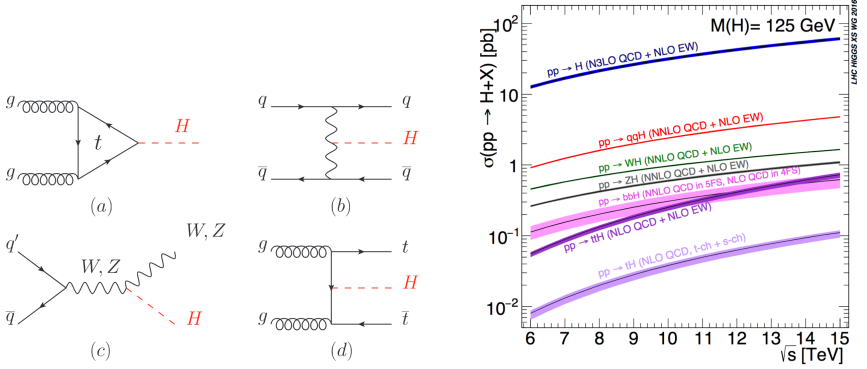


Figure 1.3 – Left) Diagram of the main production mechanisms at the LHC. Right) Their related cross section at the LHC [20].

top quark. However, if the p_T of the Higgs boson is high enough: $p_T \sim 2m_t$ the loop is resolved providing an indirect way to probe the top-H coupling at high- p_T . In this regime, a series of theories beyond the standard model predict the existence of new particles entering the loop. These effects can be formalized using effective quantum field theories and will be discussed in the following section.

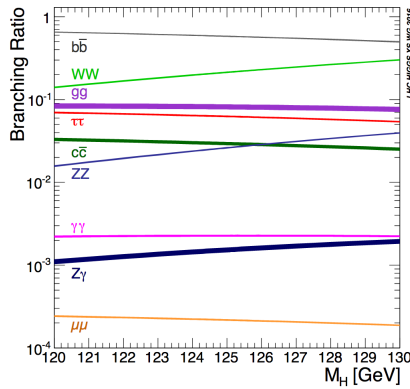


Figure 1.4 – Branching ratios of the Higgs boson [20].

1.3 Theories for physics beyond the standard model

A large variety of BSM models are searched for at the LHC, where the high center-of-mass energy allows one to set limits on new physics at world-leading scales. In this thesis, two searches for new physics will be discussed. One search targets mediators with very high masses beyond ~ 1 TeV while the other looks for resonances with a lower mass of ~ 100 GeV. Both searches are interpreted within the context of dark matter searches. The high mass analysis is also interpreted as a search for heavier Z' bosons and b^* models, while the low mass one is also presented as a search for boosted SM Higgs bosons. Such an interpretation, despite being an interesting alternative to test the SM Yukawa couplings, allows one to probe new physics differently compared to the other interpretations looking for resonances mostly produced via s-channel processes which would manifest themselves as a *bump* in the invariant mass spectrum. New physics can be probed in the Higgs boson search utilizing the fact that the Higgs boson cross section at high transverse momentum is distorted by new physics phenomena [21], such modifications are parametrized using an effective field theory approach.

1.3.0.1 Dark Matter

Many astrophysical measurements such as the velocity determination of spiral galaxies and anisotropies in the Cosmic Microwave Background (CMB) give compelling evidence for dark matter [23–25]. While the existence of DM is well motivated, a direct measurement of DM particles still remains elusive. Several complementary strategies are currently employed: direct detection in underground detectors, indirect detection with satellites, ground-based telescopes and finally direct production of DM particles at the LHC [20]. The latter in particular can be sub-divided into searches featuring missing energy (the so called "mono-X" signatures), characteristic of models with direct production and subsequent decays of DM mediators to DM particles producing missing energy in the event, or by dark sector mediators that feature DM particles decaying into SM particles. The two approaches offer complementary sensitivities to different kinematic regions. A summary of dark sector mediator searches performed by the ATLAS experiment is shown in Figure 5.6.

The model utilized for all of the analyses shown in the Figure is a *lepto-phobic* Z' , as recommended by the ATLAS and CMS Dark Matter Forum to maintain consistency between searches, as described in detail in [27]. The same model is also used in the analyses presented in this thesis.

1.3.0.2 An effective field theory approach to the SM

A search for inclusive Higgs bosons decaying into pairs of bottom quarks is interesting not only to probe the SM Yukawa couplings to the third family of quarks but also to investigate the Higgs boson's cross-section at high- p_T . In this kinematic regime the

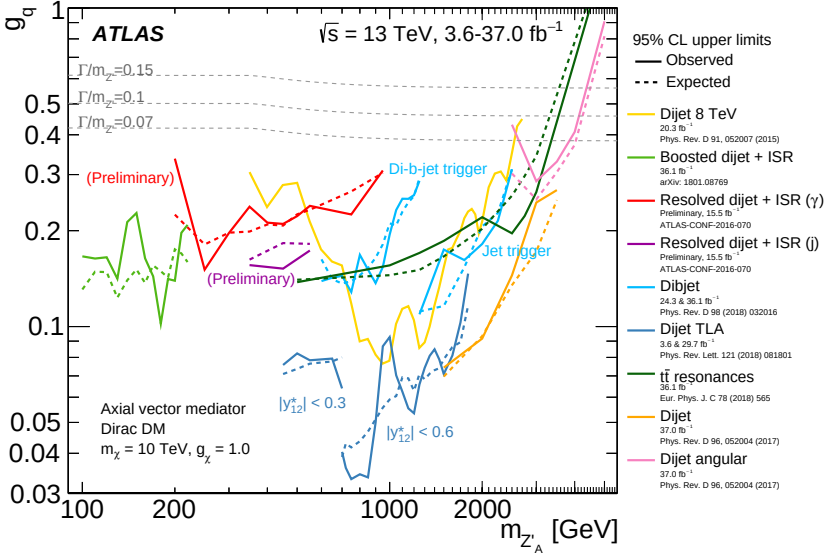


Figure 1.5 – 95 % exclusion limits for di-jet analyses searching for a Z' DM mediator. g_q represents the coupling between the Z' and the SM particles. In order to explore large mass ranges, many different experimental techniques need to be explored [26]. For this thesis, two analyses at the edges of the spectrum will be presented: a boosted analysis where the Z' recoils against an ISR particle used for triggering and a search for a massive Z' where the lower mass bound is dictated by trigger requirements. Both analyses look for pairs of bottom quarks in the final states.

gluon-gluon fusion process allows one to indirectly probe the t - H interactions via quantum loops. In fact when the initial radiation carries away a large amount of energy and boosts the Higgs boson, the process effectively probes the ultraviolet structure of the top loop. This effect is particularly relevant within the context of SMEFT, where the SM is expanded by means of an effective field theory. The general idea is that the SM Lagrangian is expanded using effective operators with dimensions higher than 4 [20]:

$$\mathcal{L}_{eff} = \mathcal{L}_{SM} + \sum_i \frac{c_i}{\Lambda^2} \mathcal{O}_i + \text{higher dimensional operators} \quad (1.28)$$

recently a NLL³+NLO calculation of the high- p_T cross-section of the ggF production mechanisms, including the effect of dimension six operators, has been computed [28]. Three main coefficients acting on dimension six operators have been studied: c_g , c_t and c_b . The first coupling represents a deviation from the gluon-top vertex entering

³NLL stands for next-to-leading log, a formalism used to compute emissions during parton shower.

the loop, c_t affects the coupling between the top quark and the Higgs boson which is indirectly accessible in the ggF process and c_b is H - b interactions and can modify either the quantum loop occurring via bottom quarks or the direct decay $H \rightarrow b\bar{b}$. The effect of these operators on the differential Higgs boson cross section as a function of the H_{p_T} is depicted in Figure 1.6. It is remarkable that the effects of the EFT operators are only appreciable at very high transverse momentum of the Higgs boson. The theoretical and experimental machinery needed to perform a global fit to constrain all the EFT parameters is still under investigation, nevertheless these kinds of searches represent a new way of looking at new physics at colliders and will be one of the major physics interests at the HL-LHC. In this thesis, a search for boosted Higgs bosons (H_{p_T} larger than approximately 480 GeV) decaying into a pairs of b -quarks, conducted for the first time by the ATLAS experiment, will be presented.

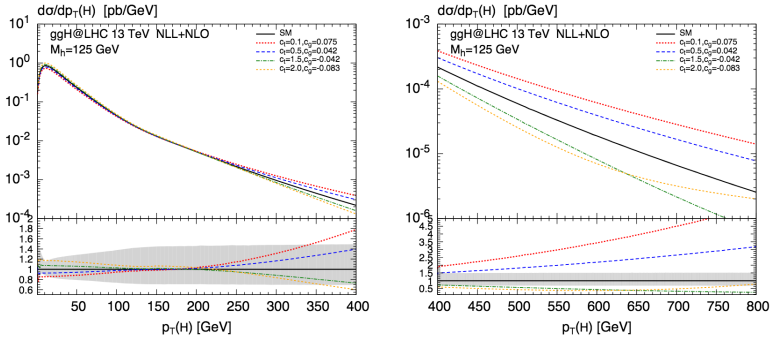


Figure 1.6 – Higgs boson transverse-momentum spectrum in the SM (black, solid) compared to separate variations of the dimension-six operators. The lower frame shows the ratio with respect to the SM prediction. The shaded band in the ratio indicates the uncertainty due to scale variations [28].

CHAPTER 2

The ATLAS detector

This chapter discusses the main characteristics of the Large Hadron Collider (LHC) accelerator and the ATLAS detector. The analysis presented in this thesis are based on the data collected in the 2015, 2016, 2017 and 2018 data-taking periods. Since December 2018, the LHC has been shut-down to undergo a major upgrade which may enable to collect up to 300 fb^{-1} at a c.o.m. energy of 14 TeV until 2023. After that, a second major upgrade is planned to the LHC which will increase the interaction rate by a factor of 10, where this upgrade is called High-Luminosity LHC (HL-LHC).

The first section of this chapter presents the main properties of the LHC and its operation until 2018. The second section is devoted to the description of the ATLAS experiment and its sub-detectors. In the third section, the main features of the HL-LHC are described.

2.1 The LHC accelerator

The Large Hadron Collider (LHC) [29] is a hadron accelerator and collider located at CERN. The choice of a hadron collider comes from the need to explore physics processes at the highest possible energy. The energy loss of a particle in a circular accelerator is: $\frac{dE}{dt} \propto \frac{E^4}{m^4 R}$ where R is the bending radius and m is the mass of the accelerated particle traveling at an energy E . Protons represent the most natural choice for a high-energy circular collider since they are at the same time heavy (the energy-loss is reduced compared to lighter particles) and stable (proton decay is yet to be observed, the upper bound on its lifetime is $\sim 10^{33}$ years [30]).

The LHC is located in the tunnel initially constructed for the CERN LEP electron-positron accelerator in between 1984 and 1989. Before reaching the highest possible energy at the LHC, the protons undergo subsequent acceleration steps. The overall accelerator complex is shown in Figure 2.1.

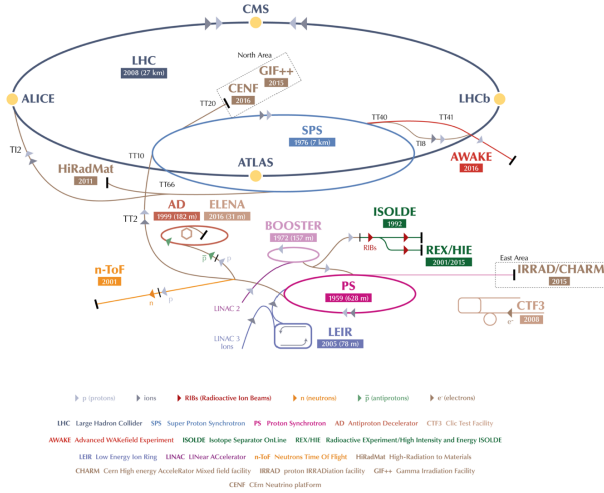


Figure 2.1 – The overall layout of the CERN accelerator complex [29].

The LHC is designed to accelerate two beams of proton (or heavy ions) traveling in opposite directions. The accelerator chain begins with the LINAC 2, where protons obtained from hydrogen gas are accelerated up to 50 MeV. The protons are then injected into the Proton Synchrotron Booster (PSB) where their energy is increased to 1.8 GeV. The beam is further injected into the Proton Synchrotron (PS) which pushes the beam to 25 GeV. The acceleration chain continues with the Super Proton Synchrotron (SPS) where the protons are accelerated to 450 GeV. Finally, the beam is injected from the SPS into the LHC in two pipes running in opposite directions. The LHC is designed to accelerate each beam at an energy of 7 TeV thanks to a complex system of dipole and higher order magnets. Four main interaction points are used as collisions points corresponding to the location of the four detectors: ALICE, ATLAS, CMS and LHCb.

The LHC beams are composed of bunches of protons colliding at a rate up to 40 MHz. A typical bunch train corresponds to 2808 bunches for each beam with 25 ns separation and with $\sim 1.15 \times 10^{11}$ protons per bunch.

One of the main parameters of a collider is the luminosity. It is a measure of the collisions per unit of area per unit time. The overall number of collisions per unit area is a crucial parameter in all LHC measurements as it is directly related with the cross-section (σ) of a process of interest: $\frac{dN}{dt} = \mathcal{L}\sigma$ where $\mathcal{L}$ is the instantaneous luminosity.

$\mathcal{L}$ can be parametrized with characteristic parameters of the collider:

$$\mathcal{L} = \frac{F n_b N_b^2 f_r \gamma_r}{4\pi \beta^* \epsilon_n} \quad (2.1)$$

where n_b is the number of bunches circulating in the machine, f_r is the revolution frequency of the bunch, N_b the number of protons circulating in the machine, γ_r represents the relativistic gamma factor, ϵ_n is the normalized transverse emittance, β^* is the beta function at the point of collisions and F is a constant factor taking into account the geometrical reduction factor due to the crossing angle at the interaction point. In order to quantify the amount of data collected over a certain period of time, the integrated luminosity is used. The integrated luminosity is obtained integrating the instantaneous luminosity over a period of time T , $L = \int_0^T dt \mathcal{L}$. The total integrated luminosity over the full LHC data taking-period running at $\sqrt{s} = 13$ TeV is depicted in Figure 2.2. The main design parameters of the LHC are summarized in Table 2.1.

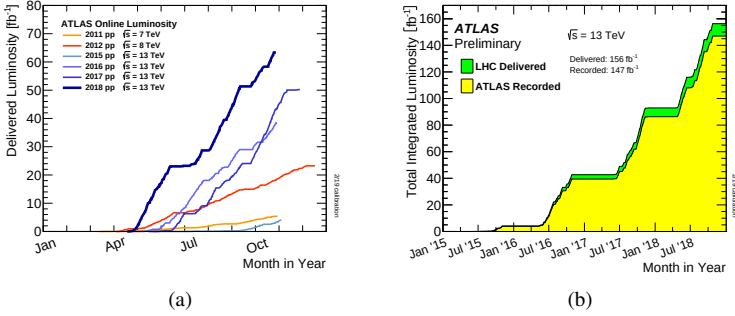


Figure 2.2 – a) Integrated luminosity as a function of time for different data-taking years. b) Integrated luminosity as a function of the time delivered to ATLAS (green) and recorded by ATLAS (yellow) during collisions at $\sqrt{s} = 13$ TeV [31].

Table 2.1 – Summary of the main beam parameters of proton-proton collisions. As a comparison, the design parameters and the parameter value during the operation in 2017 are shown. The peak luminosity in 2017 exceeded the design value.

parameter	Design value	2017
beam energy [TeV]	7	6.5
Max number of bunches	2808	2550
Max. number of protons per bunch [$\times 10^{11}$]	1.15	1.28
Peak luminosity [$cm^{-2}s^{-1}$]	1×10^{34}	1.5×10^{34}
Bunch spacing [ns]	25	25

The luminosity reached by the LHC implies a large number of multiple interactions taking place between the proton bunches (pile-up). Pile-up originates from two sources: in-time and out-of-time pile-up. The first occurs when multiple collisions take place in a single bunch crossing while the latter is mostly due to finite read-out time resolution of the sub-detectors, often slower than 25 ns. Because of this, residual energy from a previous bunch crossing could potentially enter into a single read-out stream of the relevant sub-detector. The amount of pile-up is parametrized using the average number of interactions per bunch crossing ($\langle\mu\rangle$). The distribution of $\langle\mu\rangle$ for the different data-taking periods is shown in Figure 2.3.

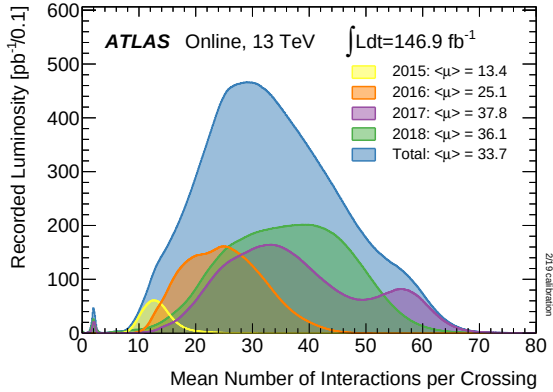


Figure 2.3 – The mean number of interactions per crossing for the different data-taking during collisions at $\sqrt{s} = 13$ TeV [31].

2.2 The ATLAS detector

ATLAS is a multi-purpose apparatus whose primary goal is to identify and measure the properties of particles produced in p - p collision. Several complementary sub-detectors are needed to achieve this goal. A typical p - p collision produces a large variety of final state particles which interact differently within the various detector volumes. In addition, magnetic fields are employed to bend the trajectories of electrically charged particles to measure their electric charge and momentum. The overall ATLAS detector is shown schematically in Figure 2.4. The detector placed closer to the collision point requires high granularity to ensure a high efficiency of the tracking algorithms and good resolution of a series of fundamental quantities such as the reconstruction of the primary vertex (where the hard-scattering took place), the reconstruction of secondary vertices which originates from decay in-flight of long-lived particles and more. This is achieved with silicon-based tracking detectors. Charged particles release charge through ioniza-

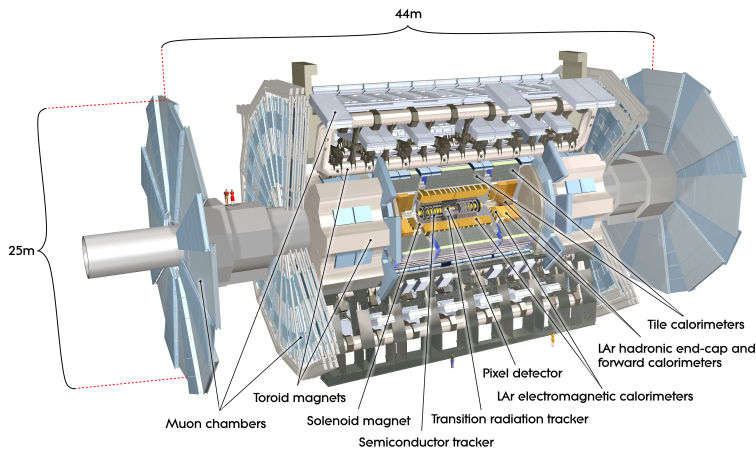


Figure 2.4 – Schematic view of the ATLAS detector [32].

tion producing *hits* which are used to reconstruct the particle trajectory traversing the detector. During the hadronization of colored partons, a spray of particle (*jet*) is produced. A *jet* is also composed of neutral particles which are not directly detectable in silicon layers. Therefore, to correctly measure the energy and transverse momentum of the resulting *jet* and of other neutral particles, such as the photon, a calorimeter system is needed. A large coverage of these detectors is crucial to reconstruct the missing transverse energy of events, which is a characteristic signature of neutrinos escaping the detector or other weakly interacting particles, predicted by extensions of the SM, such as dark matter candidates. Finally, muons interact electromagnetically but only weakly with matter. They can penetrate the calorimeters releasing only a fraction of their energy. A dedicated detector system is therefore used to measure muon-tracks. Summarizing, the main characteristics provided by the ATLAS detector are:

- fast, radiation-hard electronics and sensors, and high granularity detectors to handle the large occupancy produced by LHC collisions. These concepts will be largely discussed in Chapter 7;
- large coverage of the calorimetric systems to ensure a good resolution of the energy and direction of the *jets* as well as a good estimation of the missing transverse momentum;
- good reconstruction efficiency and resolution of charged particles in the tracker;
- precise measurement of the impact parameters resolution for the identification of long-lived particles, where a detailed discussion on this topic will follow in Chapter 4;

- efficient identification and measurement of photons and electrons in the electromagnetic calorimeter;
- high muon reconstruction efficiency and momentum resolution;
- the rate of data produced by a typical collision at the LHC need to be reduced to manageable levels. This is achieved by a fast and flexible trigger system which selects events in a wide range of topologies of interest.

In the following, the coordinate system used by the ATLAS detector is defined and a more detailed description of each of ATLAS sub-detectors is given.

Coordinate system

ATLAS uses a right-handed coordinate system whose origin is placed at the interaction point. The z -axis corresponds to the beam pipe while the x and y directions define the transverse plane. Profiting from the detector geometry, a cylindrical coordinate system is often used. ϕ is the azimuthal angle in the xy -plane. Instead of using directly the polar angle θ , which is not invariant under a Lorentz boost, the pseudorapidity η is defined as:

$$\eta = -\ln(\tan(\frac{\theta}{2})) \quad (2.2)$$

with θ being the polar angle measured between the momentum of the particle and the beam-axis. η is an approximation of the *rapidity*¹ for small masses. In this approximation, the $\Delta\eta=\eta_1-\eta_2$ between two particles in the event is invariant under a Lorentz boost along the z -axis.

The momentum computed in the transverse plane is called the transverse momentum $p_T = \sqrt{p_x^2 + p_y^2}$. The sum of the transverse momenta of all particles in the event is expected to be 0 for momentum conservation. The angular distance between a pair of reconstructed objects is defined as $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

2.2.1 Magnet system

The ATLAS magnet system is made of a thin superconducting solenoid surrounding the inner detector and three large superconducting toroids arranged with an eight-fold azimuthal symmetry around the calorimeters to provide bending power for the muon spectrometer. The central solenoid has an inner radius of 1.23 m and a total length of 5.8 m. It provides a 2 T axial magnetic field along the beam axis for the inner tracker and it is designed to minimize the amount of material in front of the calorimeter to have a small impact on the energy measurement. This is achieved by hosting the solenoid and the cryostat in the same vacuum vessel of the electromagnetic calorimeter. The toroids

¹The rapidity is defined as $y = \ln(\frac{E+p_z}{E-p_z})$

extend the magnet system to a total of 26 m length and 20 m diameter. They provide an average magnetic field intensity of 0.5 T and 1 T in the barrel and in the end-cap regions, respectively [33].

2.2.2 The inner detector

The ATLAS Inner Detector (ID) consists of three independent but complementary sub-detectors: the PIXEL, the SCT, and the TRT. Its overall layout is depicted in Figure 2.5.

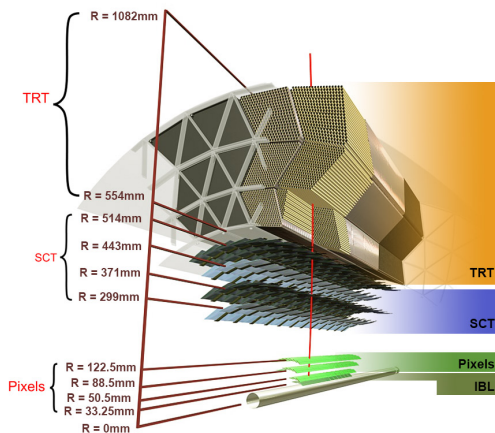


Figure 2.5 – Schematic view of the barrel of the ATLAS inner tracking system [32].

The ID is designed to provide robust pattern recognition, to reconstruct track parameters with high resolution and to measure primary and secondary vertices with high precision. Particle trajectories (tracks) are reconstructed from the *hits* in silicon layers. Tracks are reconstructed with $p_T > 400$ MeV and within a $|\eta| < 2.5$, the latter condition in particular is dictated by the acceptance of the ID. The pixel sub-system is composed of 4 cylindrical layers and 4 layer of disks to ensure coverage of the high- η region. The innermost layer, named the IBL, has been recently installed in 2015. It is made of two families of *hybrid* sensors: planar and 3D sensors, both of which are coupled with a dedicated front-end chip via a metallic bump. In *hybrid* assemblies the charge is generated on a dedicated silicon sensor and the signal is further processed and read-out by a separated chip. A detailed discussion on the main limitations of this approach will be given in chapter 8.

Planar sensors are a well-known technology for large tracking systems since they ensure robustness against radiation damage and provide a fast read-out. 3D sensors are installed at high- η region of the IBL stave. They feature electrodes which extend into the silicon bulk, hence the name 3D. Both types of IBL pixel sensors have a pixel

size of $250 \times 50 \mu\text{m}$ with the shorter pixel direction in the r - ϕ plane to optimize the impact parameter resolution in the transverse plane. The Front-End (FE) chip used to process the analog signal generated in the bulk of the detector is called FE-I4 and will be described in more details in Section 8.1.3. Pixel sensors in the other layers are characterized by a planar sensors coupled with the previous version of the front-end chip, the FE-I3. The overall assembly of a planar pixel detector is shown in Figure 2.6. The coupling between the FE chip and the sensor is done via bump-bonding, which consists in solder bumps that are deposited onto the chip pads to form ohmic contact between the two sensors.

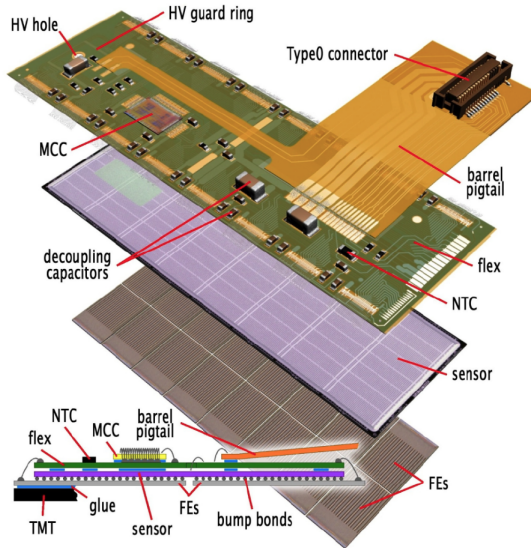


Figure 2.6 – Schematic view of the pixel assembly. Two FE are coupled via bump-bonding to a single silicon sensor.

Radiation damage usually increases the leakage current of the sensors, which in turn dissipates more power and heats the sensor more. At the same time, a higher internal temperature of the silicon produces even more leakage current due to thermal excitation of electron-hole pairs. This effect is called thermal runaway. To avoid this, a dedicated cooling system is employed to remove the heat load of typically 4 W from each module and maintain the sensors at a low temperature thus ensuring their stable operation.

The Pixel sub-system is followed by a silicon tracker based on strips (SCT) which consists of four radial layers in the barrel covering the pseudorapidity range $|\eta| < 1.4$ and

nine end-cap discs on either side covering $1.4 < |\eta| < 2.5$. The detection technique of the SCT relies on the same principle as for the pixel detector, however long strips are used compared to the rectangular pixels due to the smaller particle density in the outer layers. To resolve ambiguities, two fired strips are used to form a single *hit* used in the track fitting algorithm. The SCT is made of 4088 modules for a total of 15912 strip sensors with a length of 6.4 cm and a strip pitch of $80\ \mu\text{m}$.

The outermost sub-system of the ID is the Transition Radiation Tracker (TRT). The detecting principle consists of the collection of photon emitted when a charged particle traverses regions with different dielectric constants. The photon rate is dependent on the mass of the traversing particle so particle identification is possible. In fact, the TRT is mainly used to discriminate between pions and electrons. It consists of straw tubes, filled with a gas mixture of 70% Xe, 27% CO₂ and 3% O₂, with a diameter of 4 mm, and it can provide up to 36 hits per track in the region $|\eta| < 2$.

The overall momentum measurement provided by the ID system is:

$$\frac{\sigma_{p_T}}{p_T} = 0.05\% \cdot p_T \oplus 1\% \quad (2.3)$$

Another important track parameter is the impact parameter. As it is one of the main variables used for the identification of heavy-flavoured jets, it will be discussed in more detail Section 4.

2.2.3 The calorimetric system

The calorimeter system provides accurate measurements of high energy photons, electrons, jets and missing transverse energy. The interaction of energetic particles with matter produces a cascade (shower) of particles. The shower characteristics, such as its depth, are used to estimate the direction and energy of the reconstructed object.

The ATLAS calorimeter system is composed of two main sub-systems, the electromagnetic calorimeter and the hadronic calorimeter, as depicted in Figure 2.7.

Calorimeters must provide good containment for electromagnetic and hadronic showers to accurately measure the object energy and to limit punch-through of jets into the muon system. To this end, interaction lengths X_0 and λ are defined as the amount of material needed to decrease the initial energy of incoming object by a factor $1/e$ for electromagnetic and hadronic initiated showers, respectively. The thickness of the electromagnetic calorimeter is around $22\ X_0$ while the hadronic calorimeter has a thickness of more than 10 radiation lengths λ .

The electromagnetic calorimeter is divided into barrel $|\eta| < 1.475$ and end-cap regions ($1.375 < |\eta| < 3.2$), and are based on a lead-LAr detector. The electrodes are designed with accordion-shaped kapton and lead absorption plates to provide a complete ϕ symmetry without azimuthal cracks. Liquid argon was chosen as an active medium because of its intrinsic radiation hardness and good energy resolution. A pre-sampler is

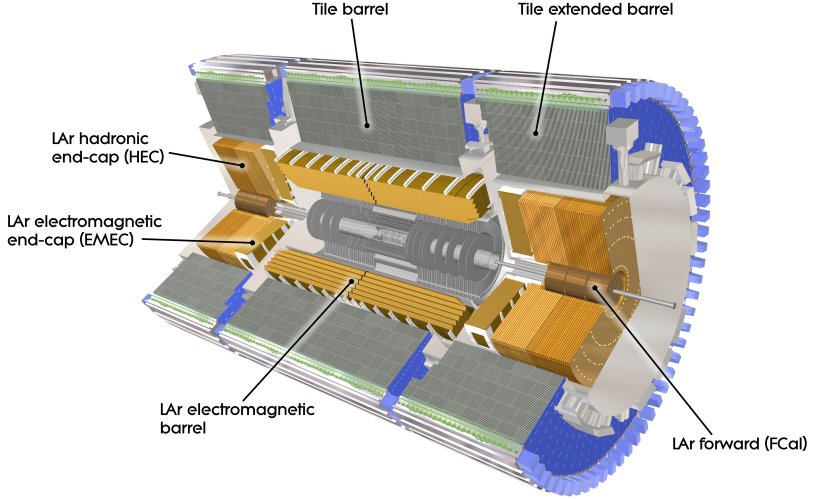


Figure 2.7 – Overall layout of the ATLAS calorimetric system [32].

instrumented to recover the energy loss in dead material in front of the calorimeter. In the region $|\eta| < 2.5$ the EM calorimeter is segmented in depth in three sections. The first is finely segmented in η to discriminate between isolated photons or photons produced by the decay of neutral hadrons, such as $\pi^0 \rightarrow \gamma\gamma$. The segmentation of the subsequent layer was chosen mainly to ensure a good spatial resolution to measure $H \rightarrow \gamma\gamma$. A schematic representation of the EM calorimeter in the barrel and its main construction parameters are shown in Figure 2.8.

The hadronic calorimeter is placed after the EM calorimeter. As for the EM calorimeter, the hadronic one is divided into different region depending on the pseudorapidity: the barrel covers $|\eta| < 1$, the two extended barrels $1 < |\eta| < 1.7$ and the end-cap region $1.5 < |\eta| < 3.2$. The barrel and extended barrel calorimeters use steel plates as absorber and plastic scintillating tiles as active material, a particle traversing the active medium produces scintillation lights which is collected with wavelength-shifting fibers running on the tile edge. PMTs are coupled to the fibers to ensure a fast and efficient collection of the emitted photons. The hadronic end-cap calorimeter consists of two cylindrical wheels which are placed behind the electromagnetic calorimeter. The hadronic end-cap technology is similar to that of the electromagnetic one in the end-cap region, the active medium is LAr, but the absorption medium is made of copper rather than lead.

In the forward region, $3.1 < \eta < 4.9$, a larger number of soft particles producing

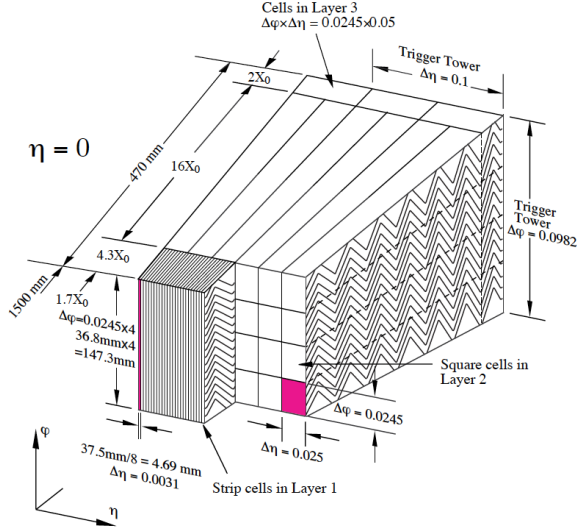


Figure 2.8 – Sketch of the EM calorimeter structure [34].

radiation damage are expected. To cope with this, a dedicated forward calorimeter system is employed. It consists of three layers in each of the end-caps, the first used as electromagnetic calorimeter and the remaining as hadronic calorimeters. For all layers, the active material is liquid argon but different absorbing material are used for the three layers: the first is made of copper while the second and third layers are made of tungsten.

One of the major figure of merit in calorimetry is the energy resolution which is parameterized as:

$$\frac{\sigma_E}{E} = \frac{S}{\sqrt{E}} \oplus \frac{N}{E} \oplus C \quad (2.4)$$

The first term represent the stochastic contribution of the intrinsic fluctuations of the number and energy distribution of particles in the shower evolution. The second term represents the effect of noise originating from the read-out electronics and the effect of the pile-up. The constant term C is due to systematic effects such as mis-calibrations of the detector as well as dead detector material. At low energy the dominant source of uncertainty is linked with the high pile-up levels achieved by the LHC whereas at high energy, the constant term becomes the leading uncertainty. In the barrel, the analysis of test-beam data [35] shows that the electromagnetic (hadronic) calorimeter achieves a resolution with $S = 10\%$ (50%) and $C = 0.17\%$ (3%).

2.2.4 Muon spectrometer

The Muon Spectrometer (MS) is placed at the outermost part of the ATLAS detector. It is primarily used to identify muons and to measure their momenta. The MS is composed of four sub-detectors that make use of different technologies: Monitored Drift Tubes (MDTs), Cathode Strip Chambers (CSCs), Resistive Plate Chambers (RPCs) and Thin Gap Chambers (TGCs). The MDT chambers are used to measure muon trajectories and to measure their momentum. A MDT chamber is made of cylindrical aluminum drift tubes of 3 cm diameter with a central wire serving as anode. These detectors reconstruct the distance between the collecting wire and the muon utilizing the drift time of the generated carriers in the active material of the chamber. MDT are designed to cover a pseudo-rapidity region of $|\eta| < 2.7$. At larger pseudo-rapidity, $2.0 < |\eta| < 2.7$, CSCs are used to cope with the higher particle flux. CSCs are radially oriented multi-wire proportional chambers, with strips placed in orthogonal directions to provide a single space point measurement for the estimation of the muon track.

The RPCs are used in the trigger system (see next section) thanks to their fast time and good spatial resolution. RPCs consist of two resistive electrode-plates placed at a distance of 2 mm and filled with a gas mix. In the higher pseudo-rapidity region $1.05 < |\eta| < 2.4$, TGCs are used to complement the RPCs in the triggering system. TGCs rely on the same working principle of the CSCs which are multi-wire proportional chambers. Both TGCs and RPCs can achieve a read-out time below 25 ns [36].

2.2.5 ATLAS trigger

The bunch spacing provided by the LHC in Run2 is 25 ns, resulting in a collision frequency of 40 MHz. The overall collision rate, which takes into account the number of protons per bunch and the inclusive cross-section of p - p collisions, is around 10^9 Hz. This high rate precludes a collection of the full event produced in each collision. A trigger system is devoted to reduce the rate to ~ 1 kHz. The trigger is designed to select the most interesting events to be further analyzed, which are typically high energetic photons, leptons, jets or events with large missing transverse momentum. The ATLAS trigger system is composed of a purely hardware-based trigger called *level-1* (L1) which selects events based on simple information from the calorimeter and muon systems. The event rate is reduced to below 100 kHz in this first triggering step. The L1 is complemented with a software-based trigger called the *high-level trigger* (HLT). The HLT provides a more complete examination of the whole event using not only muon and calorimeter information but also tracking information from the ID. Within a second, the HLT selects about 1000 events which are assembled into an event record and passed to the offline storage facilities for a complete off-line reconstruction [37].

2.3 The LHC upgrade program

The LHC underwent alternating operating periods and dedicated shut-downs, used to upgrade the accelerator machine and the detectors. A summary of the LHC operation timelines is shown in Figure 2.9. Recently, at the end of 2018, the LHC was shut-down to enter an upgrade period of two years which aims to bring the center-of-mass energy to its design value of 14 TeV and plans to collect 300 fb^{-1} , almost double the currently available statistics collected in Run2. After this period, the LHC physics program will be extended by another decade in the so-called High-Luminosity LHC (HL-LHC). The HL-LHC, with an expected integrated luminosity of 3000 fb^{-1} , will enable a series of key measurements mostly related with rare phenomena. Among them, the Higgs boson self-coupling and the Yukawa coupling between the Higgs boson and muons.

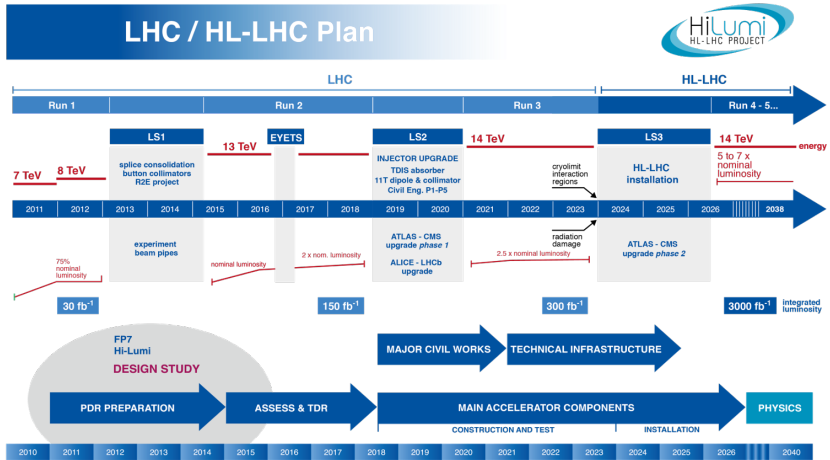


Figure 2.9 – Schedule of the LHC upgrades and operation [38].

A major upgrade of the ATLAS experiment is also expected to cope with the high luminosity of the HL-LHC. In particular, the currently installed inner tracker will be replaced by a new full-silicon tracker called ITk. Figure 2.10 shows the expected radiation fluences in the ITk. Due to the higher amount of multiplicity of particles in the vicinity of the interaction point, the inner detector layers will have to survive fluences up to $2 \cdot 10^{16} \text{ n}_{eq}/\text{cm}^2$, while for the outermost detector layers the fluence is decreased to $1 \cdot 10^{15} \text{ n}_{eq}/\text{cm}^2$. These high radiation fluences, combined with the high collision rate of 40 MHz, pose challenging requirements for silicon sensors operated at the ITk. In particular, the ability to withstand high radiation levels preserving high detection efficiency and fast time response sensor are two fundamental properties of the detectors. For this thesis, studies assessing the performance of CMOS pixel sensors, which rep-

resent a viable alternative to the currently used planar devices, will be presented and discussed.

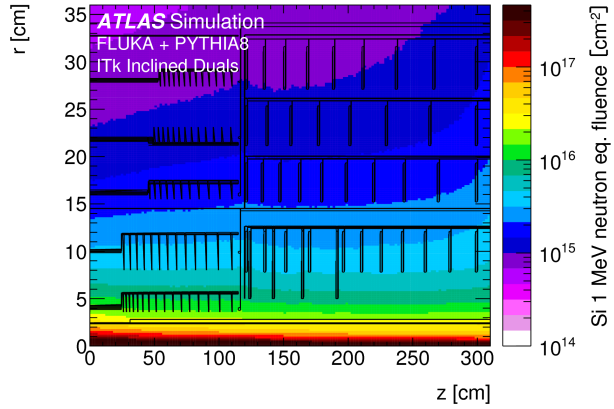


Figure 2.10 – Expected radiation fluences in the ATLAS ITk at the HL-LHC [39].

CHAPTER 3

Jets at the LHC

Quarks and gluons represent the majority of particles produced in a p - p collision. When a colored parton is produced, a spray of collimated particles is formed. To cluster together these particles into a single *jet*, dedicated algorithms are used. The set of properties that these algorithms must satisfy are the following [40]:

- simple to implement in an experimental analysis and in the theoretical calculations;
- defined at any order of perturbation theory;
- yields finite cross sections at any order of perturbation theory;
- yields a cross section that is relatively insensitive to hadronisation.

while the first point is of more practical use, the last three characteristics define the theoretical properties of a jet algorithm. These properties are embedded into the definitions of *infrared* and *collinear* safe jet algorithms. These effects are schematically demonstrated in Figure 3.1 where the soft gluon emission, in the case of collinear unsafe algorithms, splits the partons in two separate jets compared to the loop matrix element process where one parton undergoes a virtual gluon correction. This results in an artificial increase of the number of jets which is no longer representative of the initial parton [41].

The *infrared* and *collinear* safe jet algorithms used at LHC experiments are called Sequential Recombination Algorithms and will be introduced in the following.

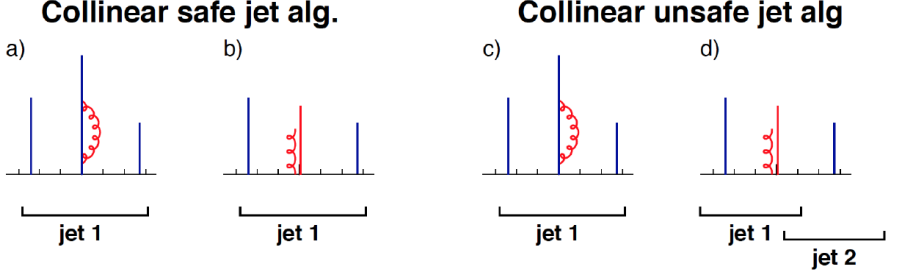


Figure 3.1 – Comparison of two processes, demonstrating the difference between collinear safe and unsafe algorithms. The parton p_T is represented by the height of the line, while the horizontal axis represents the parton rapidity. For both type of algorithms, the correction to the quark propagator (a and c) is well controlled. However, in the case of collinear emission, the gluon correction should be cancelled in perturbation theory by the gluon radiation. This feature is provided by collinear safe algorithms (b), but not collinear unsafe algorithms (d). Similar arguments can be made for infrared divergencies [41].

3.1 Sequential Recombination Algorithms

The Sequential Recombination Algorithms iteratively identify the components of a jet using a measure of the distance between them. The input to these algorithms are typically calorimeter clusters, tracks or truth particles. The distance in hadron colliders is defined to be a function of the transverse momentum and the angular separation between the different input candidates. Two distances are introduced: d_{ij} is the distance between two inputs to the algorithm and d_{iB} is the distance between the input i and the beam axis. If $d_{ij} < d_{iB}$ the inputs i , and j are combined together into a single component. The jet i is then defined when $d_{ij} > d_{iB}$ for all the remaining elements j . The distance measures used at hadron colliders are defined as follows:

$$d_{ij} = \min(p_{T,i}^{2p}, p_{T,j}^{2p}) \frac{\Delta R_{ij}}{R} \quad (3.1)$$

$$d_{iB} = p_{T,i}^{2p} \quad (3.2)$$

where ΔR_{ij} is the angular distance between component i and j , R is the radius parameter of the jet and the parameter p defines how the inputs are combined. Three jet algorithms can be built based on $p = 1, -1, 0$. The Cambridge-Aachen algorithm ($p=0$) recombines the inputs based purely on their angular distances. The k_t algorithm ($p = 1$) favors soft particles to be merged first in contrast with the anti- k_t algorithm (p

= -1) where the jets are built starting from the highest p_T components [42]. The latter algorithm is widely used by both ATLAS and CMS since it is not only less susceptible to the underlying event and pile-up but also easier to calibrate [43].

3.2 Jet Mass

In a typical search for new resonances beyond the standard model, the mass is usually reconstructed using the leading and sub-leading jet using the following relation:

$$m^2 = 2p_{T_{\text{lead}}}p_{T_{\text{sublead}}}(\cosh(\eta_{\text{lead}} - \eta_{\text{sublead}}) - \cos(\phi_{\text{lead}} - \phi_{\text{sublead}})) \quad (3.3)$$

However, when the resonance acquires high transverse momentum by recoiling against initial state radiation, the system is boosted and, when the p_T of the resonance is larger than twice its mass, the two jets are reconstructed within a single jet with a radius parameter of 1.0 (large-R jet). The mass of the jet is thus a crucial variable in analyses featuring boosted objects. One of the subject of this thesis is a search for boosted Higgs boson where the jets formed from the decay products of the Higgs bosons are merged into a single jet, and the mass of the jet is therefore one of the key discriminants against QCD jets for this and similar analyses featuring boosted object. The mass is defined based on the inputs which form the jet:

$$m^2 = (\sum_i E_i)^2 - (\sum_i \vec{p}_i)^2 \quad (3.4)$$

For a QCD singlet such as H , Z and W bosons, the jet mass is expected to peak to the nominal mass of its originating particle.

The theoretical definition of a mass for QCD-jets is more complex. QCD-jets originate from approximately massless partons, however a large fraction of jets have a significantly larger mass than zero. The differential jet mass distribution at leading order is approximately given by:

$$\frac{1}{n} \frac{dn}{dm^2} \sim \frac{1}{m^2} \frac{\alpha_s C_i}{\pi} (\ln \frac{R^2 p_T^2}{m^2} + \mathcal{O}(1)) \quad (3.5)$$

where C_i is the color factor for either a quark or gluon-jet. Due to soft emissions the mass diverges at zero. Higher order corrections are needed to cure these divergences which cause the peak of the mass distribution to shift to higher values (Sudakov peak), thus resulting in non-zero masses of the jet [44]. At higher masses, the expected distribution of the invariant mass of QCD jets is steeply falling; this is one of the main properties used to estimate the background in many analyses with hadronic final states where QCD is usually the leading background component.

3.3 Modeling Proton-Proton collisions

The modeling of p - p collision is a complex task. It involves several steps ranging from the definition of the structure of the proton to the hadronization processes. In particular, a large number of soft QCD interactions take place forming the *underlying event* which consists of multiple-parton interactions and beam remnants interactions. A schematic representation of a typical collision is shown in Figure 3.2.

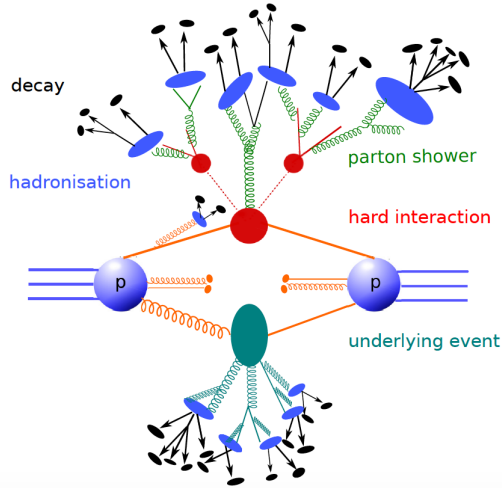


Figure 3.2 – Schematic view of a Monte Carlo simulated event including the hard scattering process, parton shower, hadronisation and underlying event.

The first step towards a formal description of the collision is to understand the structure of the proton. The proton is a composite system made of three valence quarks and a *sea* of quarks and gluons. Parton Distribution Functions, PDFs, are defined to describe the probability to find a constituent of the proton carrying a fraction of momentum x of the proton momentum. They are not process dependent and cannot be predicted by perturbative QCD, hence they need to be measured by experiments. In general, their evolution with x and Q^2 ¹ can be determined using splitting functions, formally expressed by the DGLAP-equations [45, 46]. The second fundamental step in the description of p - p collision is the factorization theorem [20]. The theorem allows one to treat the short distance components of the hard scattering process independently from the non-perturbative formation of final state particles. In view of these considerations, the hard-scattering process between two incoming partons a and b at leading order can be written as:

¹Q is the characteristic scale of the physics process of interest. It is usually defined by the momentum transfer in the physics process.

$$\sigma_{pp \rightarrow X} = \sum_{ab} \int dx_a dx_b \int f_a(x_a, \mu_f^2) f_b(x_b, \mu_f^2) \times \hat{\sigma}_{ab \rightarrow X}(x_a, x_b, \mu_f^2, \mu_r^2) \quad (3.6)$$

where $f_a(x_a, \mu_f^2)$ and $f_b(x_b, \mu_f^2)$ are the PDFs of the incoming particles, μ_f^2 is the factorization scale and $\hat{\sigma}_{ab \rightarrow X}(x_a, x_b, \mu_f^2, \mu_r^2)$ is the hard-scattering cross-section which depends not only the kinematics of the incoming partons but also on μ_f and the renormalization scale μ_r . The next step in the modeling of the collision is the *Parton Shower* (PS). PSs can be initiated from initial or final state radiation as well as from the hard-scattered quarks or gluons. Particles are emitted and produced until a certain energy scale is reached at which point the hadronisation process starts and colorless hadrons are formed. These hadrons then decay into lighter particles.

In order to produce an accurate description of the process of interest with Monte-Carlo (MC) simulations, these different steps are defined within the event-generation process. Different simulation packages are used by ATLAS and CMS. In general, two types of generators exists depending if they are able to simulate all the processes mentioned above, such as Pythia [47], Herwig [48] and Sherpa [49], or if they are able to only simulate the hard-scattering part, such as Alpgen [50] and MadGraph [51].

The truth generated event is then passed to GEANT4 [52] which simulates the interactions of these particles with the detector. At this stage, also pile-up interactions are added to the simulation with a $\langle \mu \rangle$ profile which is as close as possible to the one observed in real collision data. A model for the collection mechanisms of the detectors and sub-sequent electronic processing is employed and finally the reconstruction algorithms are run on these simulated events.

The identification of heavy-quark initiated jets

The ability to identify jets originating from b - and c -quarks (b - and c -tagging) is key to many aspects of the physics program pursued by the high energy physics experiments. First, it is fundamental to study the physics of the top-quark given its large decay rate to the b -quark. Second, it allows for the study of the Yukawa coupling of the Higgs boson to the heaviest fermions: t - and b -quarks. Third, b -quarks arise in many searches looking for super-symmetric particles. Fourth, many theories beyond the standard model predict new massive particles with an enhanced coupling to b -quarks. These different analyses require an highly efficient b -tagging performance over a broad region of momentum and pseudo-rapidity, as well as in challenging topologies, such as the dense environment resulting from the decays of boosted particles.

When a b -quark is produced during a collision event, it hadronizes to form a jet in the detector, the so-called b -jet. b -tagging exploits the properties of the weak-decay modes of the b -hadron using the reconstructed tracks associated to the corresponding b -jet. Due to the challenging reconstruction environment, b -tagging represents one of the most complex uses of tracking detectors. Since the proper life-time (τ) of a b -hadron is around 1.5 ps, in the reference system of the hadron the average decay distance is $c\tau \approx 400 \mu m$. In the laboratory frame of reference, instead, the b -hadron life-time is further increased by the boost, assuming a b -hadron with transverse momentum of around 50 GeV, the decay distance is on average $\langle l \rangle = \beta\gamma c\tau \approx 3 \text{ mm}$. The resulting displaced topology can be exploited experimentally by reconstructing the secondary vertex associated with the weak decay of the heavy-hadrons and the impact-parameters of the tracks reconstructed from its decay products. Therefore, an efficient reconstruction of

secondary vertices and a good resolution of the track parameters within a jet is crucial to achieve efficient b -tagging performance.

In the following, the latest b -tagging algorithms used by the ATLAS collaboration for the Run2 data-taking period, named 2017 b -tagging configuration throughout this chapter, will be described and compared to the previous b -tagging configuration, referred to as 2016 b -tagging configuration. Particular emphasis will be also given to the performance of high- p_T b -tagging.

4.1 Track reconstruction using the ATLAS detector

The identification of heavy-hadrons relies on the performance of the track reconstruction algorithms. A concise description of the track reconstruction in the ATLAS experiment and the main relevant track parameters for heavy-flavour tagging are described in the following. A more detailed discussion can be found elsewhere [53]. When a charged particle traverses a silicon sensor, free carriers are generated and collected, if the related amplitude is larger than a given threshold (see chapter 7), a silicon *hit* is produced. In case neighbouring pixels are fired, a dedicated clustering algorithm is used to group them together. The clustering algorithm used by the ATLAS collaboration relies on a neural network which is able to classify cluster generated by multiple charged particles. Such merged clusters mostly originate from highly energetic objects, such as high p_T b -jets as described in more detail in Ref. [54]. Reconstructed clusters are then used as input to the tracking algorithms.

Track reconstruction in multi-purpose experiments is usually divided into two steps: the track-finding or pattern recognition and the actual fit used to extract the track parameters and their uncertainties. Track-finding is the ability to correctly identify all of the clusters pertaining to the same charged particle that traversed the detector without including any clusters from other particles. This task is particularly challenging at the LHC due to the large combinatorial background arising from the high particle multiplicity produced in the many simultaneous p - p collisions. Track-finding in the ATLAS experiment is assessed using a Kalman filter technique which iteratively updates the clusters in the detector layers associated to the track candidate. The algorithm starts from seed clusters in the innermost layer and progresses upstream until the outermost silicon layer is reached; this is the so called inside-out pattern recognition. Once the clusters associated to a candidate track are found, the track fitting is performed. The trajectory of a charged particle in a magnetic field generated by a solenoid is described by a set of five parameters. Two parameters are needed to describe a straight-line trajectory in the longitudinal plane, where no magnetic field is present, and three parameters to describe the circular trajectory in the transverse plane. The parametrization of these five parameters chosen by the ATLAS experiment is: $(d_0, z_0, \phi, \cot(\theta), Q/p_T)$, the corresponding definition is shown in Figure 4.1. The five parameters are expressed with respect to the point of closest approach to the primary vertex, the perigee. In particu-

lar, d_0 and $z_0 \sin \theta$ are the Impact Parameters (IP), and they are the distance of closest approach in the transverse and longitudinal planes. They also represent the baseline variables used in the discrimination of heavy-flavoured jets. It is therefore interesting to discuss in more detail the dependency of these parameters on the detector geometry. It can be shown that in a simplistic case consisting of 2 measuring silicon-planes and no magnetic field, the uncertainty on z_0 can be expressed as [55]:

$$\sigma_{z_0}^2 = A \oplus \frac{B}{p_T} = \frac{\sigma^2(r_1^2 + r_2^2)}{(r_1 - r_2)^2} \oplus \frac{B}{p_T} \quad (4.1)$$

where A is the contribution related to the detector geometry and B/p_T is the multiple-scattering which deteriorate the z_0 resolution at low track- p_T . r_1 and r_2 are the distance of two detector planes with respect to the primary vertex and σ is the uncertainty on the measurement, which, in case of a single hit in the cluster, is proportional to the longitudinal pitch of the pixel, $\sigma = \text{pitch}/\sqrt{12}$. When the p_T of the tracks is large enough (around 1.5 GeV in the ATLAS detector), the IP resolution saturates to A which represents an intrinsic limitation depending only on the geometry of the detector. Although the previous parametrization was derived for a simplistic case, the overall conclusions do not change compared to the parametrization derived from a more complete description of the detector geometry. In general, three main design principles must be respected to minimize the uncertainty on the IP:

- excellent spatial resolution. This is directly related to the size of the pixel pitch and it is one of the main reasons to characterize innovative detector technologies such as CMOS pixel sensors as described in Chapter 8.
- place the innermost layer as close as possible to the interaction point to improve the track extrapolation uncertainty at the primary vertex.
- minimize the amount of material since the impact of multiple scattering is dominant at low energy.

4.2 The Run2 b -tagging algorithms

The main algorithms used to discriminate between b -, c - and light-jets¹ rely on the properties of heavy hadrons decaying via weak interactions:

- As already mentioned, heavy-hadrons are long-lived. A b -hadron with ~ 50 GeV of transverse momentum typically travels a few mm before decaying. This leads to macroscopic observables linked with the displaced topology.

¹A light-jets is a jet originated by a $u/d/s$ or gluon-jets.

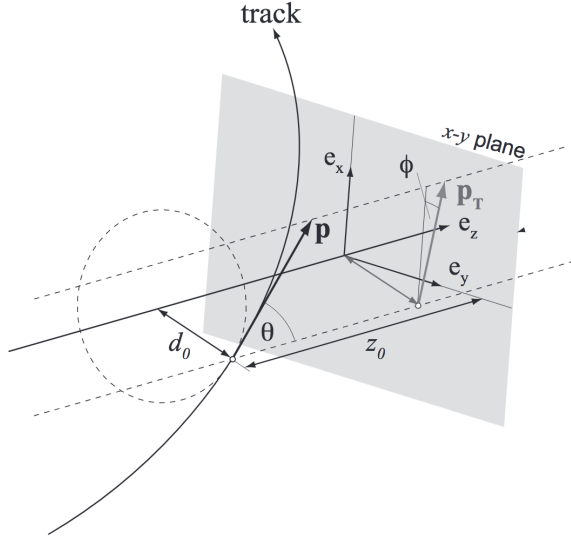


Figure 4.1 – Illustration of helix parameters of a charged tracks defined using the ATLAS coordinate system [56].

- The fragmentation function of the b -hadron is hard. Around 70% of the energy carried by the initial b -quark is transferred to the final hadron.
- b -hadrons are the heaviest pseudo-stable particle in the SM. Their decay products carry a larger p_T compared to the one produced by lighter long-lived particles such as K_s or Λ .

Given these properties, identification algorithms are constructed to exploit the presence of displaced secondary and tertiary vertices as well as tracks with IP values which are not compatible with the primary vertex. An event display outlining the most representative quantities used for b -tagging is shown in Figure 4.2.

The algorithms used by the ATLAS collaboration can be divided into three main categories:

- IP-based: Two main classes of algorithms exploit the IPs of the tracks associated to the jet. The first is made of IP2D and IP3D. Both algorithms are based on Log-Likelihood-Ratio (LLR) discriminants relying on template distributions of the transverse and longitudinal IPs of tracks in the jet. This is a well-known algorithm which was employed by several early high-energy physics experiments.

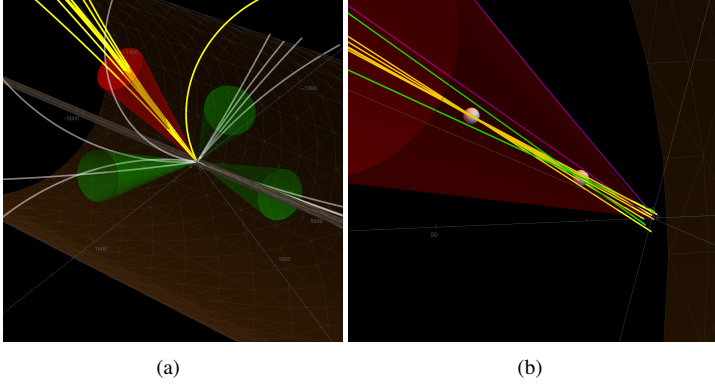


Figure 4.2 – a) Event display of a simulated $t\bar{t}$ event. The b -jet with largest p_T in the event is marked in red. The tracks produced by the hadronization and subsequent decay of the b -hadron are shown in yellow. b) A zoom inside the leading b -jet. The spheres indicate the reconstructed vertices from the decay of the b - and c - hadrons. The tracks marked in green are generated by the b -decay while the ones shown in yellow are produced by the decay of the c -hadron.

A more innovative approach is based on a Recurrent Neural Network (RNNIP) which takes tracks as input to deliver a single output score per jet. As opposed to the IP-tag algorithms, RNNIP exploits the correlations between the impact parameters of the tracks in the jet.

- Vertices-based: Two algorithms are based on vertex reconstruction, The SV1 algorithm aims at reconstructing a single secondary vertex in the jet. The Jet-Fitter algorithm, instead, reconstructs the full weak decay chain of the b -hadron. It is based on the initial assumption that the jet-axis corresponds to the b -decay flight, secondary and tertiary vertex can be built and the assumption is iteratively corrected using a modified Kaman-filter technique. Both algorithms use the tracks associated to the vertex to exploit the distinctive features of the b -hadron such as its hard fragmentation function and the multiplicity of its decay products.
- Soft-muons: An algorithm based on the semi-leptonic decay of heavy hadrons to soft muons was also implemented and characterized in simulation. Improvements of the b -tagging performance are achieved thanks to discriminative variables which are built from kinematic and quality requirements of the muon track associated to the jet.

The outputs of such algorithms are then combined using multivariate techniques: a boosted decision tree (MV2) and a deep neural network (DL1) are used as final b -tagging algorithms, referred to as high-level taggers in the following. To optimize and

characterize the b -tagging performance at high p_T , a dedicated sample, enriched with high- p_T b -, c - and light-jets was produced.

Tracks used for flavour tagging are associated to the jet using a ΔR matching criteria. ΔR is chosen to be a function of the jet- p_T to profit from the fact that decay products of energetic hadrons are more collimated. As a reference, a ΔR of 0.45 is chosen for a jet- p_T of 20 GeV and it shrinks to 0.26 for a jet- p_T of 150 GeV [2].

Finally, to characterize the b -tagging performance in simulation, a truth-based labeling is needed. The labeling scheme used for the reconstruction of RUN2 data associates the jet to the flavour of the original hadron: a jet is labeled as b -jet if a b -hadron with $p_T > 5$ GeV is found within a cone of radius 0.3 around the jet-axis. If no b -hadron is present, the procedure is repeated first for c -hadrons and then for τ -leptons. The remaining jets with no such matching are defined as light-jets.

In the following, a more detailed description of the b -tagging algorithms and their performance will be given.

4.2.1 Impact parameter algorithms

The transverse and longitudinal IPs are among the most powerful discriminanting variables used in b -tagging. The IP3D and IP2D algorithms rely on the information from these impact parameters and their significance, defined as the impact parameter divided by its uncertainty. In particular, IP2D makes use of the transverse IP significance, d_0/σ_{d_0} , whereas IP3D makes use of both the transverse and the longitudinal IPs. In both cases, a sign is associated with the impact parameters of the tracks used by the algorithms which replace the geometrical definition of the sign of the impact parameters. This is done to improve the discrimination of tracks that most likely originate from heavy-hadron decays. The sign is defined positive (negative) if the point of closest approach of the track to the primary vertex is upstream (downstream) of the primary vertex with respect to the jet direction.

In order to improve the purity of tracks originating from heavy-hadron decays, a track selection is implemented based on the following requirements:

- track- $p_T > 1$ GeV;
- $|d_0| < 1$ mm and $|z_0 \sin\theta| < 1.5$ mm;
- seven or more silicon hits, with at most two silicon holes, at most one of which is in the pixel detector, where a hole is defined as a hit expected to be associated with the track but not present.

IP2D and IP3D are based on a Log Likelihood Ratio (LLR) which uses tracks to provide a per-jet score assuming there are no correlation among them. The LLR is defined as:

$$LLR = \sum_n^{\#tracks} \log\left(\frac{p_{b,n}}{p_{l,n}}\right) \quad (4.2)$$

Where $p_{b,n}$ is the template probability that the n -th track in the jet belongs to a b -jet, similarly $p_{l,n}$ represents the light-flavor hypothesis. Since it is assumed that tracks are uncorrelated, template pdfs are uniquely defined for each jet flavor. Such distributions are taken from reference histograms of the transverse impact parameter significance and a joint 2D distribution of the transverse and longitudinal impact parameter significances for IP2D and IP3D respectively. The reference histograms used to define the probability distribution function (pdf) are derived from MC simulation. To further increase the discriminating power, pdfs are divided into exclusive categories based on the hit pattern of the track. A total of 14 categories are used as shown in Table 4.3. The fraction of these track grades as a function of the jet- p_T is shown in Figure 4.4 for b -flavored jets. For jets at high energy, the categories featuring expected, shared or split hits increases due to the displaced and boosted topology of high-energy b -hadron decays².

Figure 4.5 shows the IP significance in the transverse and longitudinal planes for the *good* category defined in the table. The jets originating from b - and c -quarks shows a larger tail towards high positive values due to their displaced decays. The negative side forms approximately a gaussian distribution since most of the negative signed tracks are due to mis-reconstruction effects caused by the finite resolution of the IPs. The distribution of light-flavoured jet also shows large, non gaussian tails in the distribution of the IP significances, S_{d_0} and S_{z_0} . This is due to tracks from Λ , K_s , photon conversions and interactions in the detector material. The LLR score evaluated on a $t\bar{t}$ sample is shown in Figure 4.6 for both, IP2D and IP3D algorithms. A clear separation is achieved.

4.2.2 A Recurrent Neural Network based on tracks

In the decays of heavy particles the impact parameters are intrinsically correlated among themselves. If one track is found with large impact parameters, it is likely to find a second track with large impact parameters since both tracks originate from a common source [57]. Figure 4.7 shows the correlation of the leading and sub-leading IP tracks for b -jets. Recurrent Neural Network (RNNIP) can be used to profit from these properties. RNN are used to learn sequential dependencies between variables, therefore they are particularly suited to approach the identification of heavy-hadrons.

²It is worth mentioning that in the ATLAS simulation infrastructure the interactions with the detectors of charged b - and c -hadrons are not simulated by default. This is particularly relevant for high-energy hadrons which can eventually decay beyond the IBL.

#	Category	Fractional contribution [%]		
		<i>b</i> -jets	<i>c</i> -jets	light-jets
0	No hits in first two layers; expected hit in IBL and b-layer	1.9	2.0	1.9
1	No hits in first two layers; expected hit in IBL and no expected hit in b-layer	0.1	0.1	0.1
2	No hits in first two layers; no expected hit in IBL and expected hit in b-layer	0.04	0.04	0.04
3	No hits in first two layers; no expected hit in IBL and b-layer	0.03	0.03	0.03
4	No hit in IBL; expected hit in IBL	2.4	2.3	2.1
5	No hit in IBL; no expected hit in IBL	1.0	1.0	0.9
6	No hit in b-layer; expected hit in b-layer	0.5	0.5	0.5
7	No hit in b-layer; no expected hit in b-layer	2.4	2.4	2.2
8	<i>Shared</i> hit in both IBL and b-layer	0.01	0.01	0.03
9	At least one <i>shared</i> pixel hits	2.0	1.7	1.5
10	Two or more <i>shared</i> SCT hits	3.2	3.0	2.7
11	<i>Split</i> hits in both IBL and b-layer	1.0	0.87	0.6
12	<i>Split</i> pixel hit	1.8	1.4	0.9
13	<i>Good</i>	83.6	84.8	86.4

Figure 4.3 – Description of the track categories used by IP2D and IP3D along with the fraction of tracks in each category for a $t\bar{t}$ sample. The categories are constructed with respect to the track quality, which is defined by the clusters (referred to as hits in this table), from the silicon layers of the Inner Detector, used in the track reconstruction. The clusters in the innermost (IBL) and next-to-innermost (*b*-layer) layer of the pixel detectors are of particular importance, as is the knowledge of whether a cluster was expected (exp.) or not, based on the detector coverage and dead module maps. Shared hits are clusters which are shared among more than one track, degrading track quality, while split hits are clusters which have been identified as originating from overlapping tracks and have therefore be split into sub-clusters. In case the track does not represent any of the previous 13 categories, it is defined as good [1].

The RNN algorithm is based on a total number of five input variables per track: S_{d_0} and S_{z_0} , the fraction of transverse momentum carried by the track relative to the jet- p_T , the angular distance between the track and the jet-axis and the grades of the tracks. The tracks are ordered by their S_{d_0} which is the most discriminating variable, for this reason the algorithm has been named RNNIP. The NN returns three output variables per jet, corresponding to the *b*-, *c*- and light-jet probabilities. These outputs are combined into the discriminant function, which is defined as follows:

$$D_{RNN} = \ln \frac{p_b}{f_c p_c + (1 - f_c) p_{light}} \quad (4.3)$$

where the f_c is the *c*-fraction. This fraction can be tuned to weight the relative importance of one jet flavor with respect to another to enhance the discrimination of *b*- vs *c*-jets or *b*- vs light-jets.

As already mentioned, the IP2D and IP3D are based on similar inputs, namely the impact parameters of the tracks. To address the complementarity between the two algorithms, a study was performed by removing one of the algorithms at a time from the MV2 training. It was found that RNNIP improves the performance in the case of

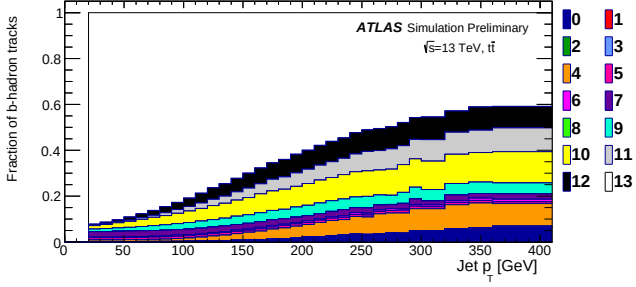


Figure 4.4 – Fraction of tracks from b -hadron decays as a function of the jet- p_T for $t\bar{t}$ events for IP categories reported in Figure 4.3 [1].

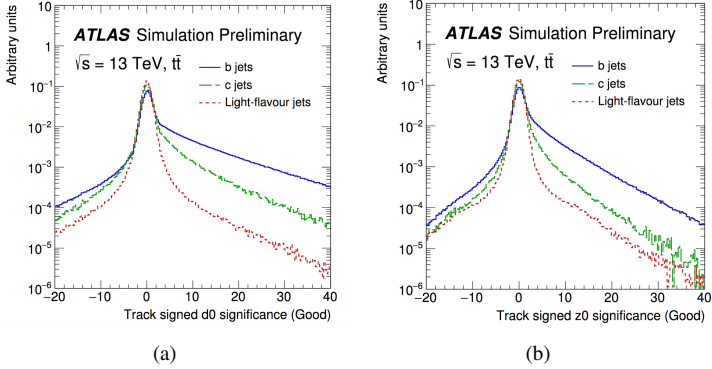


Figure 4.5 – The transverse (a) and longitudinal (b) signed impact parameter significance of tracks in $t\bar{t}$ simulated events [2].

jets with high multiplicity of tracks and large displaced vertices but it does not fully overcome the LLR-based tagger at low jet- p_T . In fact, when removing IP3D from the MVA training, a decrease of efficiency of around 15% was observed in jets featuring low track-multiplicities. As a results, both algorithms were used in the training of the high-level taggers. In the future, a training of the RNNIP tagger on a more inclusive sample will help to remove this loss of performance.

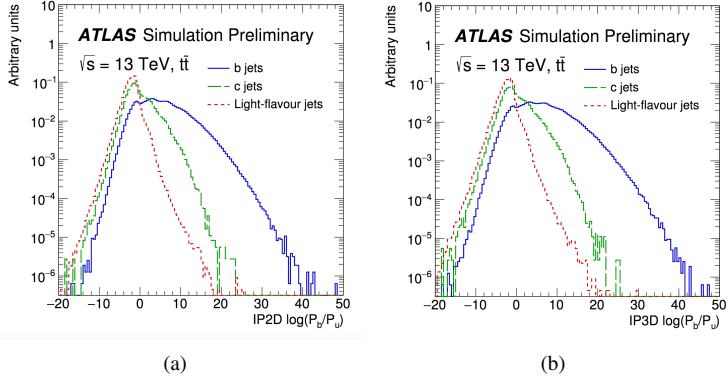


Figure 4.6 – The LLR distribution for the (a) IP2D and (b) IP3D b-tagging algorithm for b (solid blue), c (dashed green) and light-flavour (dotted red) jets in $t\bar{t}$ simulated events [1].

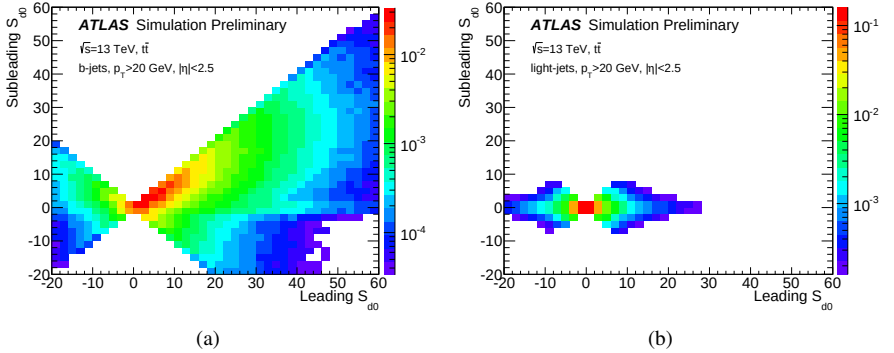


Figure 4.7 – The distribution of the d_0 significance for the leading d_0 significance track and sub-leading d_0 significance track in b-jets (left) and light jets (right). Each distribution is normalized to unity [57].

4.2.3 Inclusive secondary-vertex reconstruction algorithm

The secondary vertex finding algorithm (SV1) reconstructs a single secondary vertex in the jet. An exclusive reconstruction of the possible b -decays would drastically limit the tagging efficiency of the algorithm due to high numbers of neutral particles involved in the weak b -hadron decay chain. In addition, particles originating in the subsequent decays of the c -hadron generically carry a low transverse momentum leading to degradation of the relevant track parameters used to build the vertex. For these reasons, the algorithm reconstructs an inclusive vertex within the jet with minimal assumptions on the number of tracks involved in the decays [58].

The reconstruction starts from a two-track vertex hypothesis formed by combinations of track pairs in the jet. Cleaning cuts are applied to the two-track vertices to reject decays of K_s and Λ , photon conversion and hadronic interactions with the detector material. Two additional cuts are applied to address the most complicated topologies arising from high- p_T jets and high- η jets. To cope with the former, tracks in jets with $p_T > 300$ GeV are ordered based on their measured p_T and the first 25 tracks are used in the vertex finding strategy. This is done to remove the large number of fragmentation tracks originating at high-energy while still retaining all reconstructed tracks from the b -hadron decays, including the case where jets containing a gluon split to $b\bar{b}$. In the case of high η regions, the track reconstruction suffers from an increasing amount of detector material leading to worse resolution of the track parameters. To increase the quality of these tracks, a minimal number of required silicon-hits of 7 (including pixels and SCT) is used at the expenses of a slight decrease of efficiency. Finally, only tracks with $S_{d_0} < 2$ and $S_{z_0} > 6$ are used to mitigate the effect of pile-up. Once the tracks are finally selected, a global χ^2 minimization procedure is used to determine the vertex parameters.

The algorithm builds a total of eight discriminating variables from the reconstructed secondary vertex, including: the number of two-track vertices reconstructed within the jet, the transverse decay length, the 3D decay length significance, the energy fraction, the invariant mass and the number of tracks associated with the vertex. Figure 4.8 shows the distribution of these variables in $t\bar{t}$ events for b -, c - and light-jets.

The reconstruction rate of the algorithm as a function of the jet- p_T is also shown in Figure 4.9; the combinatorial background arising from the larger number of fragmentation tracks increases at high- p_T , thus decreasing the rate of vertices in b -jets. At the same time the higher collimation of the particles in the jet increases the probability of producing fake vertices.

4.2.4 The JetFitter algorithm

JetFitter (JF) is a decay chain multi-vertex reconstruction algorithm. In contrast to the SV1 algorithm, JF is based on a priori assumption which allows it to resolve the topological vertex structure of heavy hadron decays inside a jet. It is initially assumed that the b and c -hadrons decay on the same line defined by the jet-axis. This hypothesis is

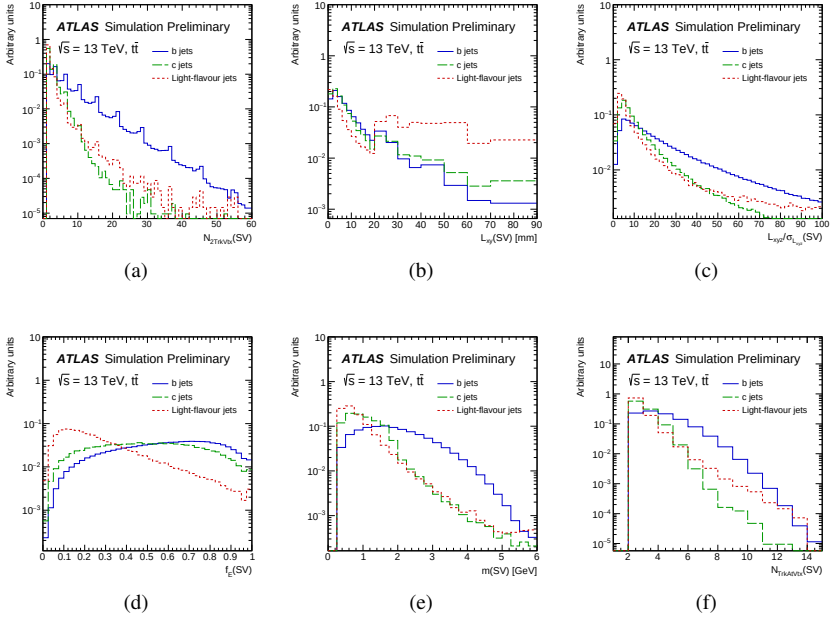


Figure 4.8 – (a) The number of two-track vertices reconstructed within the jet, (b) the transverse decay length, (c) the 3D decay length significance, (d) the energy fraction, (e) the invariant mass and (f) the number of tracks associated with the vertex [1].

justified through the kinematics of the particles involved as defined through the hard fragmentation function of heavy quarks [60]. There are three main advantages to the use of this method:

- Incomplete topologies can be reconstructed, including topologies with a single track from the b -hadron decay and a single track from the c -hadron decay.
- The fit evaluates the compatibility of the given set of tracks with a $b \rightarrow c$ -like cascade decay topology, increasing the discrimination power against c - and light-flavoured jets.
- Constraining the tracks to lie on the b -hadron flight axis reduces the number of degrees of freedom of the fit, increasing the chance of separating the b - and c -hadron decay vertices [61].

The vertexing task is mathematically implemented in JetFitter as an extension of the Kalman filter formalism for vertex reconstruction. While in a conventional Kalman filter vertex fit the variables to be iteratively updated in the fit are the three-dimensional

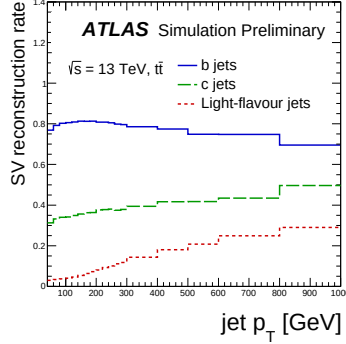


Figure 4.9 – Secondary vertex reconstruction rate as a function of jet- p_T [59].

components of the vertex position, in the case of JetFitter the variables that are iteratively updated describe the full decay chain [61].

Distributions of some of the most important output variables are shown in Figure 4.10. The vertex reconstruction efficiency is shown in Figure 4.11 for different requirement on the minimal number of tracks forming the vertex. It is observed that the efficiency to have at least a single-track vertex is significantly higher than the efficiency to have a vertex with at least two tracks. However this is also seen in case of the light-jets, especially at high p_T where the probability to form a single track vertex increases rapidly due to the higher number of tracks produced during the fragmentation process of energetic hadrons.

4.2.5 Tagging with soft muons

The Soft Muon Tagger (SMT) aims to reconstruct the muons from semi-leptonic b -decays. These muons usually carry a sizable p_T in the weak decay chains of heavy-hadrons, though smaller than the typical p_T of prompt muons produced from vector boson decays, hence the label "Soft". The b -tagging performance of SMT is intrinsically limited by the decay branching ratios of b -hadrons to muons $\text{BR}(b \rightarrow \mu\nu X \approx 11\%)$ and by the branching ratio of the subsequent semi-leptonic decay of the c -hadron to muons: $\text{BR}(c \rightarrow \mu\nu X \approx 10\%)$. However, in semi-leptonic decays the IP- and vertex-based taggers suffer from the number of charged particles and their invariant mass and energy. The SMT algorithm, while being intrinsically limited by the BR, provides a useful complement to the other taggers for jets featuring semi-leptonic decays to muons.

SMT uses muon tracks which feature clusters from the inner tracking detector and the muon spectrometer. Muons are associated with the jet based on an angular requirement of $\Delta R(\text{muon}, \text{jet}) < 0.4$. In addition, muons are required to have a minimum p_T

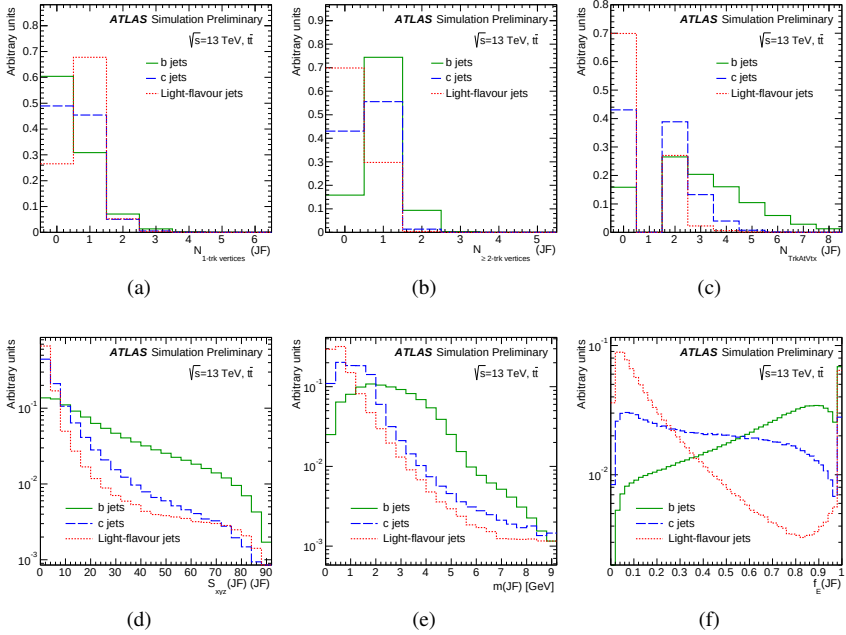


Figure 4.10 – Properties of the decay topology and secondary vertices reconstructed by JetFitter for b - (solid green), c - (dashed blue) and light-flavour (dotted red) jets in $t\bar{t}$ events: (a) the number of 1-track vertices, (b) the number of vertices with at least two tracks, (c) the number of tracks from vertices with at least two tracks, (d) the average flight length significance of the reconstructed vertices, (e) the invariant mass of tracks fitted to one or more displaced vertices and the (f) energy fraction, defined as the energy from the tracks in the displaced vertex relative to all tracks reconstructed within the jet [62].

of 5 GeV, $d_0 < 4$ mm and $|\eta| < 2.5$. The latter cut is based on the acceptance of the ID, the IP cut rejects muons from long-lived particle decays and the p_T cut is dictated by the energy loss of muons traversing the calorimetric system of around 3 GeV.

Six discriminating variables are then built for muons passing these quality criteria and a BDT is used to provide a single output score per jet. Out of these variables, three are based on the quality of the tracks and the other three cover the kinematics of the semi-leptonic decays. Table 4.1 shows a summary of the variables used while Figure 4.12 shows the BDT score distributions for the different jet-flavours.

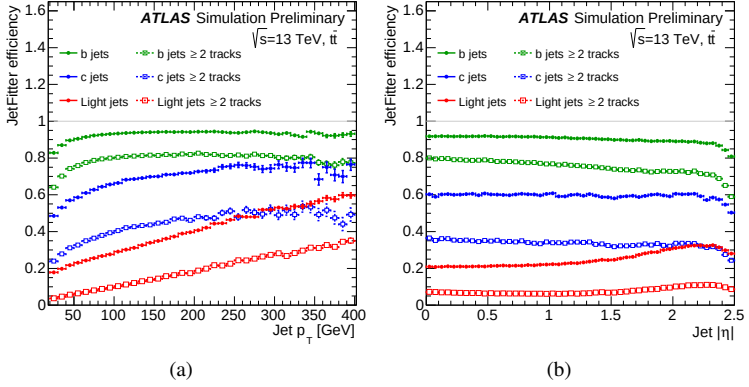


Figure 4.11 – JetFitter vertex reconstruction efficiency as function of (a) jet- p_T and (b) η for b - (green), c - (blue) and light-flavour (red) jets in $t\bar{t}$ events. The solid lines with closed markers represent the efficiency to reconstruct any JetFitter decay chain, the dashed line with open markers requires that at least one vertex has two or more tracks [59].

Table 4.1 – The input variables of the SMT algorithm.

algorithm	description
$\Delta R(\mu - jet)$	angular distance between the muon and the jet-axis.
d_0	transverse impact parameter of the muon track.
$p_{T,rel}$	projection of the muon momentum in the direction perpendicular to the jet-axis.
$\sum_i \frac{\Delta\phi_i}{\sigma_{\Delta\phi_i}}$	significance of the angular difference $\Delta\phi$ between pairs of adjacent hits along the track.
$(\frac{q}{p})_{ID}/(\frac{q}{p})_{MS}$	ratio of the curvature of the muon track in the magnetic field in the inner detector divided by the one obtained in the muon spectrometer.
$\frac{E_{ID}-E_{MS}}{\sigma E_{ID+MS}}$	difference between the momentum measured in the spectrometer and inner detector normalized to the energy loss in the calorimeter.

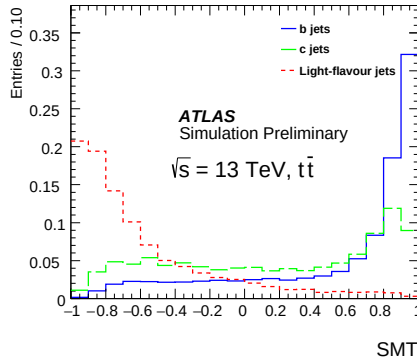


Figure 4.12 – Output of the BDT used to combine the soft-muon tagging discriminating variables [2].

4.2.6 The High-level taggers

The outputs of the b -tagging algorithms are combined together by means of multivariate techniques. A boosted decision tree is used to provide the final discrimination power in ATLAS and it is called MV2. MV2 is built from the ROOT Toolkit for Multivariate Data Analysis (TMVA) [63]; more details on the BDT parameters can be found in [1]. Similarly to what was discussed for RNNIP in section 4.2.2, it is possible to modify the performance of the light- versus c -jet rejection for a given b -jet efficiency. In a BDT-based tagger this is achieved by changing the fraction of c -jets when performing the training. The MV2 variants of the tagger were all trained using a fraction of c -jets equal to 7%.

In addition to MV2, a novel high-level discriminant was developed based on a Deep Neural Network, named DL1. DL1 is built using Keras [64] with the Theano [65] back-end and utilises the Adam optimizer [66]. The NN architecture and the optimization of its hyperparameters are defined in more detail elsewhere [67].

The following discussion describes the high-level tagger characterization performed in 2017. The two families of high-level taggers, MV2 and DL1, were optimized in parallel and results were produced for both of them independently. For simplicity, only the MV2 family of taggers will be discussed in detail. Similar features and conclusions were also found for DL1, as reported in [67]. The advantages of using a NN instead of a BDT are presented in section 4.2.6.3.

Given the availability of several low level taggers, three different variants of MV2 were implemented and studied:

- **MV2**: a reference option, based on the inputs from the IP2D, IP3D, SV1 and JetFitter algorithms. Table 4.2 summarizes the 21 input variables for this default configuration. In some of the Figures, MV2 is also called with the name used in the 2016 b -tagging configuration, MV2c10. Figure 4.13 shows the output score of the BDT used to characterize the b -tagging performance in MC simulated events.
- **MV2mu**: SMT is added to MV2.
- **MV2muRnn**: RNNIP is added to MV2mu.

In addition to these high-level tagger variants, a novel training strategy was adopted to tune the b -tagging algorithms. A Z' sample was designed and characterized specifically to optimize the performance at high- p_T . In the following, a more detailed description of the training strategy will be given.

4.2.6.1 The Training strategy

Previous versions of the high-level taggers were trained on $t\bar{t}$ sample, as described in Ref. [2]. The jet- p_T spectrum of this sample is steeply falling, leading to insufficient

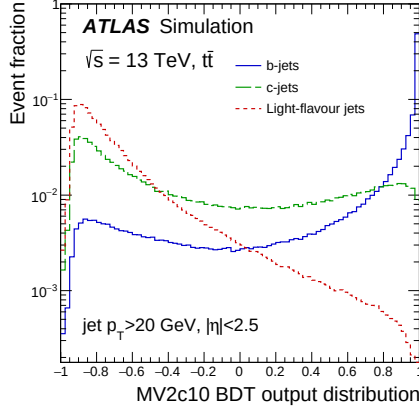


Figure 4.13 – The MV2c10 output for b -jets (solid line), c -jets (dashed line) and light-flavour jets (dotted line) in simulated $t\bar{t}$ events [1].

Table 4.2 – The 21 input variables used by the MV2 b -tagging algorithm.

algorithm	variable	description
Kinematics	jet- p_T	Jet transverse momentum
	jet- η	Jet pseudorapidity
IP2D,IP3D	$\log(p_b/p_{light})$	Likelihood ratio between the b - and light-jet hypotheses
	$\log(p_b/p_c)$	Likelihood ratio between the b - and c -jet hypotheses
	$\log(p_c/p_{light})$	Likelihood ratio between the c - and light jet hypotheses
SV1	$m(SV)$	invariant mass of tracks at the secondary vertex assuming pion masses
	$f_E(SV)$	fraction of the charged jet energy in the secondary vertex
	$N_{trkAtotx}(SV)$	number of tracks used in the secondary vertex
	$N_{2trkVtx}(SV)$	number of two track vertex candidates
	$L_{xy}(SV)$	transverse distance between the primary and secondary vertices
	$L_{xyz}(SV1)$	distance between the primary and secondary vertices
	S_{xyz}	distance between the primary and secondary vertices divided by its uncertainty
	$\Delta R(\text{jet},SV)$	ΔR between the jet axis and the direction of the secondary vertex relative to the primary vertex
JetFitter	$N_{2trkVtx}(JF)$	number of 2-track vertex candidates (prior to decay chain fit)
	$m(JF)$	invariant mass of tracks from displaced vertices assuming pion masses
	$S_{xyz}(JF)$	significance of the average distance between the primary and displaced vertices
	$f_E(JF)$	fraction of the charged jet energy in the secondary vertices
	$N_{1-trackvtx}$	number of displaced vertices with one track
	$N_{>1-trackvtx}$	number of displaced vertices with more than one track
	$N_{trkAtotx}(JF)$	number of tracks from displaced vertices with at least two tracks
	$\Delta R(\vec{p}_{jet}, \vec{p}_{vtx})$	ΔR between the jet axis and the vectorial sum of the momenta of all tracks attached to displaced vertices

statistics above ~ 250 GeV. This results in sub-optimal performance for the higher p_T regime. A Z' sample with an artificially wider jet- p_T spectrum was designed to cope with kinematic regions not accessible when training on a $t\bar{t}$ sample. This is achieved thanks to a dedicated reweighting employed at truth level for particles originating from the hard-scatter process. The reweighting strategy was derived in two steps: first the hard-scatter component was removed by applying a weight corresponding to the inverse of the Breit-Wigner distribution, then the remaining dependency originating from the PDFs was parametrized to obtain a wider transverse momentum distribution of the de-

cay products of the Z' . The reweighted cross-section is fed into Pythia8 which offers the possibility to internally modify on the fly the cross-section of the hard-scattered partons before the actual event generation. The branching ratios of this sample were set to 33.3% for each b -, c - and light-jets. In particular, the rates of light-jets were set to 11.1% for u -, d - and s -quarks, and no gluons or leptons from hard-scattering were simulated. Figure 4.14 shows a comparison of the Z' and the standard $t\bar{t}$ samples for light- and b -jets.

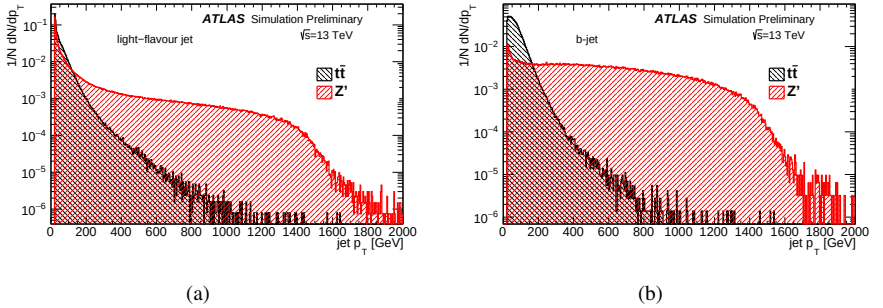


Figure 4.14 – Jet- p_T distributions for $t\bar{t}$ and the wide Z' sample for light-jets (a) and b -jets (b). The distributions are normalized to unity [2].

The $t\bar{t}$ and Z' events are split to form orthogonal samples for training and evaluating the performance of the algorithm. Half of the statistics of each sample is used to train the BDT and the other half is used to evaluate its performance. The performance is then quantified using a ROC curve, where the b -jet efficiency is computed as a function of the light- or c -jet rejection, which is defined as the inverse of the efficiency of mis-tagging a light- or c -jet as a b -jet.

A comparison of the b -tagging performance on the $t\bar{t}$ sample for different training samples is shown in Figure 4.15 for jets with $p_T > 20$ GeV and $|\eta| < 2.5$, the same selection being applied to all the plots in this section. It is worth mentioning that the simple kinematic differences between the two samples in the training were reduced thanks to a dedicated reweighting procedure which normalizes all of the jet-flavors to the same p_T - η distribution to ensure that the discrimination power is only based on the b -hadron properties and not on the kinematic characteristics of the training sample. An increase of the b -tagging performance when training on the same sample used for evaluation is observed. This was attributed to a difference between the light-jets initiated by gluons or light-quarks. The former has on average a larger number of tracks in the jet which leads to an increase of fake vertices found by the vertex-based algorithms. This information is exploited during the training of the BDT that becomes sensitive to the number of gluon-jets in the training sample.

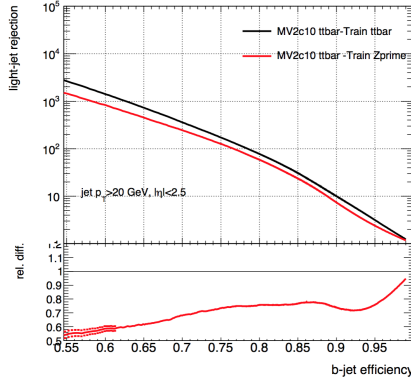


Figure 4.15 – The Light-jet rejection vs b -jet efficiency of the MV2 algorithm trained on the $t\bar{t}$ and Z' samples and evaluated on the $t\bar{t}$ sample.

In view of the previous consideration, it was decided to keep the b -tagging performance invariant at low p_T . To do this, a sample, referred to as *hybrid* sample, was made of $t\bar{t}$ events at low p_T and by Z' events at high p_T . Figure 4.16 shows the correlation plots between the b -hadron and the jet- p_T for both samples. For the $t\bar{t}$ sample, a loss of correlation is visible for high- p_T jets due to the W -boson decay products merging into the b -jets. On the other hand, the correlation on the Z' sample is also ensured for jets with high- p_T values. The *hybrid* sample was obtained by including b -jets from $t\bar{t}$ if the corresponding b -hadron $p_T < 250$ GeV and from Z' sample otherwise. For c - and light-flavour jets, the same mixing strategy is applied by considering the jet- p_T . Figure 4.17 shows the so-called *hybrid* sample used to train all of the multivariate techniques used for flavor tagging in ATLAS.

The b -tagging performance was evaluated on $t\bar{t}$ and Z' events separately. Light-jet rejection as a function of the b -jet efficiency is shown in Figure 4.18 for trainings on *hybrid* and $t\bar{t}$ samples. While the performance on $t\bar{t}$ shows similar results between the two different training configurations, a gain of around a factor of 2.2 at a b -jet efficiency of 77% is observed when training on the *hybrid* sample and evaluating on the Z' sample.

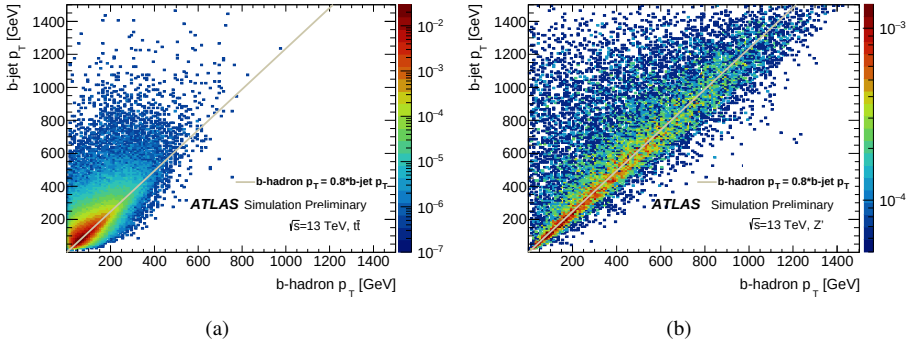


Figure 4.16 – Scatter plot showing the relation between the B -hadron and the jet- p_T for the $t\bar{t}$ (a) and the wide Z' samples (b). The continuous line represents the most probable value of the b quark fragmentation function used in the simulation that controls the relation between the b quark and the b hadron energy [2].

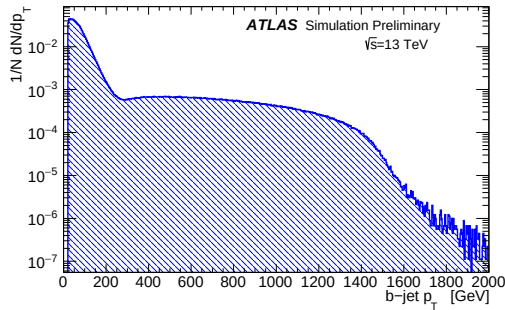


Figure 4.17 – Jet- p_T distribution of the *hybrid* training sample [2].

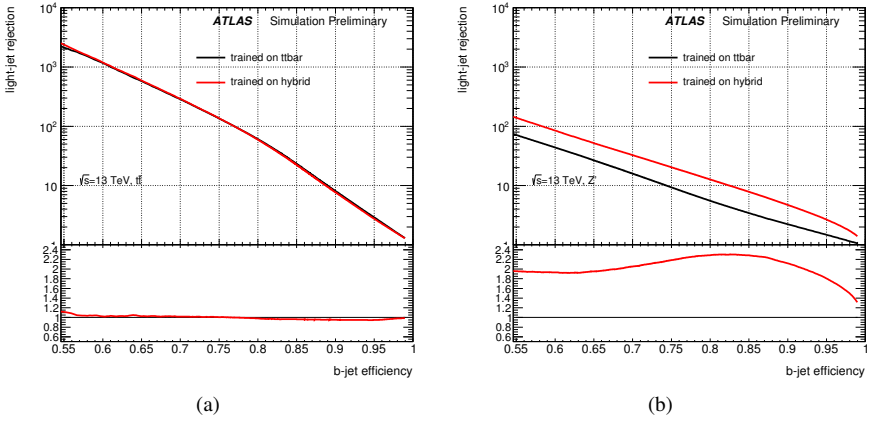


Figure 4.18 – Light-flavour jet rejection as a function of b-jet efficiency using the MV2 b -tagging algorithm when comparing the nominal $t\bar{t}$ training (black line) with a training using the hybrid configuration (red line), evaluated on the $t\bar{t}$ (a) and the Z' (b) samples. The ratio reported on the bottom of the figure is calculated between the $t\bar{t}$ -based training and the *hybrid*-based configuration [2].

4.2.6.2 Performance results

This section focuses on the evaluation of the performance of the MV2 family of high-level taggers. Similar results were obtained for DL1 as described in detail here [67].

The performance of the different MV2 variants, evaluated on the $t\bar{t}$ sample, is shown in Figure 4.19. The performance at low p_T shows an improvements thanks to the SMT discriminant of around 20% in light-jet rejection. The c -jet rejection, instead, shows no gain from the SMT tagger, this is due to the similar topology and BR of c -hadrons and b -hadrons. For RNNIP, no improvements are observed for light-jets indicating that no additional information is brought by the neural network to the one already used by the standard taggers. On the other hand, RNNIP improves the performance of c - vs b -jets discrimination by around 15% at a 77% b -jet efficiency. RNNIP is particularly beneficial in this case as it exploits the correlation between the IPs of the decay products of both b - and c -hadrons. As this information is not fully used in the other low level taggers, an improvements of the performance is observed. The improvement is flat in the jet- p_T range considered as shown in Figure 4.20.

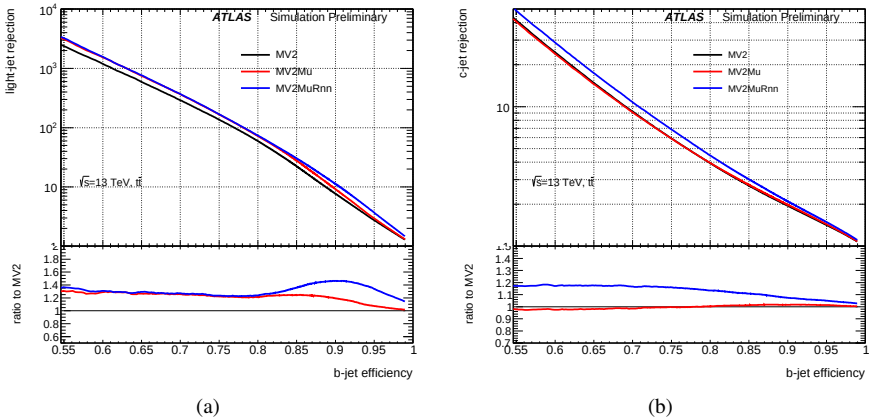


Figure 4.19 – Light-flavour and c -jet rejection as a function of b -jet efficiency for MV2 (black line), MV2Mu (red line), MV2MuRnn (blue line). The algorithm evaluation is performed on $t\bar{t}$ events. The ratio reported on the bottom of the figure is calculated for each MV2 variant (MV2Mu, MV2MuRnn) with respect to MV2 [2].

The high- p_T performance is evaluated on the Z' sample as shown in Figures 4.21. Contrarily to the low jet- p_T case, the RNNIP tagger significantly improves the rejection of light-flavoured jets. The performance as a function of the jet- p_T is shown in Figure 4.22. The 2016 b -tagging configuration is also shown in these plots. A decrease of light-jet rejection is observed in the first jet- p_T bin between the 2016 and 2017 configurations. This is due to a different description of the charge collection mechanism in

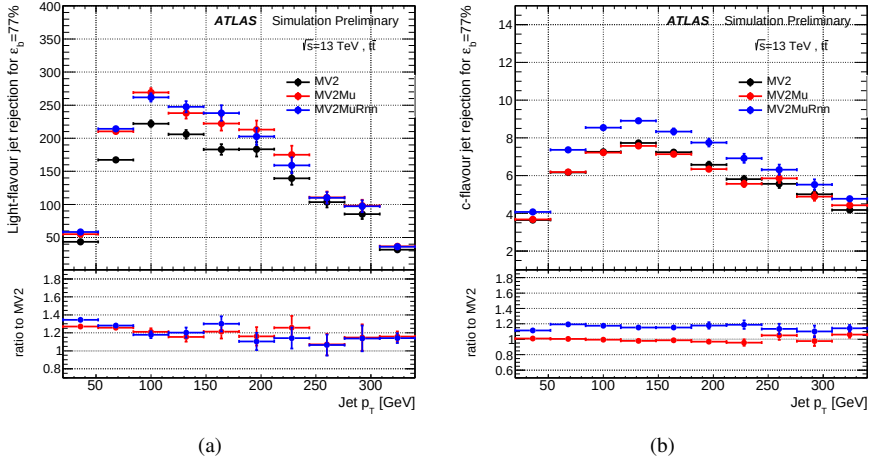


Figure 4.20 – a) Light-flavour and (b) c-jet rejection as a function of the jet transverse momentum for MV2 (black markers), MV2Mu (red markers), MV2MuRnn (blue markers). The algorithm evaluation is performed on $t\bar{t}$ events for a flat b -jet efficiency of 77% for each p_T bin. The ratio reported on the bottom of the figure is calculated for each MV2 variant (MV2Mu, MV2MuRnn) with respect to MV2 [2].

silicon pixels that was implemented in 2017. This new algorithm [68] degraded the b -tagging performance in MC simulations but improved the overall agreement of the simulations with respect to the data, as described in detail elsewhere [2]. At intermediate p_T regime, the SMT algorithm improves the light-jet rejection by 50%, until around 400 GeV, where its performance decreases due to the high collimation of the muon track with the jet-axis becoming comparable with the resolution of the relevant track parameters. The main improvements in the high transverse momentum regime is due to the RNNIP algorithm which is able to tag jets in this more challenging environment, where the track multiplicity in jets increases and the correlation of the tracks parameters plays a crucial role. Figure 4.23 shows the number of tracks in b -jets as a function of the jet- p_T for a $t\bar{t}$ sample. The number of fragmentation tracks increases rapidly; these are tracks originating from the hadronization process of the b -quarks with an impact parameter compatible with the primary vertex. In contrast, tracks from b -hadron decays decreases at high jet- p_T . Such a decrease in reconstruction efficiency is due to two factors: the dense environment and the very displaced vertex, both originating from the high γ factor associated with energetic b -hadrons. Under these conditions, a RNN-based tagger is complementary to the IP2D and IP3D algorithms. In fact, the discrimination power of the latter algorithms is reduced at high jet- p_T due to the large number of fragmentation tracks which enter directly in the definition of the LLR. Since the tracks in the jet are assumed to be uncorrelated in these algorithms, the addition of tracks whose IPs are

compatible with the primary vertex deteriorates significantly their discrimination power. In addition, the vertexing efficiency of the JF and SV1 algorithms decreases at high- p_T while the rate of fake vertices increases degrading their overall performance. The RNN-based tagger, on the other hand, is able to capture the correlation of the tracks in the jet such that, even if the number of fragmentation tracks increases, the properties of the decay products of the b -hadron are still exploited.

In terms of c -jet rejection, as already noted when evaluating on the $t\bar{t}$ sample, RN-NIP improves the discrimination performance across the full p_T range.

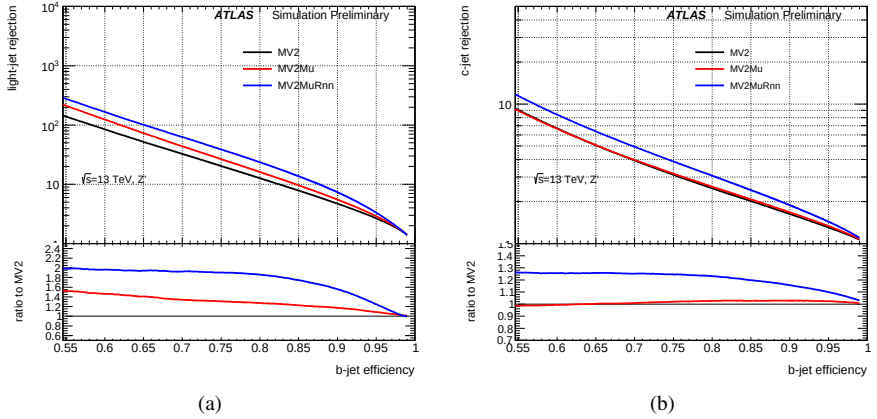


Figure 4.21 – (a) Light-flavour and (b) c -jet rejection as a function of b -jet efficiency for MV2 (black line), MV2Mu (red line), MV2MuRnn (blue line). The algorithm evaluation is performed on Z' events. The ratio reported on the bottom of the figure is calculated for each MV2 variant (MV2Mu, MV2MuRnn) with respect to MV2.

In summary, the identification of heavy-flavor jets was improved at high transverse momentum by a factor of 3 in terms of light-jet rejection and by 50% for the rejection of c -jets at a b -jet efficiency of 77%.

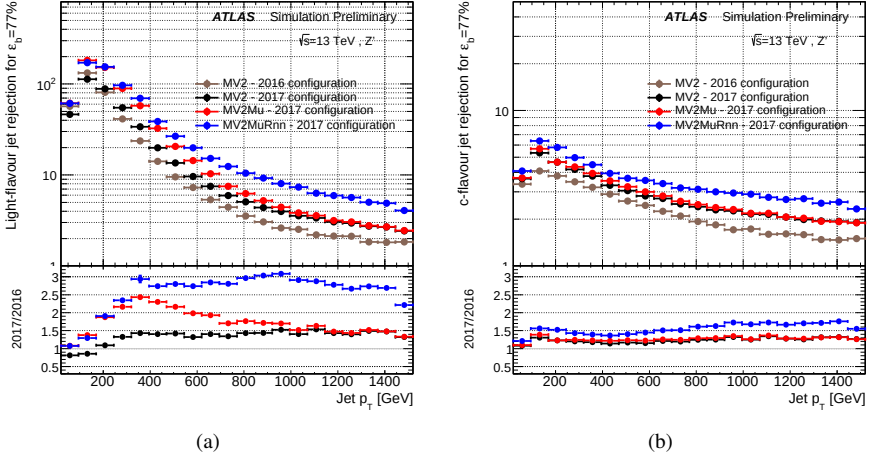


Figure 4.22 – (a) Light-flavour and (b) c -jet rejection as a function of the jet- p_T for MV2 in the 2016 configuration (brown markers), MV2 (black markers) in the 2017 configuration, MV2Mu (red markers) and MV2MuRnn (blue markers). The algorithm evaluation is performed on Z' events for a flat b -jet efficiency of 77% for each p_T bin. The ratio is calculated with respect to the 2016 configuration [2].

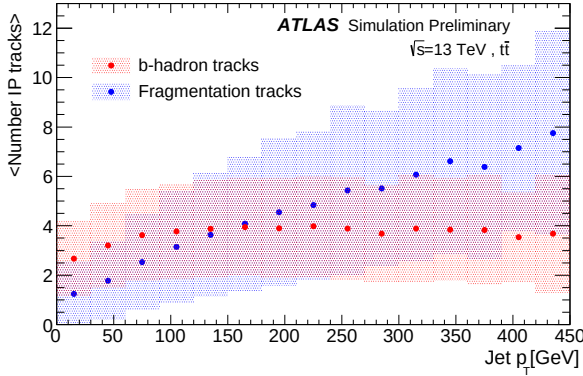


Figure 4.23 – Average number of b -hadron and jet fragmentation tracks selected for the IP algorithm as a function of the jet- p_T . The shaded band around the two contributions represents the RMS of the distribution in each bin, not the statistical uncertainty [1].

4.2.6.3 A deep neural network as high level tagger

As already mentioned, in addition to a BDT-based discriminant, a new, high-level tagger based on a Deep Neural Network (DL1) was implemented. It is expected that for a large number of input variables a NN would outperform a BDT. However, a comparisons between the two high-level taggers showed similar performance with poor complementarity between the two multivariate approaches, i.e. the two algorithms tag approximately the same jets for all the different variants of the taggers.

DL1 provides a set of three different outputs, in contrast to the single score provided by a BDT, defined as the probability of a jet to be tagged as a b -, c - or light-jet. These probabilities are then combined into a single discriminant:

$$D_{DL1} = \ln \frac{p_b}{f_c p_c + (1 - f_c) p_{light}} \quad (4.4)$$

Similar to the case of RNNIP, f_c is a constant parameter which define the relative importance to enhance the rejection of c - or light-jets.

Despite the similarity in terms of b -tagging performance, the DL1 algorithm presents some advantages compared to MV2:

- c -tagging: Similar to the case of b -tagging, analyses featuring c -quarks in the final state rely on c -jet identification algorithms. Thanks to the multi-dimensional output of DL1, a single training can be used to define a discriminant for b or c tagging by simply replacing $p_b \leftrightarrow p_c$ in equation 4.4. BDT-based discriminants need a specific training to optimize the c -tagging performance thus doubling the work load.
- The curve describing the b -jet efficiency as a function of the jet- p_T was found to be smoother in DL1 algorithm with respect to MV2. This feature is particularly useful for analyses looking for heavy resonances decaying into b -quarks as it facilitates the estimation of the QCD background. This is further discussed in the next chapter.
- Additional R&D: The multi-dimensional outputs allow one to extend the usage of the network to different physics processes. DL1 could potentially cover many topologies with a single training allowing to define a posteriori different tagging strategies based on a unique training process which is inclusive enough to contain of all the topologies of interest. One example is b -tagging in a very boosted environment where two b -hadrons can eventually merge into a single jet. Such a topology could correspond to one additional output of the network, p_{bb} , that can be set to zero a posteriori for any analysis which does not feature boosted objects. Similarly, the probability of a light-flavor jet can be further divided into probability of light quarks, namely, u -, d - and s -quarks, and the probability of gluons, p_g .

Depending on the composition of gluon-jets in a given physics analysis of interest, these probabilities may be tuned a posteriori to optimize the sensitivity of the analysis. In addition, the DL1 machinery makes it possible to further incorporate developments coming from the machine-learning community.

4.3 Calibration of the b -tagging algorithms

Mis-modelling of the variables used for the identification of heavy quarks in MC simulations would be reflected as different tagging rates for data and MC. To correct for these effects, the performance in simulation is matched to the data by means of dedicated calibration analyses. The operating Working Points (WP) provided to physics analysis are defined with a cut, constant as a function of the jet- p_T , corresponding to 60%, 70%, 77% or 80% b -jet tagging efficiency. These sets of cuts are derived using a $t\bar{t}$ sample. The corresponding b -efficiency profile is shown in Figure 4.24 for the DL1 tagger, similar profiles were produced for all set of high-level taggers described in the previous Section.

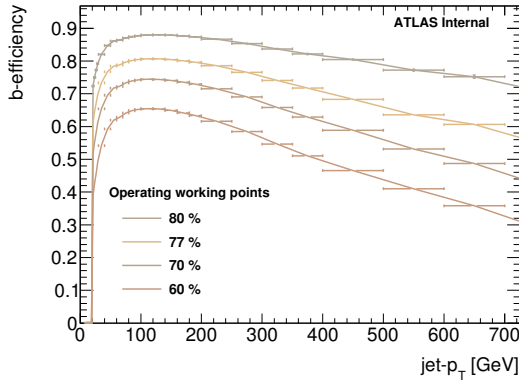


Figure 4.24 – Efficiency profile corresponding to the working point described in the text for the DL1 algorithm. The evaluation was performed on a $t\bar{t}$ sample.

Scale factors are then defined, for each of the WP, as the ratio of efficiency in data and MC:

$$SF_{b,c,light} = \frac{\epsilon_{\text{DATA}_{b,c,light}}}{\epsilon_{\text{MC}_{b,c,light}}} \quad (4.5)$$

Each jet-flavour needs to be calibrated using an independent analysis which optimizes the purity of the flavor of interest in data. The main sample used to calibrate the

b -jet efficiency and c -jet mis-tagging rate is a $t\bar{t}$ sample, either in a single-lepton or di-lepton topology. The $t\bar{t}$ sample provides a pure selection of b -jets given that $V_{tb} \sim 1$. c -jets are calibrated using the hadronic decay of the W bosons in single-lepton $t\bar{t}$ events. However, as already described, a $t\bar{t}$ sample is limited in terms of its maximum transverse momentum and a dedicated extrapolation based on MC simulation is needed. The isolation of a pure sample of light-jets, instead, is challenging due to the high rate of light-jet rejection achieved by the algorithm. This means that after tagging, the number of remaining light-jets is comparable to the one of heavy-favored jets which makes a direct calibration of light-jets inaccurate. This problem is overcome by making an assumption on the origin of the light mistag rate. It is assumed that most of the mis-tagged jets originate from resolution effects of the detector. Under these assumptions, an algorithm emulating the distribution of light-jets is constructed by flipping the transverse impact parameter $d_0 \rightarrow -d_0$ of the tracks in jets and the b -tagging performance is re-evaluated. More details about this and other calibration methods can be found elsewhere [62]. A summary of the calibration analyses used for the Run2 b -tagging configuration is shown in Table 4.3.

Table 4.3 – Brief summary of the calibration analyses.

jet-flavour	sample	Summary
b -jets	$t\bar{t}$	Two calibration analyses are performed: one based on di-leptonic $t\bar{t}$ events and the other using single-lepton $t\bar{t}$ events.
c -jets	$t\bar{t}$	The analysis relies on single-lepton $t\bar{t}$ events profiting from the $W \rightarrow cs$ decay while the leptonic signature in the opposite hemisphere is used for triggering.
light-jets	di-jets & Z+jets	Both analyses are based on the assumption that the main source of mis-tag rate is due to resolution effect of the detector. A control sample which mimics light-jets is obtained as described in the text.

When the statistics is limited at high- p_T , a MC-based extrapolation is used to infer the uncertainty on the SF. The central value of the SF is assumed equal to the latest calibrated jet- p_T bin. This additional uncertainty is based on underlying quantities that

are known to affect the b -tagging performance. Namely, the reconstruction of tracks and jets, the modeling of the b -hadrons and the interaction of long-lived b -hadrons with the detector material. Each uncertainty source is varied independently in the simulation and the b -jet tagging efficiency is recomputed. The difference with respect to the b -jet tagging efficiency obtained in the nominal case is then taken as an additional systematic uncertainty. The related uncertainty on the SF are scaled proportionally to their respective values in the highest- p_T bin of the data measurement and added in quadrature to the pre-existing data-based uncertainty, more details are available in [to be published shortly]. Figure 4.25 shows the b -jets SF for DL1 at an operating point of 70% b -jet efficiency.

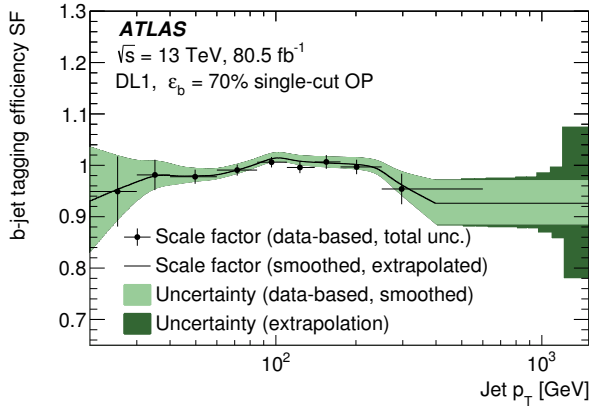


Figure 4.25 – The scale factor uncertainties as a function of the jet- p_T . The two uncertainty components described in the text are shown for DL1 algorithm. The simulation-to-data scale factors are smoothed in jet- p_T using a local polynomial kernel estimator. The bin centers are used for the smoothing whereas the dots are located at the mean of the b -jet p_T distribution in each p_T bin [69].

In the 2016 b -tagging configuration, the extrapolation uncertainty was computed using $t\bar{t}$ MC events. In the high energy regime, the available statistics of the $t\bar{t}$ MC was the dominant source of uncertainty. In the Run2 configuration, the Z' sample was used, where its wide p_T spectrum sufficiently covers the high-energy regime, and the uncertainty was reduced compared to the previous b -tagging configuration. These improvements are further outlined in the next Chapter.

CHAPTER 5

Search of new physics with very energetic b -jets

In this chapter, the improved performance of the b -tagging algorithms is evaluated in the context of an analysis looking for heavy resonance decaying into one or two b -quarks. The analysis probes the highest kinematic regime provided by the LHC center-of-mass energy of 13 TeV. It is thus a natural analysis candidate to study the impact of the improvements of high- p_T b -tagging.

The chapter also includes a discussion on a novel tagging algorithm, investigated for the first time by the ATLAS experiment, for further improving the identification of heavy-flavor jets in the highest transverse momentum regime. This algorithm exploits the boosted topology of the b -hadron to build discriminating variables based on the *hits* in the tracking detector rather than the reconstructed track parameters. For this reason it is named *trackless* b -tagging.

The chapter is organized as follows. In the first section the analysis is presented along with the analysis improvements related to the upgraded b -tagging performance. The second chapter is devoted to studying the novel approach to b -tagging at extreme energies.

5.1 Search for high mass resonances decaying into a pair of b -quarks

Searches for high mass resonant signals over a steeply falling QCD background have been performed since the beginning of hadron collider experiments. In particular, ATLAS and CMS have been looking at new resonances decaying into quarks since the beginning of the LHC collisions [70–73]. In this section, results of a search for resonant signals decaying into b -quarks are presented using the full data-set collected by the ATLAS experiment in Run2, which corresponds to 139 fb^{-1} . The analysis largely relies on the ability to b -tag jets with the highest transverse momentum achievable at a center-of-mass energy of 13 TeV. Figure 5.1 shows an event display of the event with highest invariant mass events with two b -tagged jets recorded in 2015.

A variety of BSM models predict high mass resonances with preferred couplings to b -quarks. Examples include an excited bottom quark $b^* \rightarrow bg$ postulated by compositeness models and a fourth generation of vector boson $Z' \rightarrow b\bar{b}$ decaying into b -quark pairs. These examples are considered as benchmark for this analysis. Feynmann diagrams for these models are shown in Figure 5.2. To accomodate both final states, b -tagging is applied to the leading and sub-leading jets in the event and the analysis is divided into a single b -tagged region and a double b -tagged region.

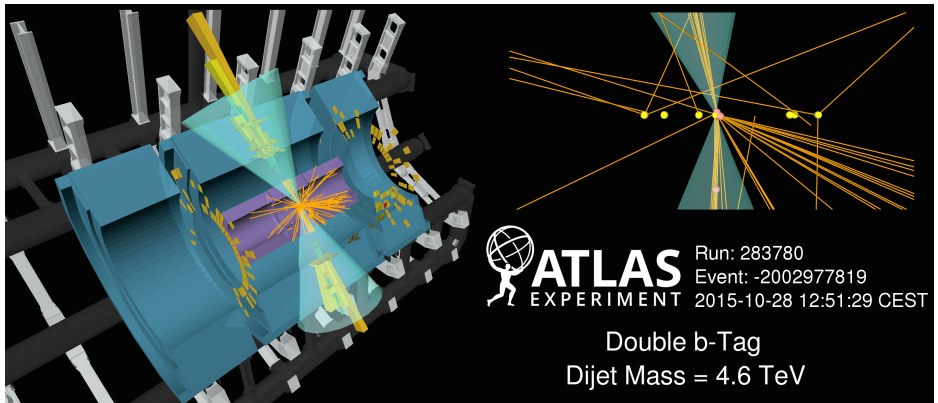


Figure 5.1 – The highest mass di-jet event collected in 2015 passing the event selection and entering in the 2 b -tag category. The two central high- p_T jets have a transverse momentum of around 2 TeV. The upper right panel shows a magnified view of reconstructed inner detector tracks with primary vertex candidates, shown as yellow points, and reconstructed secondary vertices, shown as red points [72].

¹Some of the figures in this section, mostly related with MC samples, indicate 140 fb^{-1} instead of 139 fb^{-1} .

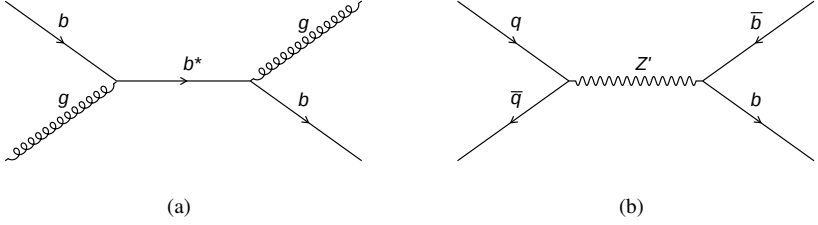


Figure 5.2 – Feynmann diagram for the (a) b^* model and the (b) Z' model [72].

In the following, the benchmark models used in the analysis are further discussed.

5.1.1 Simulated signal models

b^* models

Excited quarks are a typical signature of composite quark models. In these models quarks are not elementary particles, but are in fact a bound state of constituent particles similarly to the hadrons in the SM. This family of models could help to explain the mass hierarchy of quarks. The simulated events corresponding to this model are generated with the PYTHIA8 event generator [74], using the A14 tune [75] and NNPDF2.3 PDF set [76]. Figure 5.3 shows the invariant mass distribution for several values of the b^* signal mass.

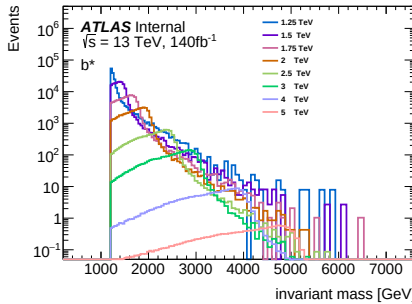


Figure 5.3 – Invariant mass distribution for the b^* model.

Heavy Z' bosons

Heavy spin 1 bosons are predicted in many theories with additional gauge groups such as Grand Unified Theories (GUT). The particular case considered for this thesis is a Z'

bosons from the Sequential Standard Model [77], in which the new bosons are heavier versions of the Standard Model bosons with the same couplings. The simulated events corresponding to this model were generated using PYTHIA8 with the A14 tune and NNPDF2.3 PDF set. Figure 5.4 shows the invariant mass distribution for several nominal mass values.

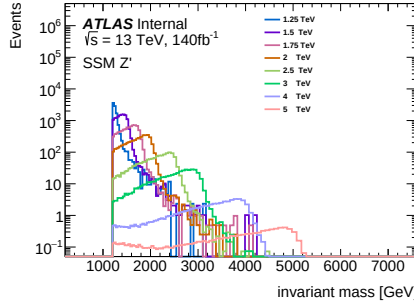


Figure 5.4 – Invariant mass for the SSM Z' model.

Dark Matter mediators

This analysis is also sensitive to DM mediator refereed to as Z' . In the models used in this analysis the Z' decay to invisible particles is kinematically suppressed. As already discussed in section 1.3.0.1, the Z' mediates interactions between the SM and DM particles. The mass of these particles, m_χ , is set to 10 TeV such that the decay of the Z' into SM particles is favored. Figure 5.5 shows the Feynman diagrams for the production of the mediator and its subsequent decay to DM or SM particles. The Z' is assumed to be leptophobic and with spin 1 to facilitate comparisons with other di-jets searches using the same model. The Z' simulated events are generated using MadGraph [51] and showered with PYTHIA8 with several values of the coupling to the SM particles, g_{SM} , ranging from 0.05 to 0.25 in steps of 0.05. To increase the statistics of the samples, only Z' decays to pairs of b -quarks are simulated. Figure 5.6 shows the invariant mass distribution for several mass values at the largest coupling of 0.25.

Graviton

According to the Randall-Sundrum (RS) model [78–80], the gravitational force is diluted into higher space-like dimensions. It is one of many new physics models which can solve the large hierarchy problem of the weak and the Planck scale. The model considered in this analysis is a Kaluza-Klein spin-2 Graviton that can interact with the SM fields via the graviton sector of the RS model. The KK graviton signal templates are generated for different mass values with the PYTHIA8 event generator, using the A14

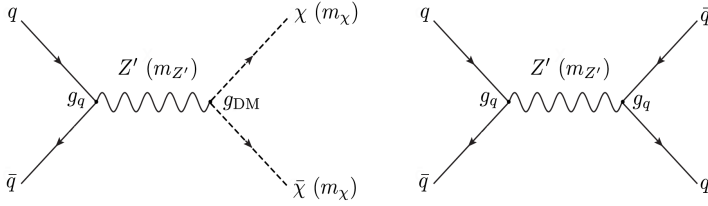


Figure 5.5 – Feynman diagrams showing the production of a Z' DM mediator decaying into invisible (left) DM particles and into (right) SM particle. The latter configuration is the focus of this analysis.

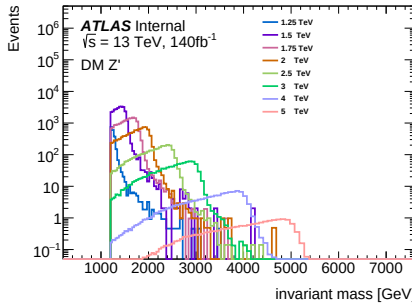


Figure 5.6 – Invariant mass for the DM Z' at the largest coupling of 0.25.

tune and NNPDF2.3 PDF set. Figure 5.7 shows the Graviton invariant mass distribution for the considered mass points.

5.1.2 Event Selection

The possible resonant signals of the di-jet search would appear as a narrow resonance peak in the invariant mass of the di-jet system formed from the two highest- p_T jets in the event. The main source of background in the analysis is the two-to-two scattering of QCD processes. The search exploits two key properties of the background to enhance its sensitivity to new physics signals:

- The background at high m_{jj} is a smooth and continuously falling spectrum, contrarily to the expected narrow resonance of the signal models considered.
- The background at high mass peaks in the forward direction due to the fact that QCD multi-jets are mainly produced through t - and u -channels, while signals are produced via s -channel, which peaks in the central region.

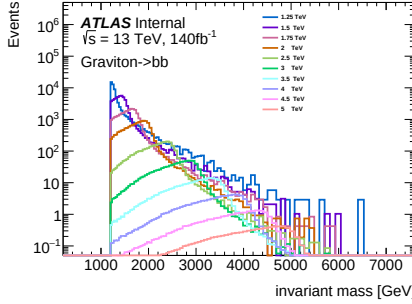


Figure 5.7 – Invariant mass for the $G \rightarrow b\bar{b}$ samples.

The latter property is exploited in the analysis by using the pseudo-rapidity difference of the two leading jets in the events as a discriminating variable, defined as:

$$y^* = (y_1 - y_2)/2$$

Where $y_{1,2}$ are the rapidity of the leading and sub-leading jet respectively. A $y^* < 0.8$ cut was used where the value was chosen to reject t -channel QCD while preserving the potential signals.

The lowest usable transverse momentum of the leading jet in the analysis is dictated by the trigger. The trigger selects events requiring at least one reconstructed jet with a $p_T > 420$ GeV (HLT-j420). During the years of Run2, the p_T cut of the trigger was changed from 360 GeV in 2015 to 420 GeV in 2018. To keep a consistent p_T cut across the different years, the cut dictated by the tighter trigger, corresponding to 420 GeV, was chosen. This decision was also driven by the fact that at the lowest mass points, other di-jet analyses [73] already exclude with lower cross-section values the same benchmark models. The ratio panel of Figure 5.8 shows the trigger turn-on using a subset of 2018 data of 5 fb^{-1} as a function of the invariant mass formed by the two leading jets.

In addition to the cuts on y^* and jet- p_T , b -tagging is applied to the leading and sub-leading jets. A single b -tag region is defined in cases where at least one of the two leading jets is b -tagged. Similarly, the double b -tag region is defined in cases where both jets are b -tagged.

As mentioned already in section 4.3, a dedicated calibrations which correct differences in the b -tagging performance between data and Monte-Carlo must be derived for and used in physics analyses. The SMT algorithm, in particular, poses additional challenges to the derivation of the calibration. Since the SMT algorithm does not have significant contribution at high p_T , it was decided to define a new version of the tagger without the inclusion of SMT but including the RNNIP algorithm which brings the largest improvements at high p_T , referred to as DL1r or MV2r. Effectively, the gain of

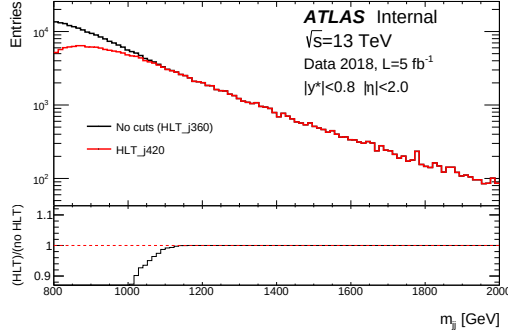


Figure 5.8 – Trigger turn-on as a function of the invariant mass using the HLT-j420 trigger described in the text and the HLT-j360 trigger used as reference to define the turn-on.

the performance at high transverse momentum, where SMT improvements are negligible, is still present as shown in Figure 5.9. The DL1 family of tagger was used in the analysis due to the smooth distribution of the efficiency curves which facilitate the QCD background estimation. A cut corresponding to 77 % b -tagging efficiency was used in the analysis. The corresponding event tagging efficiency for different analysis regions and related benchmark models is shown in Figure 5.10.

5.1.3 Background estimation

It is known from first principles that QCD processes result in a steeply falling m_{jj} spectrum. Because of this, functional forms can be used to describe the invariant mass spectrum arising from QCD events. One of the largest limitations of this approach is related to the statistics used for fitting. The higher the statistics, the more difficult it is to find a function that correctly accomodates the data points. One solution, which was already adopted by other similar searches, is to reduce the range of m_{jj} which is actually used for fitting. This way, a fit is performed on different windows and smooth boundary conditions ensure a continuously falling spectrum. Figures 5.11 shows the basic concept of this method, also called the sliding window fit or simply SWift. In general, the largest window size which ensure a good fit quality is chosen to maximize the statistical power of the fit and to avoid overfitting of signal templates which can occur especially for signals featuring large widths. The optimal number of bins used to slice the full range was found to be 46 as shown in Figure 5.12.

The functional form used to describe the QCD background in each window is given by:

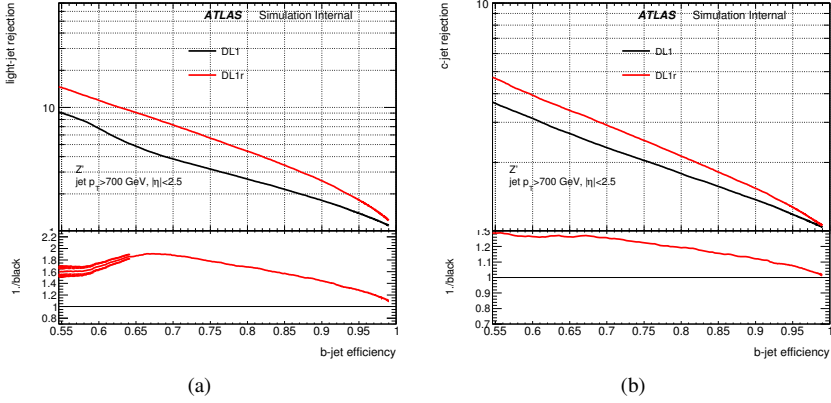


Figure 5.9 – (a) light-jet rejection and (b) c -jet rejection as a function of the b -jet efficiency. The evaluation is performed on a Z' sample designed to populate a large range of jet- p_T (see Section 4.2.6.1). Jets are required to have a $p_T > 700$ GeV which correspond roughly to a decay of a resonant particle with a mass of 1.4 TeV.

$$f(x) = p_1(1-x)^{p_2}x^{p_3+p_4 \ln x}, \quad (5.1)$$

where $x = m_{jj}/\sqrt{s}$. The same parametric form was used in several other di-jets analyses [70–73]. The number of parameters needed to describe the background were chosen based on Wilks’ test. The results of this test showed that the functional form with three parameters ($p_4 = 0$) describes poorly the data in both single and double tag analysis categories.

In order to validate the background estimation a dedicated invariant mass spectrum which is independent of and serves as a proxy of the invariant mass spectrum in signal region is needed. Usually, this is done using Monte-Carlo simulations. However, it was found that the statistics of the QCD sample after applying b -tagging is not sufficient to perform any meaningful fitting studies. To cope with this, ABCD control regions using data were defined for the single and double b -tag categories. The regions were defined by inverting the b -tagging and y^* requirements:

- Region A: Two jets with $|y^*| > 0.8$, two($\geq$ one) of them are b -tagged
- Region B: Two jets with $|y^*| < 0.8$, two($\geq$ one) of them are b -tagged (Signal region)
- Region C: Two jets with $|y^*| > 0.8$
- Region D: Two jets with $|y^*| < 0.8$

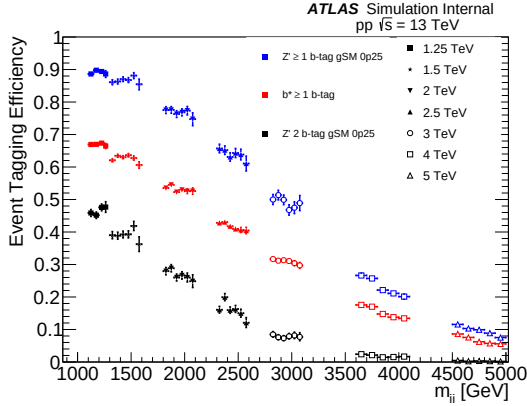


Figure 5.10 – The per-event b -tagging efficiencies after the event selection of the analyses as a function of the reconstructed invariant mass for simulated samples with six different b^* and Z' resonance masses.

It was shown the correlation between these two variables is small and that the contamination from signal hypotheses is negligible in regions A, C and D. In order to define a region that can be used as a proxy for the signal region, efficiencies maps were derived from regions A and C for both the 1- and 2-tags categories:

$$\epsilon_{\geq 1b} = \epsilon_{j1} + \epsilon_{j2} - \epsilon_{j1}\epsilon_{j2\text{conditional}}$$

$$\epsilon_{2b} = \epsilon_{j1}\epsilon_{j2\text{conditional}}$$

where $\epsilon_{\geq 1b}$ and ϵ_{2b} is the efficiency of the events in the one and two tag categories, respectively. ϵ_{j1} is the efficiency of the leading jet in the event and $\epsilon_{j2\text{conditional}}$ is the efficiency of the second leading jet in the event given that the leading one was already tagged. Since the performance of the b -tagging algorithms depend on the kinematic variables of the jet, the efficiencies were binned in p_T and η . These efficiencies are then used to define the control regions, referred to as ABCD regions in the following, which are used as a proxy of the signal region in the single and double b -tag categories:

$$N_{ABCD} = N_D \epsilon$$

To validate the method a sub-set of the already published data, corresponding to 7 fb^{-1} , was used. Figure 5.13 shows the comparison between the ABCD regions and the data. Only the shape is compared as the normalization is taken directly from the signal region. Good shape agreement between the two regions is achieved. It is worth stressing the fact that these regions are only used for validation of the fit and are not meant to provide an actual background estimate.

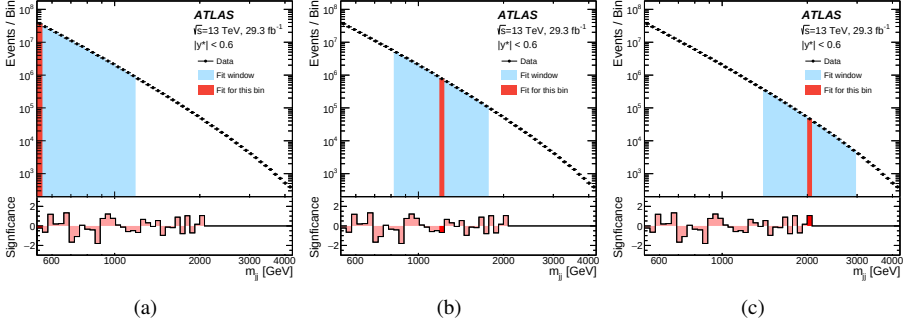


Figure 5.11 – A depiction of the SwiFit windows (shaded blue) used for the background estimate of the bins shaded in red. The data-points represents a previous iteration of one di-jet analysis which is used as an example of the procedure. Figures adopted from [73].

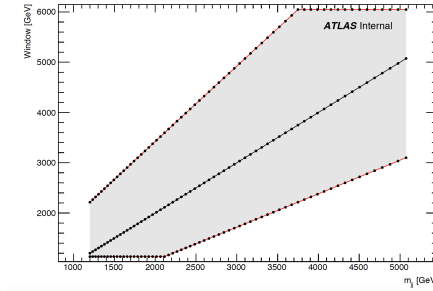


Figure 5.12 – Window sizes across the invariant mass range.

5.1.3.1 Signal Injection and Spurious signal tests

To ensure that the fitting strategy based on the SWIFT approach is sensitive to all possible signal types, signal injection tests were performed where the performance of the sliding window fit at recovering injected signal events is quantified. Signal templates were injected on the ABCD regions at various mass points, the number of recovered signal events and its related uncertainty give an estimate of the fitting performance. Results are shown in Table 5.1 and Table 5.2 for the single tag and double tag categories. The numbers quoted in the tables are an average value taken over 10 pseudo-experiments for each mass point, while the uncertainty represents an average of the statistical uncertainty from the SwiFit fits.

For low and intermediate masses of the benchmark signals, no significant bias is observed. For high mass values instead, further investigation is needed. A larger number of pseudo-experiments of ~ 500 were performed and the results were estimated by using

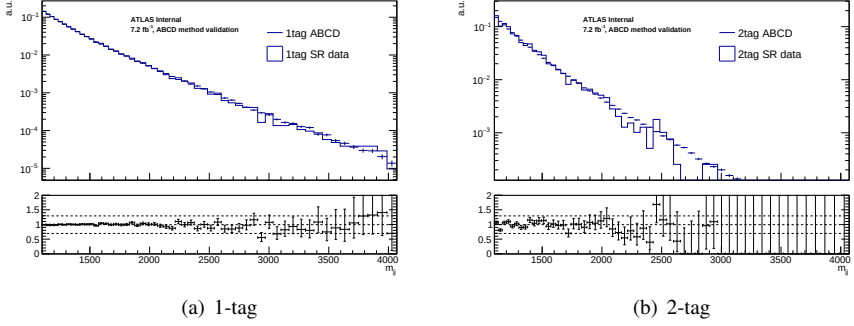


Figure 5.13 – Validation of the ABCD method using a subset with 7 fb^{-1} of the already published data. The invariant mass spectrum is shown for the (left) one and (right) two tag categories.

Signal Mass (TeV)	Injected Events	injected/recovered $\pm$ stat. unc.
1 TeV	115067	0.98 ± 0.05
1.75 TeV	57571	1.02 ± 0.07
2 TeV	26024	1.02 ± 0.10
2.5 TeV	5006	1.3 ± 0.3
3 TeV	1001	1.4 ± 0.6
4 TeV	43	-1.01 ± 4.9

Table 5.1 – Injected vs. recovered numbers of events in signal injection tests for the b^* model.

Signal Mass (TeV)	Injected Events	injected/recovered $\pm$ stat. unc.
1.5 TeV	5039	1.16 ± 0.17
1.75 TeV	2788	1.1 ± 0.2
2 TeV	1329	1.03 ± 0.28
2.5 TeV	289	0.95 ± 0.71
3 TeV	62	0.2 ± 1.2

Table 5.2 – Injected vs. recovered numbers of events in signal injection tests for the SSM Z' model.

the pull distributions as a figure-of-merit. The pull is defined as:

$$\text{pull} = \frac{\mu_{\text{fit}} - \mu_{\text{injected}}}{\sigma_{\mu_{\text{fit}}}}. \quad (5.2)$$

The pulls for each pseudo-experiment are then histogrammed and a Normal distribution

is fit to the histogram. If the fit is unbiased, then one should expect the pulls to be Normally distributed with a mean of 0 and width of 1,

$$\text{pulls} \sim \mathcal{N}(\mu = 0, \sigma = 1).$$

The deviation of the Normal distribution fit's mean from 0 is then an indicator of the bias in the extraction of signal given the choice of QCD model. Similarly, a deviation from a width of 1 indicates a bias in the estimation of the uncertainty of the fit due to the QCD model parametrization. As an example, the pull distribution is shown in Figure 5.14 for a b^* at 4 TeV when signal is injected. Figure 5.15 shows the results of signal injection tests for one tag and two tag categories for different models and mass hypotheses. The measured means and widths of the fitted gaussian distributions are shown for different mass points. No significant bias is observed.

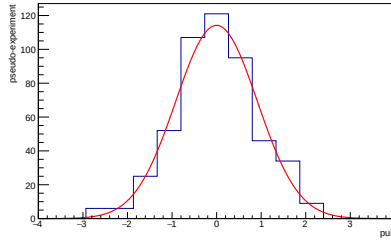


Figure 5.14 – Pull distributions for a b^* at 4 TeV. Signal was injected in the mass spectrum of the pseudo-experiments used to extract this distribution.

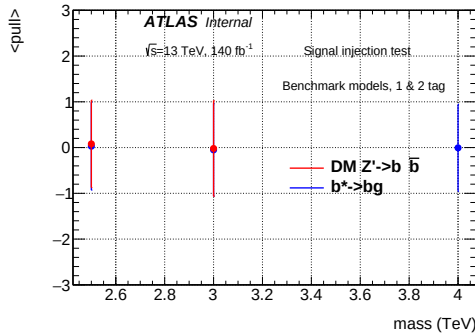


Figure 5.15 – Signal injection tests for one tag and two b -tag categories for different models and mass hypotheses.

The second test performed to assess the robustness of the functional form used to estimate the QCD background is the spurious signal test. This test quantifies whether

the choice of the function used to describe the QCD multi-jet background is sensitive to statistical fluctuations faking a possible signal. The same procedure used to study the fit performance in the presence of signal events is also used for the spurious signal test. The only difference between the two tests is that, in case of the spurious test, no signal is actually injected into the ABCD regions. Results are presented in Figure 5.16 for different signal mass hypotheses. Again, no bias is observed, providing confidence about the robustness of the QCD background estimate.

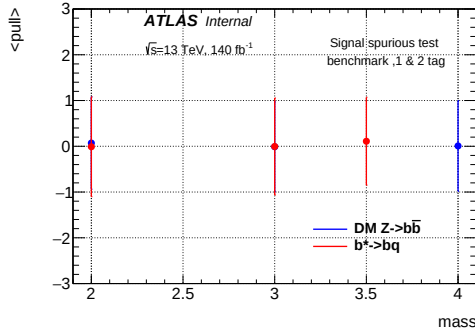


Figure 5.16 – Spurious signal tests for one tag and two b -tag categories for different models and mass hypotheses.

5.1.4 Systematic uncertainties

Systematic uncertainty are divided into uncertainty related with the QCD multi-jet estimation, these are the statistical uncertainty of the fit and the choice of the functional form used to describe the data. The second set of uncertainties deal with experimental calibrations and affects the signal templates. In general, these uncertainties modify both the normalization and the shape of signal templates. The only exception is the uncertainty on the luminosity which by definition only affects the normalization of signal models.

Uncertainties on fit function choice

The choice of the functional form used to describe the data is arbitrary. A systematic uncertainty is implemented considering the use of a different functional form to fit the data. The alternate fitting function considered in the analysis was defined as:

$$f(x) = p_1(1 - x)^{p_2 + p_3 x} x^{p_4 + p_4 \ln x} \quad (5.3)$$

The nominal and alternate background are compared and the difference between the two is used to derive the uncertainty. A collection of pseudo-data are produced from

the nominal background result, and from each pseudo-experiment both nominal and alternate backgrounds are derived. The mean of the difference between the nominal and alternate background is recorded in each bin and it is used to define the size of the uncertainty on the function choice. The resulting uncertainty is shown in Figure 5.17 for both categories, one-tag and two-tags.

Uncertainties on the fitting function parameters

The second uncertainty associated with the background estimate is the quality of the fit itself. Under ideal circumstances this would be derived as a confidence band on the function determined by the covariance matrix of the fitted parameters. However, in cases where the parameters of the function are strongly correlated, or whenever the likelihood function has a badly-behaved maximum, minimization algorithms such as Migrad or Hesse are not reliable.

Since the confidence interval on a function is meant to represent the 1σ region within which the fit would fall in the large-number limit of repeated trials, it can also be found by generating pseudo-experiments and fitting each of them. This method does not require an accurate estimation of the parameter errors; instead, the pseudo-experiments are generated using Poisson statistics based on the nominal background model after a fit to data. A large number of these pseudo-data sets (~ 10000) are generated, each is fit using the same starting conditions as the observed data, and the error on the fit in each bin is defined to be the RMS of the function value in that bin considering all of the pseudo-experiments. This method has been used since the early versions of the di-jet analyses. The resulting uncertainty is also shown in Figure 5.17.

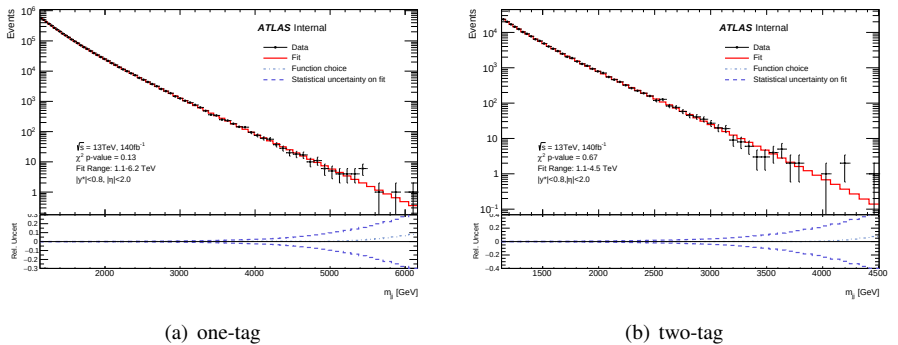


Figure 5.17 – The two fit function errors are shown along with the nominal fit (SWiFit 4-parameter) for the untagged resonant selection. The Dark blue lines are the statistical uncertainty on the fit for the (a) one tag and two (b) tag categories.

Luminosity Uncertainty

A luminosity uncertainty is applied as a scale factor to the normalization of the signal samples. The uncertainty in the combined 2015-2018 integrated luminosity is 1.7%. It is derived from the calibration of the luminosity scale using x - y beam-separation scans, following a methodology similar to that detailed in Ref. [81], and using the LUCID-2 detector for the baseline luminosity measurements [82].

Jet Energy Scale and Resolution Uncertainties

The Jet Energy Scale (JES) uncertainty is applied to the signal templates for all models. The JES uncertainty corrects for mis-modeling of the energy assigned to the jet in MC simulation compared to real collision data. A very large variety of sources contribute to this uncertainty; all of the sources are parametrized to form set of nuisance parameters which have the advantage of being orthogonal by construction. More details can be found elsewhere [83]. This analysis used the strongly reduced set of 7 nuisance parameters.

The Jet Energy Resolution (JER) uncertainty is linked with the finite experimental resolution of the calorimetric system. This uncertainty was found to be negligible in this analysis and it is therefore neglected.

Flavour tagging uncertainty

The jet- p_T range considered for this analysis is well above the typical range used to derive flavour-tagging calibrations, which usually extends up to a jet- p_T of ~ 500 GeV. To cope with this, the calibration is extrapolated from its end-point up to large p_T (see Section 4.3 for more detail).

The b -tagging uncertainties are then parametrized using a separate set of nuisance parameters. In total 9 independent NPs are used. Among them, the dominant source is expected to be due to the extrapolation uncertainty as already mentioned.

PDF and Scale Uncertainties

This uncertainty is evaluated comparing different sets of PDFs. There are in general two effects related to this uncertainty: changes in the theoretical values of the cross section of the given model of interest and changes in the acceptance of the analysis. Due to the large uncertainty of the PDFs at high x values, the change in shape of the invariant masses obtained from reweighting a signal from one set of PDFs to another was found to be significantly altered. This large difference can lead to unphysical results and it was decided not to include this as an uncertainty. In addition to this, when setting exclusion limits on new physics models, it is questionable whether there is the need to add an additional nuisance parameter in the fit which is related with a theoretical uncertainty on the cross-section of a model that is not yet observed. The prescription used by ATLAS analyses excluding new physics models is to only account for the change in the

acceptance. This component of the uncertainty was estimated to be a 1% flat systematic across different invariant masses.

5.1.5 Statistical interpretation

The statistical interpretation of the results is divided into two steps: the search-phase and the limit-setting phase. In the first, a background-only model is used to fit the data to assess the level of compatibility of the background-only interpretation with the data points. In case of good compatibility in the first step, the second step quantifies the amount of signal that can be excluded for a given benchmark model of interest.

The search phase

The first test needed to probe the level of significance of an excess is the level of compatibility of the background-only model with the data. In this analysis, this means running a background-only fit using the functional form defined in eq. 5.3, without the inclusion of any signal template into the fit. The BumpHunter (BH) [84] algorithm is used to take into account the fact that a random fluctuation occurring anywhere in the invariant mass spectrum could lead to a disagreement with the background estimation which might potentially be mis-interpreted as a sign of new physics. This is the "Look-elsewhere effect" (LEE) [85]. The BH algorithm takes the LEE effect properly into account by defining a test-statistic which is sensitive to fluctuations in any of the m_{jj} bins; more details can be found elsewhere [84]. The BH p -value is used as a figure of merit to assess the compatibility of the background-only hypothesis with the data. If a p -value larger than 0.01 is found, the fit is accepted and the spectrum is considered to be depleted of signal events. If this is the case, the limits setting stage addresses the question of how much signal can be excluded for a given model under consideration. If the BH p -value is instead lower than 0.01, the window of maximal discrepancy is excluded from the fit, a second fit is performed with that mass region excluded and the significance of the excess is re-computed. As an example, the background-only fit on the ABCD spectra for the 1- and 2-tag categories is shown in Figure 5.18. The BH p -value is found to be 0.49 and 0.91 for the 1- and 2-tag categories. Both values are larger than 0.01, thus indicating good compatibility with the background-only hypothesis, as expected from a fit to the ABCD regions which are designed to be signal depleted.

The limit setting phase

The limit setting machinery used in this analysis is based on frequentist statistics. It relies on the HistFitter [86] package. The limits are set based on the following test-statistics:

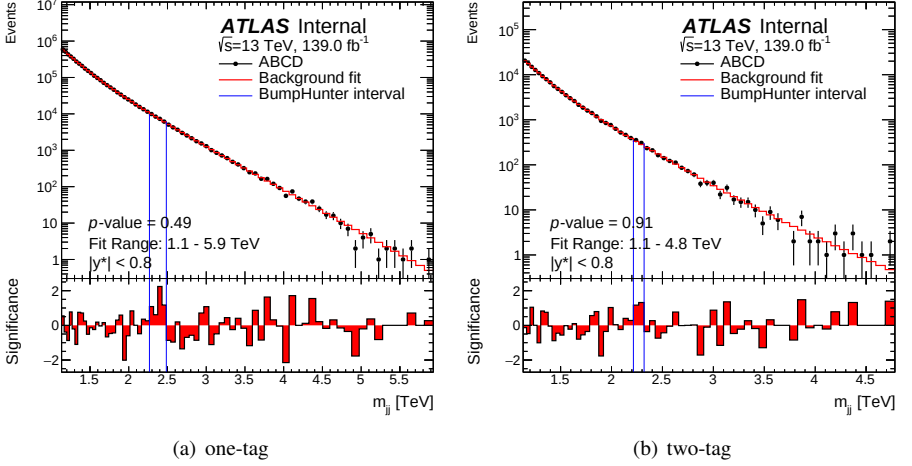


Figure 5.18 – BH results of the fit to the 1-tag (a) and 2-tag (b) ABCD regions. As expected, no significant bias is observed

$$\tilde{q}_\mu = \begin{cases} -2\ln\left(\frac{L(\mu, \hat{\hat{\theta}}(\mu))}{L(0, \hat{\hat{\theta}}(0))}\right) & \hat{\mu} < 0, \\ -2\ln\left(\frac{L(\mu, \hat{\hat{\theta}}(\mu))}{L(\hat{\mu}, \hat{\hat{\theta}})}\right) & 0 < \hat{\mu} < \mu, \\ 0 & \hat{\mu} > \mu. \end{cases} \quad (5.4)$$

where L is the likelihood, μ is the parameter of interest which in this case corresponds to the number of signal events, θ represents an ensemble of the nuisance parameters, and $\hat{\theta}$ and $\hat{\mu}$ are the global maximal-likelihood estimators for the nuisance parameters and the parameter of interest, respectively. $\hat{\hat{\theta}}(\mu)$ is the maximal estimator for a given value of μ . The test statistic is built to properly account for the fact that, given the benchmark models chosen for this analysis, negative fluctuations cannot be interpreted as a sign of new physics. Expected limits and related uncertainty bands are either computed by means of toys or by using the asymptotic approximation, which states that if the data set is sufficiently large, the distribution of the test-statistic is approximated by a non-central χ^2 distribution [87]. In the tail of the invariant mass distributions, where the statistics are lower, toys are used for both regions considered in the analysis.

5.1.6 Results

The invariant mass spectrum and the background-only fit hypothesis are shown in Figure 5.19, for both the single and double b -tag regions.

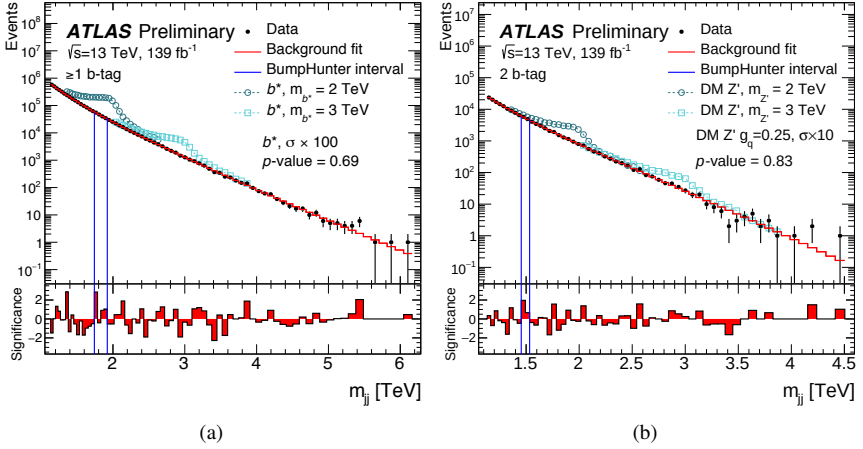


Figure 5.19 – Background-only fit to the data point. The BH p -value is much higher than 0.01 indicating good compatibility with the data points for both analyses: (a) 1-tag and (b) 2-tag. [3]

The BH p -values corresponds to 0.55 and 0.71 for the 1-tagged and 2-tagged regions, respectively. Good compatibility between the background-only fit and the data is achieved and thus exclusions limits were set. Figure 6.28 shows the exclusions limits for the different benchmark models.

To outline the effect of the improvements of the b -jet identification performance (see previous Chapter), the current expected limit at 95% CL and the limits obtained in the previous iteration of the analysis are shown in in Figure 5.21 for the DM Z' benchmark model. An extrapolation of the expected limits from the previous results to the current dataset of 139 fb $^{-1}$, assuming no change to the previous analysis strategy or its uncertainties, is also shown. To further outline the improvements of both the b -tagging algorithms and systematic uncertainties, the current version of the analysis was also repeated using the previous configuration of the b -tagging algorithm (MV2c10) and its related uncertainties as in the previous result. The ratio of sensitivities, defined as $S/\sqrt{B}$, when adopting the past or current b -tagging strategy is shown in Figure 5.22 as a function of the Z' mass. An improvement from 3 to 5, depending on the Z' mass, is observed. The uncertainty bands represent the extrapolation uncertainty (see Section 4.3) between the two b -tagging configurations. It can be seen that not only the discrimination power of the b -tagging algorithm was improved but also its related uncertainty.

In conclusion, it was demonstrated that improvements to the identification of heavy-flavor jets and related calibration analyses propagate into improvements of the analysis reach beyond the mere increase in data statistics.

Given that compelling evidence of new physics beyond the standard model in collider experiments has yet to be observed, the work to further improve the tools used in physics analysis with novel techniques and methodologies represents a crucial part of the physics program of the LHC experiments.

In the following, a novel approach designed to complement and expand the identification of jets initiated by heavy quarks at extreme energies is presented.

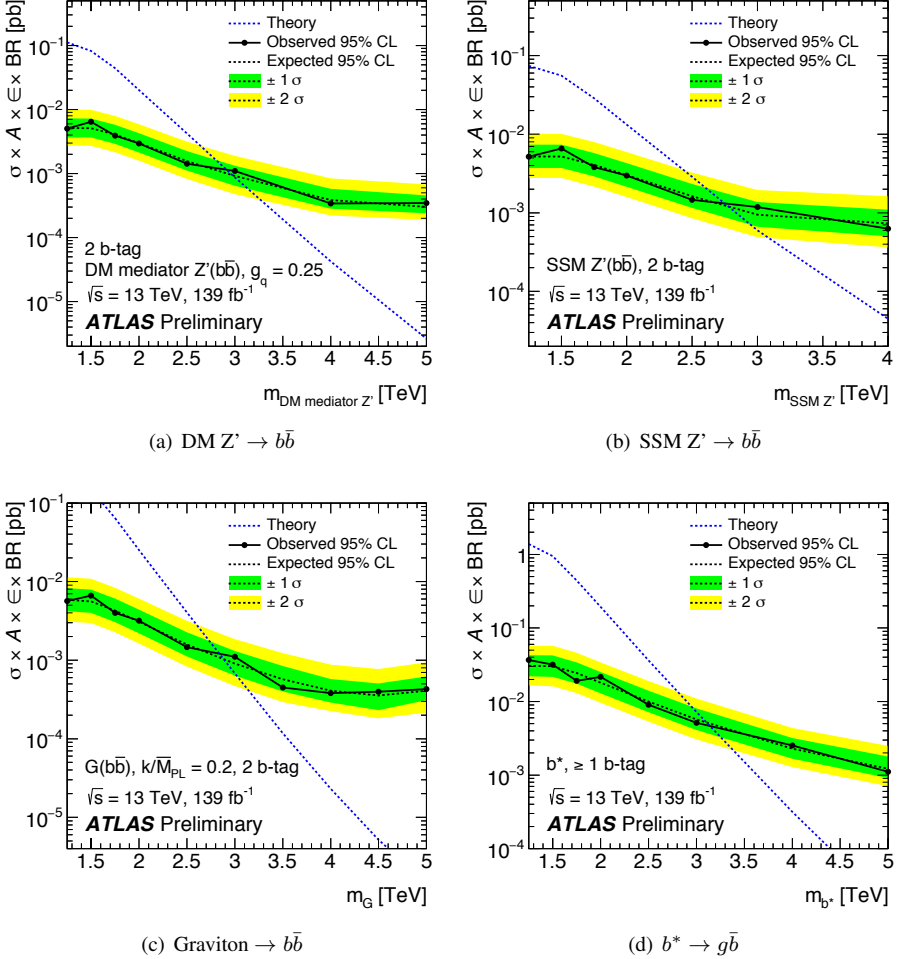


Figure 5.20 – Exclusion limits for the different benchmark models in the single and double b -tag categories of the analysis [3].

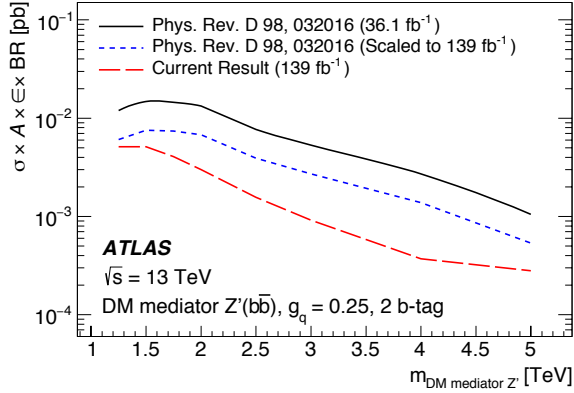


Figure 5.21 – The 95% CL upper limit on cross-section times acceptance times branching ratio times efficiency as a function of the Z' mass for the current and previous iteration of the analysis. The 95% CL upper limit of the previous result is also scaled to the 139 fb^{-1} luminosity of the current result to illustrate the analysis improvements. [3]

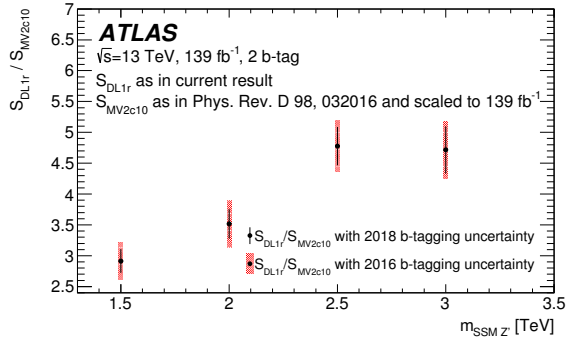


Figure 5.22 – The improvements in sensitivity brought by using the b -tagging configuration described in sections 4.2.6.2 and 5.1.2. The data-points represent the improvements with respect to the previous b -tagging configuration utilized in the previous iteration of the analysis in 2016. The uncertainty on the points are not representative of the statistical fluctuations but rather on the systematic uncertainties of the calibration analyses [3].

5.2 Investigation of trackless b -tagging for very energetic jets

The identification of heavy-hadrons at high- p_T is a challenging task. The tracking efficiency decreases for highly displaced and highly boosted topologies, such as the decay chain of heavy-hadrons. For high energy b -hadrons the lifetime increases as $\tau \rightarrow \tau\gamma$. For a b -hadron with a p_T of 800 GeV, $\gamma \sim 150$ and this high boost factor leads to a significant displaced signature of around 20 mm. The angle between the decay product and the b -hadron axis transforms under a boost as $\alpha \rightarrow \alpha/\gamma$; the decay products are thus very collimated. This boosted and displaced topology poses unique challenges in terms of tracking performance. Figure 5.23 shows the average number of tracks from the b -hadron decay chain as a function of the b -hadron decay length in the x - y plane where the z -axis is defined along the beam pipe. An evident decrease of the number of tracks is observed for highly displaced vertices. Since the b -tagging algorithms largely depends on tracking inputs, the b -tagging performance is also expected to decrease significantly for highly displaced topologies.

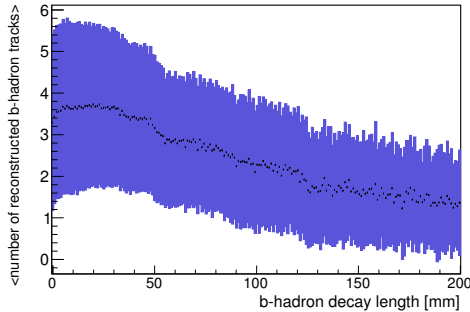


Figure 5.23 – Average number of tracks from the b -hadron decay chain as a function of the truth b -hadrons decay length using the Z' sample described in Section 4.2.6.1. The shaded band around the markers represents the RMS of the distribution in each bin, not the statistical uncertainty.

Recently, a novel approach to high- p_T b -tagging has been proposed based on the number of pixel hits in the tracker rather than tracks [88]. Using the high spatial resolution of the tracking detector, a small cone around the jet-axis of $\Delta R(\text{hit}, \text{jet-axis}) = 0.04$ is defined. This value is one order of magnitude smaller than the radius parameter used in the calorimeter to define the cone size of the jet. Due to the displaced nature of highly-energetic heavy hadrons, the number of hits on each pixel layer in the cone of 0.04 is used as a discriminating variable. Thanks to the boost of the system, the decay products of the heavy hadrons are collimated and fall within the small cone of 0.04.

This approach, referred to as trackless b -tagging, has the advantage of being simple and independent on any tracking algorithms. Despite being intrinsically limited by the percentage of heavy-hadrons decaying at least beyond the first pixel layer, the trackless approach is expected to complement the track-based algorithms for jets with very high p_T . For instance, even if a track associated to a very displaced decay is reconstructed, the resolution of its IPs at the perigee is degraded due to the large distance between the measurement points and the primary vertex and thus the discrimination power of the IP-based algorithms is also reduced. A schematic representation summarizing the main concept of the algorithm is shown in Figure 5.24. The percentage of b -hadrons decaying in between the first and last pixel layers and the average angular distance between the track produced from the decay chain of the b -hadron and the jet-axis as a function of the b -jet p_T are shown in Figure 5.25.

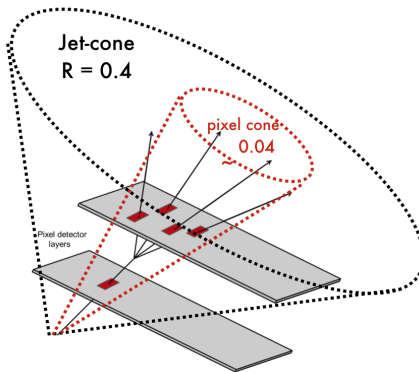


Figure 5.24 – Schematic representation of the trackless b -tagging algorithm. Figure adopted from [88].

For this thesis, the trackless b -tagging algorithm was investigated for the first time in the ATLAS experiment. An important fraction of the work was related to the generation of a suitable sample storing the hit information. By default, the hits are removed from the ATLAS data formats due to the large size needed to store them. The Z' sample, described in section 4.2.6.1, was re-produced with hits information correctly stored following all of the reconstruction steps described in section 3.3.

Figure 5.26 shows the number of clusters in the IBL and in the fourth pixel layer around a cone of 0.04 for light and b -jets with a jet- $p_T > 500$ GeV. Only the barrel is considered for this studies, i.e. $|\eta| < 1$. Given that the heavy-hadrons can pass the pixel layers before decaying, the number of clusters from the b -jets is on average smaller than the ones from light-jets in the IBL and it becomes comparable in the fourth pixel layer. The probability to have a pixel hit originating from pile-up interactions is negligible due to the small size of the cone. In fact, this approach was also demonstrated to

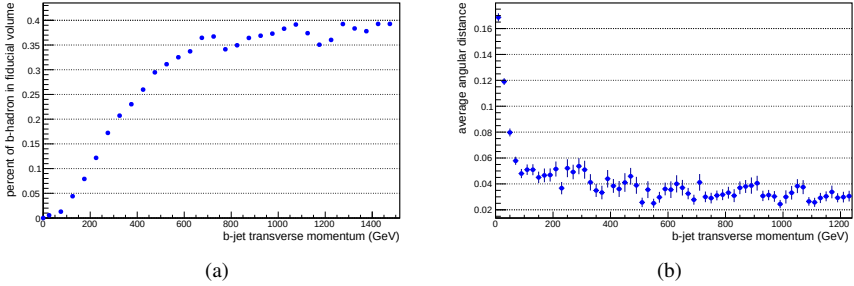


Figure 5.25 – (a) The percentage of b -hadrons decaying in between the first and last pixel layers as a function of the b -jet p_T . (b) The average angular distance between the track produced from the decay chain of the b -hadron and the jet-axis ($\Delta R(\text{b-track}, \text{jet-axis})$) as a function of the b -jet p_T . The decay products of the heavy-hadron for jet- $p_T > 400$ GeV are contained within a cone with $R = 0.04$.

be pile-up insensitive up to the expected HL-LHC pile-up values [88]².

In order to quantify the increase in performance of the algorithm, the average number of clusters in each layer was added to the MV2 training. Therefore, a total of 4 additional parameters were used, corresponding to the four pixel layers used in these studies. Figure 5.27 shows the performance in terms of light-jet rejection vs b -jet efficiency for the wide Z' sample for a jet- $p_T > 500$ GeV. An improvement in light-jet rejection of the order of 20 % is achieved for a b -efficiency of 70 % thus showing that complementarity between this new approach and the standard b -tagging techniques can be achieved.

A more sophisticated version of the algorithm was studied using simulated MC samples in the context of the identification of heavy-flavored jets at the Future Circular Collider [89]. The idea is to build an algorithm which discriminates using not only the number of clusters, but also the topological information of the cluster distribution within the cone. Due to the hard-fragmentation function of the b -quark, one would expect the decay products of the b -hadron to be very collimated and being surrounded by a more homogenous distribution originating from the softer fragmentation particles. A more complete investigation of this approach in the ATLAS experiment is currently on-going, and in the following some key distributions are shown.

Figure 5.28 shows the average ΔR of clusters in the 0.04 cone in the B-Layer for b -jets of the Z' sample, where the components arising from fragmentation and the decay products of the b -hadron decay chains are separated. As expected, the average ΔR of clusters formed by direct decay of the b -hadron is sensibly smaller compared to the

²It is worth mentioning again that in the ATLAS simulation package, the interaction of charged heavy-hadrons is not simulated. This effect is being corrected but not available at the time of this thesis.

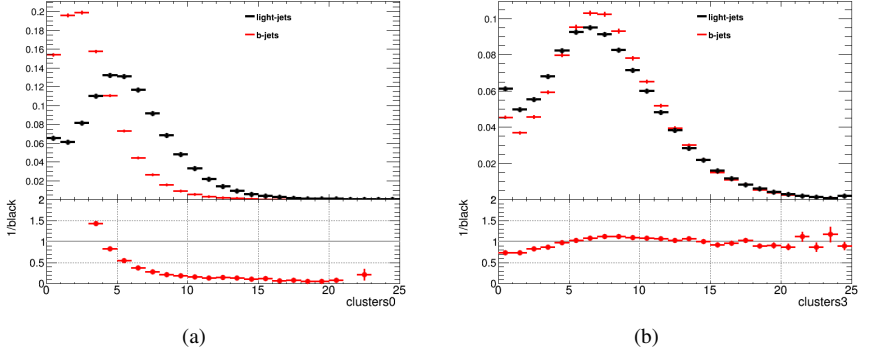


Figure 5.26 – Number of hits in the IBL (a) and in the fourth pixel layers in a cone of 0.04 with respect to the jet-axis for b - and light-jets with p_T greater than 500 GeV. The distribution for light- and b -jets were normalized to unity. A clear separation is visible in the IBL due to the fact that b -hadron are boosted enough to decay after the pixel layers. In the fourth pixel layers, instead, the number of pixel hits are comparable between light- and b -jets since at this p_T most of the heavy-hadron decays within the pixel volume.

cluster originating from fragmentation. It is also interesting to see how the number of clusters from these two components evolve vs the jet- p_T , this is shown in the right plot of the same Figure. The number of clusters increases up to jet- p_T of approximately 200 GeV, where the clusters from the b -hadron decay are contained within the cone of 0.04. After 200 GeV, the clusters from the b -hadron slowly decrease due to the high boost of the system which can results into two particles crossing a single silicon hit. The fragmentation component, instead, increases due to the higher number of particles produced at high energy. These studies, even though they are preliminary, triggered an ongoing effort for tagging high-energetic b -jets for the next LHC phase.

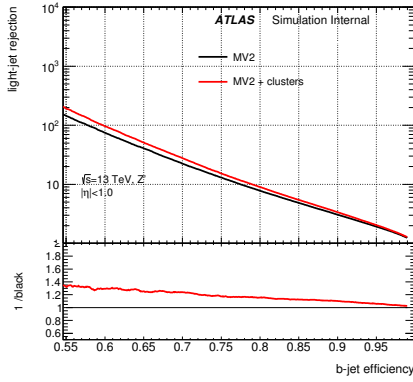


Figure 5.27 – The light-jet rejection vs b -jet efficiency for the standard MV2 configuration and the MV2 trained adding hits information.

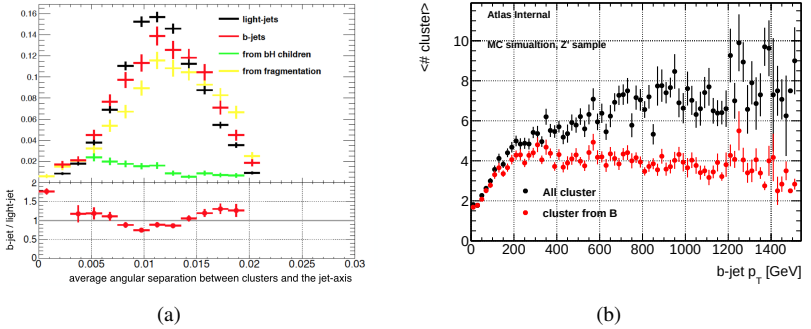


Figure 5.28 – a) The average ΔR between the clusters in the B-layer and the jet-axis in a cone of 0.04. The clusters originating from decay products of the b -hadron and clusters originated from fragmentation particles are outlined for b -jets. b) Average number of hits in the B-layer as a function of the jet- p_T for b -jets.

Search for boosted Higgs boson and other resonances decaying into pairs of b -quarks

6.1 Physics motivation

Two main motivations drive the search for low mass resonances decaying to pairs of b -quarks. The first is to search for SM Higgs Bosons at high energy and the second is to search for new particles which could explain the presence of Dark Matter in the universe. In the following a new physics analysis, targeting both interpretations, is presented.

Standard Model Higgs boson

The study of the Yukawa coupling to the third family of quarks is one of the leading measurements of the LHC experiments. Both, the ATLAS and CMS collaborations have measured this coupling in the production channel with an associated vector boson or top quarks. An inclusive measurement of the cross-section of the Higgs boson, featuring all production modes, was considered hopeless due to the large cross-section of di- b production compared to the cross-section of Higgs boson production in p - p collisions, $\sigma_{H_{bb}}/\sigma_{\text{QCD}} \sim 10^{-7}$. A new approach based on the reconstruction of boosted objects has been proposed, as already mentioned in Section 1.2.1. Other Higgs boson decay channels such as $\gamma\gamma$ or WW lack the statistics for high Higgs boson p_T . The larger BR to b -quarks allows the exploration of the highest possible p_T regime. The boosted Higgs boson analysis also represents an invaluable opportunity to study the structure of the gluon-gluon fusion (ggF) production mechanism. At high Higgs boson p_T , the

production via ggF starts to be sensitive to the top-quark loop, including possible new particles contributing to it, and to the presence of anomalous couplings that giving rise to an effective gluon-gluon-Higgs interaction [21, 22]. Figure 6.1 shows one of the Feynman diagrams contributing to the ggF production mechanism with the finite top mass contribution outlined.

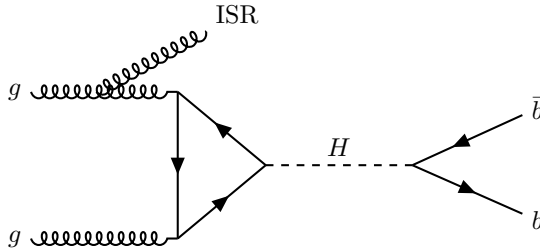


Figure 6.1 – One of the Feynman diagrams contributing to the gluon-gluon fusion production process at NLO. The Higgs boson acquires transverse momentum thanks to the recoil against an ISR particle. The quantum loop is suppressed at low transverse momentum of the Higgs boson where the mass of the top is larger than the Higgs boson mass and the interaction is considered point-like with an effective gluon-Higgs coupling. In the boosted regime, where the $H_{p_T} > 2m_{top}$ the loop becomes resolved. Effective field theories postulate BSM couplings contributing to this loop, as already discussed in section 1.3.0.2.

Due to the highly boosted system, the decay products of the Higgs boson are captured within a single jet with a radius parameter of 1.0 (large-R jet). The high spatial resolution of the tracking detector is then used to reconstruct the trajectory of charged particles which are used to identify the two prong sub-structures within the large-R jets. Finally, the sub-jets need to be identified as originating from b -quarks. The analysis also measured, for the first time in the ATLAS experiment, the $W/Z+j$ yield in the boosted regime with heavy-quarks in the final state.

Dark matter mediators

Analyses looking for resonances decaying into pairs of quarks have been thoroughly explored at the LHC experiments. As already discussed in section 5.1, a large number of BSM models predict the existence of heavy mediator particles that can be produced at the LHC, thanks to its high center-of-mass energy. While well motivated, in hadronic final states this search program is limited to resonance masses above roughly 1 TeV due to the high p_T requirement dictated by the jet-trigger. This leaves a large unexplored area at low (sub-TeV) masses. To bypass this, alternative search strategies must be explored. One way to overcome the challenge of triggering on low energy final state objects is to require that these low-mass resonances are produced with a large transverse momen-

tum by recoiling against an additional initial particle. A number of searches featuring different initial radiation such as a photon or jets have been pursued by the ATLAS experiment [90, 91]. The analysis presented in this chapter focuses on hadronic signatures. One of the Feynman diagrams contributing to such process is shown in Figure 6.2. For a resonant particle, if the resonance p_T is larger than two times its mass, the angular separation becomes small enough for the two partons from the resonance decay to be reconstructed within one large-R jet. Many models predict low mass resonances with enhanced couplings to bottom quarks. For instance, in the context of DM mediators, these are spin-0 DM particles [26].

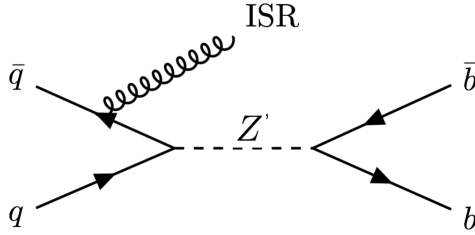


Figure 6.2 – Feynman diagram of the production modes of a DM Z' candidate. The mass of the resonance is set to be much lower than any other dark matter particle which would lead to missing transverse energy in the detector. The ISR allows to lower the minimum p_T dictated by the trigger and to search for boosted resonances in the mass range of 100-200 GeV.

6.2 Jets reconstruction in boosted environments

The analysis relies largely on the usage of jets with a large radius parameter of $R = 1$ which contains at least two associated track-jets. The calorimeter information is used to correctly extract the energy and momentum of the signal candidate while track-jets are used to resolve the two-prong topology expected from the decay of the Higgs boson, Z or Z' signals and to apply b -tagging. A brief introduction to large-R jet and track-jet reconstruction will be discussed in the following.

Thanks to the large center-of-mass energy provided by the LHC, particles originated from the hard-scatter collision are often produced with a transverse momentum much larger than their mass. Therefore, their decay products are collimated along the momentum axis of the parent particle. In case of a boosted Higgs boson decaying hadronically into quarks, the angular separation of the decay products can be expressed as:

$$\Delta R = \frac{1}{\sqrt{x(1-x)}} \frac{m_H}{p_{T_H}} \quad (6.1)$$

where x and $(1-x)$ are the momentum fraction carried by the two quarks. For the decay of a Higgs boson, the two quarks are expected to have approximately the same momentum and thus the equation simplifies to: $\Delta R \approx 2 \frac{m_H}{p_{T_H}}$. For $m_H = 125$ GeV, the minimum transverse momentum of the Higgs boson needed to produce collimated particles within a ΔR of 0.5 is $p_{T_h} \approx 500$ GeV. This p_T value roughly corresponds to the point where the trigger becomes fully efficient (see section 6.5.1). It is therefore natural to search for high energetic Higgs boson using large-R jets.

6.2.1 Large-R jet mass

The critical variable used in this analysis is the mass of the large-R jet. The mass is calculated from the energy E and momentum $\vec{p}$ of its constituents:

$$m = \sqrt{(\sum_n E_n)^2 - (\sum_n \vec{p}_n)^2} \quad (6.2)$$

Large-R jets moments, such as the mass, are in general susceptible to pile-up and soft emissions during the hadronization process which would lead to instability in the measurements. To cope with this fact, a set of grooming techniques have been proposed in recent years [92–94]. It is worth mentioning that one of the first large-R jet substructure definitions was introduced in 2008 to search for the Higgs boson in the boosted topology produced in association with a vector boson [92]. Since that time, several techniques to reconstruct the moments of the large-R jet have been employed by the ATLAS experiment. A detailed report of the different grooming techniques and their performance in ATLAS and CMS can be found in [95]. The *trimming* algorithm was used for this analysis. *Trimming* is based on the assumption that the sub-jets built from constituents corresponding to initial-state radiation and pile-up are relatively soft with respect to the sub-jets from the hard scatter process. In the ATLAS experiment, sub-jets are built using the k_t algorithm with radius parameter $R = 0.2$. Sub-jets with a transverse momentum below a certain fraction of the p_T of the large-R jet are removed: $p_{T_{sub}} < f \cdot p_{T_{jet}}$ where f is a parameter of the trimming algorithm; the typical value used in ATLAS is 5%. Figure 6.3 shows a schematic illustration of the target topology of the analysis featuring two sub-jets built from tracks which are associated to a trimmed large-R jet.

A number of different jet moments can be built from the energy distribution and the angular separation of either the constituents of the large-R jets or the sub-jets associated

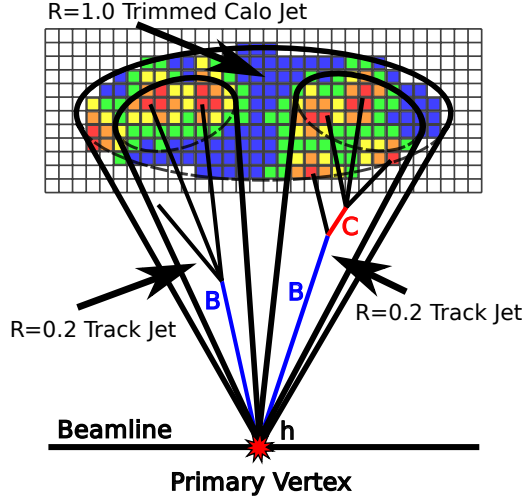


Figure 6.3 – Cartoon illustrating the reconstruction of a large- R jet with associated sub-jets originating from the hadronization of two b -quarks [97].

with them. These moments, that have been successfully used in a variety of boosted analyses, are correlated with the mass of the large- R jet itself. Given the topology of the analysis, such a correlation may lead to instability. For instance, it was found that the assumption of a falling QCD mass spectrum was not respected in case a cut on one of the large- R jet moments was employed. Dedicated algorithms have been proposed to de-correlate the mass of the large- R jets with the other moments [96]. However, it was found that the sensitivity to the boosted Higgs boson signal was not significantly improved by using these techniques and thus no cuts on sub-structure variables were used. In this analysis, the particle multiplicities expected in the boosted decay of the Higgs boson or the DM signals are determined using the number of track-jets associated with the large- R jet. This reduces the additional discrimination power when using substructure variables. However, it should still be possible to exploit the expected different color-flow connections when comparing $g \rightarrow b\bar{b}$ with QCD singlet states such as $Z, H, Z' \rightarrow b\bar{b}$ decays. In future iterations of the analysis, it may be interesting to further investigate this feature.

6.2.2 b -tagging in boosted environment: VR sub-jets

As already mentioned, the large- R jet was used to extract the kinematic information of the jet such as its mass and transverse momentum. The leading and sub-leading track-jets associated with it were required to be identified and originated by b -quarks. Track-jets are built with the anti- k_t algorithm using the tracks associated with the primary

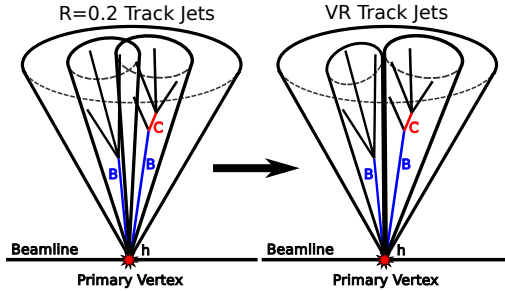


Figure 6.4 – Cartoon illustrating sub-jet reconstruction using variable radius track jets [97].

vertex as input constituents. The track-jets used in this analysis feature a variable radius parameter. At high momentum, one would expect the jets to be more collimated as their transverse momentum increases. A jet-collection which exploits this feature has been implemented in the ATLAS experiment, referred to as Variable-Radius (VR) track-jets. VR track-jets are clustered using the variable-radius jet algorithm [97]. Since the p_T of the track jets depends on the radius itself, an iterative procedure is used until all tracks contributing significantly to the jet- p_T are included in the VR-jet and convergence is reached. The effective radius parameter of the VR track-jet is defined as:

$$R(p_T) = \frac{\rho}{p_T} \quad (6.3)$$

where ρ determines how fast the jet size decreases with the transverse momentum of the jet and in the ATLAS experiment is set to 30 GeV. In addition, the VR algorithm requires two parameters to define upper and lower bounds, R_{min} and R_{max} , to impose lower and upper cuts on the jet size, respectively. The additional parameters prevent the jets from becoming too large at low p_T and from shrinking below the detector resolution at high p_T . The effective jet size varies smoothly between R_{min} and R_{max} . Figure 6.4 shows schematically the differences between a pair of fixed radius track-jets with $R = 0.2$ and VR track-jets. In the latter case the radius is adjusted to take into account possible differences in the p_T of the heavy hadrons. The effect in term of Higgs boson-tagging efficiency (only $H \rightarrow b\bar{b}$ decays were considered for these studies) as a function of the Higgs boson transverse momentum is shown in Figure 6.5 for different value of R_{max} . As the boost increases, the two fixed radius track-jets are merged together and the H -tagging efficiency quickly drops. This is due to the fact that many underlying b -tagging algorithms assume the jet axis to be the b -hadron decay length, as described in the Chapter 4. On the other hand, VR track-jets ensure high efficiency over a broad H_{p_T} range.

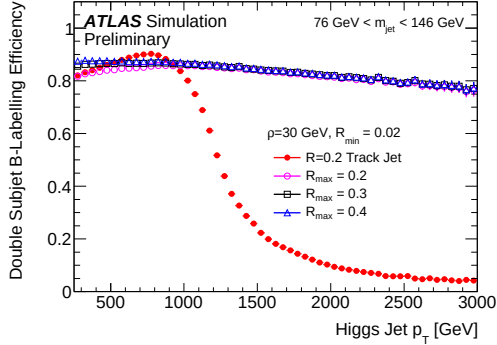


Figure 6.5 – Efficiency of double sub-jet identification as a function of the Higgs boson jet- p_T for several values of the maximal radius parameter R_{max} [97].

6.3 Analysis strategy

This analysis is based on the 80.5 fb^{-1} dataset recorded by the ATLAS experiment in 2015, 2016 and 2017 at a center-of-mass energy of $\sqrt{s} = 13 \text{ TeV}$. The structure of the analysis is based on identifying one large- R jet in the event which is compatible with a resonance decay to a pair of bottom quarks, with a resonance mass between 70 and 230 GeV.

The primary source of background is multi-jet QCD events, which is estimated with a parametric functional form. Control regions, defined by anti b -tagging requirements, are used to validate the background estimation procedure. The background from $t\bar{t}$ production is estimated from a data-driven control region. The $V+j$ process is also significant in the signal region and it is simultaneously measured together with the $H+j$ component.

6.4 MC simulated samples

QCD multi-jet sample

Simulated QCD dijet events are generated using the PYTHIA8 [74] generator with the A14 tune [75] and the NNPDF2.3 LO parton distribution function [76]. The decays of b -hadrons were performed using EvtGen [98]. To maintain a constant statistical power over a large energy range, the events are generated in different slices of transverse momentum before reconstruction. However, even then the low p_T samples have a statistical precision smaller than the Run2 dataset used in the analysis.

Top samples

Simulated $t\bar{t}$ events were generated at tree-level using POWHEGBOXV2 [99–101] and the NNPDF30 NLO parton distribution function. The hadronization was performed using PYTHIA8 with the A14 tune. The generated samples are split into events where both tops decay hadronically, when only one decays hadronically and when both tops decay leptonically.

To evaluate the uncertainty due to the choice of MC generator, a second set of $t\bar{t}$ events were generated using SHERPA 2.2.1 [102] with the NNPDF30 NNLO [103] parton distribution function. Independent samples were generated for the different decay modes of the top quark.

Vector Boson samples

Hadronically decaying W and Z events, with up to 4 additional partons at leading order, were generated using SHERPA 2.1.1 with the CT10 [104] parton distribution function. They were separated into several orthogonal datasets based on the p_T of the vector boson. Leptonically decaying W and Z samples exist with up to 2 additional partons at NLO and up to two more at LO. The hadronic sample cross sections are then corrected with k -factors by comparing to the NLO samples. The calculated k -factors are 1.28 for $W+j$ and 1.37 for $Z+j$.

Alternate samples of $W+j$ and $Z+j$, with the bosons decaying hadronically, were generated using HERWIG++ [105]. Unlike the SHERPA samples, only one extra parton was included in the matrix element. The UEEE4 underlying-event tune was used with the CTEQ6L1 [106] parton distribution function. They were also separated into several orthogonal datasets based on the truth p_T of the vector boson.

Higgs Boson samples

Higgs boson events were simulated corresponding to the three main production mechanisms; gluon-gluon fusion (ggF), vector boson fusion (VBF) and Higgsstrahlung (associated W/Z production). All contribute in a non-negligible manner to the SR, correspondingly making up 50%, 30% and 20% of the total signal.

The ggF plus jet events and VBF production mechanisms were generated at NLO with top-mass-effect corrections following the MiNLO procedure using the HJ+MiNLO prescription with finite top mass using POWHEGBOXV2 [107–109] and the NNPDF30 NNLO parton distribution function. They are showered using PYTHIA 8.212 with the AZNLO tune and the CTEQ6L1 parton distribution function. The decays of b -hadrons were performed using EvtGen.

The Higgs boson events produced in association with a W or Z boson were generated using PYTHIA 8.212 with the AZNLO tune and the CTEQ6L1 parton distribu-

tion function. The decays of b -hadrons were performed using EvtGen. The PYTHIA process does not include the $gg \rightarrow ZH$ contribution. To account for this and higher order effects, the cross-section was corrected to the LHC cross-section working group recommendation [110]. This results in k -factors of 1.25 and 1.47 for WH and ZH respectively. All decay modes of the vector bosons were enabled.

Dark Matter mediator samples

The events containing a leptophobic Z' decaying to two quarks and produced in association with a jet are generated using a Simplified Dark Matter MGMCatNLO model [111] and the NNPDF30 LO parton distribution function. The showering was done using PYTHIA8 with the A14 tune and the NNPDF23 LO parton distribution function.

To ensure high Monte Carlo statistics at large Z' p_T , all events are required to have a truth jet with $p_T > 350$ GeV before detector simulation. Independent samples were also generated for Z' decaying to light quarks and decaying to b -quarks. The two samples are orthogonal and were combined into an inclusive sample.

Signal samples were generated at several Z' masses spanning the invariant mass region of interest to the analysis. The values of $m_{Z'}$ are 100 GeV, 125 GeV, 150 GeV, 175 GeV, 200 GeV, 250 GeV and 300 GeV.

Similarly to what discussed in section 5.1.1, the simplified model defines an absolute axial coupling, g_q , to a quark-antiquark pair and was taken to be the same for all generations. The signal events are simulated with $g_q = 0.25$. The specific value should not have a significant effect on the kinematics of the reconstructed events because the natural width of the Z' is smaller than the typical large- R jet jet mass resolution in this p_T and mass range (about 10% of jet mass). The cross-section at other values can thus be obtained by scaling as g_q^2 . The calculation was implemented using the DM width calculator in Ref. [112]. The DM particle mass was set to 10 TeV to not alter the Z' branching ratios to SM particles. In the following, the Z' mediator model will be referred to as dark matter Z' signal candidate for simplicity.

6.5 Event selections

6.5.1 Offline selection

The trigger selection usually sets the minimum jet- p_T that can be used by the analysis. Triggers based on large- R jets were found to be more suitable for this analysis. This is due to their additional flexibility in the trigger decision: they can trigger on either the ISR or signal candidate jet, in contrast to the standard small- R jet triggers which only target the ISR jet. Triggers change slightly during the data-taking period. The detail of the primary triggers for each year are:

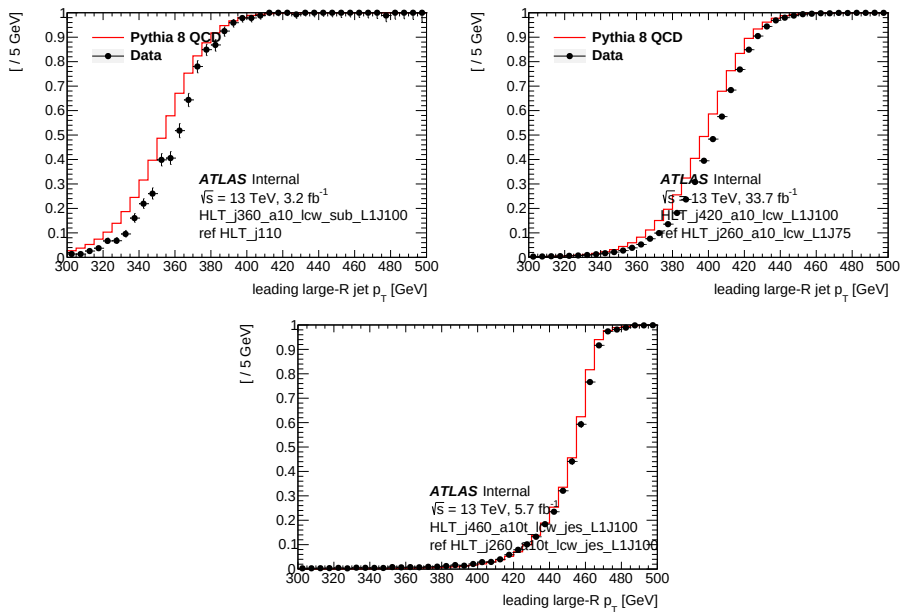


Figure 6.6 – Efficiencies of the chosen triggers for this analysis for a subset of the data collected in 2015, 2016 and 2017.

- 2015 - ungroomed¹ large-R jet with $p_T > 360$ GeV,
- 2016 - ungroomed large-R jet with $p_T > 420$ GeV,
- 2017 - trimmed large-R jet with $p_T > 460$ GeV.

The corresponding trigger turn-ons are shown in Figure 6.6. The analysis-level leading jet p_T cut selects events for which all of the triggers are fully efficient, and it was set to $p_T > 480$ GeV for all years to gain some margin from the turn-on and to avoid sculpting of the QCD invariant mass spectrum due to different p_T selections. An additional selection of jet- $p_T > 250$ GeV was employed on the sub-leading large-R jet to explicitly select a recoiling system.

To ensure good quality of the reconstructed events, events with noise bursts in the LAr calorimeter, as well as events with data corruption in either the tile or LAr calorimeters were rejected.

The decay products of the signal candidates must be contained within the large-R jet. To ensure this, a set of pre-selections are applied to all large-R jets in the events.

- the large-R jet must contain at least 2 VR sub-jets with $p_T > 10$ GeV.
- $\Delta R_{VR} / \min R_{VR} > 1$, with R_{VR} the radius of the two VR track sub-jets and ΔR_{VR} the distance between them. It was observed that VR sub-jets can be reconstructed within each other. This requirement removes large-R jets with these pathological cases to prevent anomalous b -tagging response.
- $2m_J/p_{T,J} < 1$ was required to ensure a boosted jet configuration.

The large-R jets passing these selections are ordered in jet- p_T for each event and the the highest p_T jet in the list was taken to be the signal candidate.

The last set of selections used to define the signal candidate enforce orthogonality with the control region designed to extract the top contribution in the SR described in section 6.8. Any events with muons opposite to the signal candidate jet were removed. Such muons were required to have a $p_T > 40$ GeV and $\Delta\phi > \frac{2}{3}\pi$ from the signal candidate jet.

With the jet identified as a signal candidate, different b -tagging selections were used to define different regions in the analysis. At the time of the analysis, the different b -tagger variants (see Section 4.2.6.2) were not fully calibrated, and thus the standard MV2 configuration had to be used. Table 6.1 summarizes the sensitivities of the different b -tagging working points. The 77% WP was used to define the SR.

¹Ungroomed is defined as the large-R jets before any grooming procedure such as Trimming. In 2015 and 2016, only ungroomed large-R jet triggers were available.

Table 6.1 – The signal significance as a function of different available b -tagging algorithms and working points. The significance is defined using $s/\sqrt{b}$ at 80.5 fb^{-1} , with s corresponding to the Higgs boson signal and b corresponding to the QCD background modeled using PYTHIA8. The event count is taken within a $\pm 25 \text{ GeV}$ window around signal candidate large- R jet mass of 125 GeV .

	MV2c10
85% WP	0.43
77% WP	0.49
70% WP	0.49
60% WP	0.45

6.5.2 Event classification

The available MC statistics of the QCD sample are not sufficient to validate the background estimation technique. To cope with this feature, control regions are defined in data by dividing the events based on the number of b -tags in the two leading sub-jets of the signal candidate:

- Events with exactly 0 *loose* b -tags form the QCD control region (CR).
- Events with exactly 0 *tight*, but 1 or 2 loose b -tagged sub-jets, form the QCD validation region (VR).
- Events with exactly 2 *tight* b -tagged sub-jets form the 2-tag signal region (SR).

Where the *loose* working point corresponds to 85% b -tagging efficiency and the *tight* working points corresponds to 77% b -tagging efficiency

Table 6.2 lists the $S/\sqrt{B}$ significance for the different resonance components in the different regions considered in the analysis. The SR is the only region where the Higgs boson signal is not negligible. On the other hand, the Z' signals have similar significance in the CR and SR. For this reason, only the 2015 and 2016 datasets were used to form the CR and VR as the Z' model was previously excluded in these datasets by the untagged version of this analysis [91]. The analysis in these regions was then performed on 1.2 fb^{-1} datasets to have a comparable number of events between the CR, used as a proxy for fitting studies, and the actual SR.

6.5.3 Signal and background shapes

The QCD background and signal shapes based on MC simulation in the different regions are described in the following.

Table 6.2 – The signal significance of the different peaking components in the different analysis regions. The significance is defined as $s/\sqrt{b}$ in a ± 25 GeV window around the resonance mass at 80.3 fb^{-1} . It is also worth mentioning that the sensitivity to Z' signals is comparable between the CR and SR. This is due to the fact that the chosen Z' benchmark sample has an axial coupling to SM particles. A spin-0 mediator, with enhanced couplings to b -quarks, is expected to change this picture and will be considered for future iteration of the analysis.

Sample	Control Region	Validation Region	Signal Region
W	33.24	16.59	1.66
Z	12.30	5.62	10.78
Higgs	0.02	0.02	0.47
$Z'(100)$	17.05	7.83	17.29
$Z'(125)$	16.76	8.06	16.65
$Z'(150)$	16.37	7.57	16.24
$Z'(175)$	15.28	7.15	14.49
$Z'(200)$	13.87	6.76	13.45

Background shapes

In Figure 6.7, the SR mass spectrum is shown for the QCD background. A clear kink in the spectrum at ~ 250 GeV is observed. This kink happens at the place where the boost from the p_T requirement of 480 GeV is not large enough to merge two hadrons into a single large-R jet ². On the other end of the spectrum, the lower bound was selected to avoid the turn-on region, which would have complicated the QCD background estimation. Therefore, the mass range considered in the analysis is from 70 GeV to 230 GeV in mass.

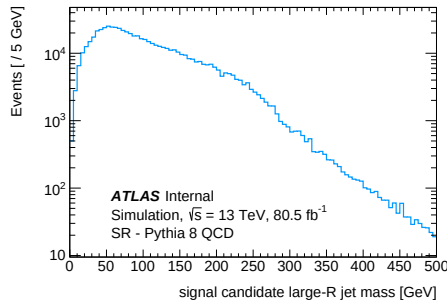


Figure 6.7 – This figure shows the SR mass spectrum for the QCD background.

² Assuming that, in a two body decay, $\Delta R \lesssim 2m/p_T$, then $m \lesssim p_T/2$, which means that, for a selection of $p_T > 480$ GeV, masses below 240 GeV are favored.

The simulated QCD shapes of the signal candidate mass spectrum in the CR, VR and SR are compared in Figure 6.8. This comparison indicates that the shape of the QCD background is similar in all regions for the mass range considered. This feature allows to use the different regions as a proxy of the SR for validation of the fitting procedure.

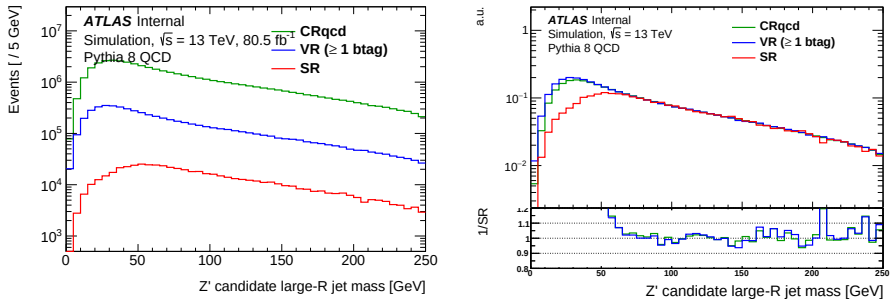


Figure 6.8 – The expected yield and shape of the invariant mass of the QCD background in the different analyses regions. The distributions in the right figure have been normalized to the same event count between $100 \text{ GeV} < m_J < 200 \text{ GeV}$.

It is also interesting to discuss the flavor composition as predicted by Pythia8 in the SR for the multi-jet QCD background. Figure 6.9 shows how the background in the SR is dominated by double b -quarks and combinations of (b - or c -) quarks. Events with no heavy (b - or c -) quarks make up only 5%. Therefore, the background is most likely formed by gluon-splitting into heavy quarks and a high energy heavy quarks emitting a lighter quark. The latter most likely originates during the fragmentation process of the heavy hadron or from nearby hadronic activity.

Signal shapes

The resonant signals are shown in Figure 6.10 in the SR. The W and Z boson templates were merged together to form a single V template to facilitate the fit. A sizable $t\bar{t}$ component is present in the SR. This is due to mis-tagging of the c -jets from the W decay, in addition to the direct b -jet produced from t decays, which merge into a single large-R jet. The yield of the samples represents the expected number of events in the SR. In between the $V+j$ and $t\bar{t}$ peaks, a small contribution from $H+j$ is visible. The Z' signals are also shown in the Figure for different mass hypotheses. To reduce statistical fluctuations of the MC templates, a functional form was used to smooth the distributions and the related systematic variations. It was found that a sum of three gaussians plus a constant is able to correctly smooth all of the templates of interest. As an example, Figure 6.11 show the $H+j$ and $Z'(m = 175 \text{ GeV})$ templates with the corresponding results of the fit outlined. In addition, the Z' signals were morphed using *RooMomentMorph*

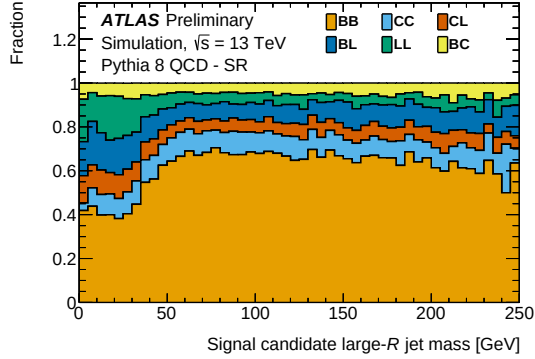


Figure 6.9 – Predicted flavour composition of the dijet background in the SR based on the truth-matched hadron content of the two leading- p_T track-jets associated to the signal candidate large-R jet, with the B/C labels indicating the presence of a b/c -quark and L indicating the presence of a light quark or a gluon [4].

to increase the available mass points to be probed for the exclusion limits.

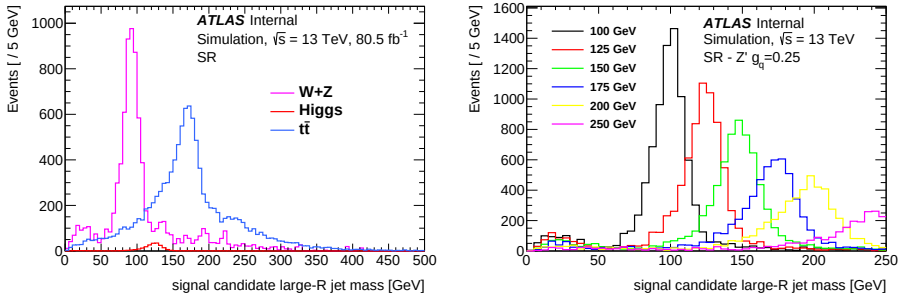


Figure 6.10 – The expected SM resonances (a) and the dark matter Z' signal candidates (b) for mass hypotheses in the SR.

To further investigate the yields of the different production mechanisms of the Higgs boson in the SR, the $H+j$ components are depicted in Figure 6.12. The majority of the signal candidates are formed by the ggF production mode as expected, followed by the production in association with a vector boson and VBF. It is also interesting to note that in the associated production with a Z boson, a second peak at around 90 GeV is seen. This is due to selections which define the signal candidate as the leading large-R jet with 2 b -tagged associated with it. If the Z boson produced in association with the Higgs boson decays into a pair of b -quarks, it can be reconstructed as the signal candidate.

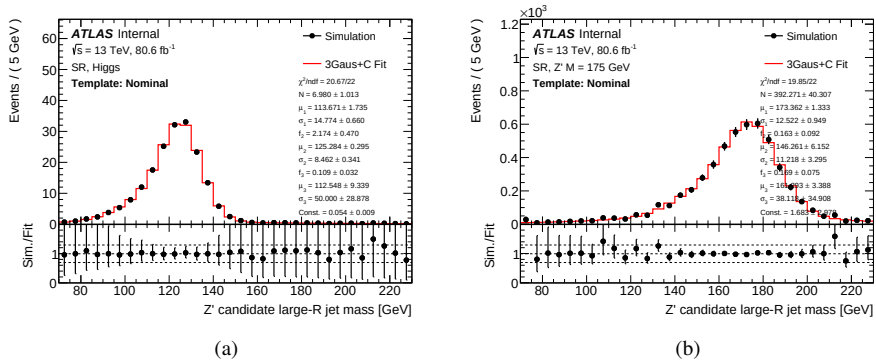


Figure 6.11 – (a) The $H+j$ template and the (b) Z' signal model at a nominal mass of 175 GeV. The functional form used to smooth the two spectra is outlined in red.

This effect is small and is not significant given the sensitivity of the analysis. However, in the future, a more sophisticated event selection exploiting also the information of the recoiling jet could be foreseen.

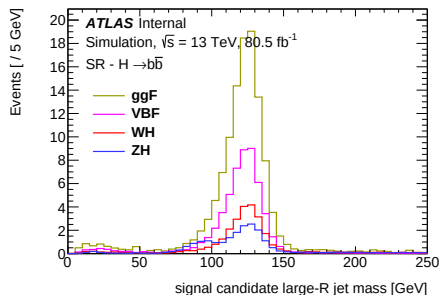


Figure 6.12 – Component break down of $H+j$ components in the SR.

The relative yield of the resonant templates in the different regions is detailed in Table 6.3. The vector boson component is dominated by the W boson in the CR. However, as expected by imposing the double b -tagging requirement, $Z \rightarrow b\bar{b}$ is the main contribution in the SR. The $t\bar{t}$ contribution is divided equally between the two regions with $\sim 60\%$ coming from hadronic decays, $\sim 40\%$ from semi-leptonic events and only a small percentage from di-leptonic decays of the top quarks. The $H \rightarrow b\bar{b}$ component is mainly produced via ggF in all regions, contributing 53% of the Higgs boson signal in the SR. The alternative production mechanisms also contribute in a non-negligible manner: VBF production contributes 25% and Higgs-strahlung the remaining 22%. This indicates that a dedicated Higgs boson analysis with selections optimized for each of

Table 6.3 – The fractional composition of the different resonant contributions in the defined regions [4].

		CR	SR
$V+j$	$Z+j$	0.28	0.80
	$W+j$	0.72	0.20
$t\bar{t}$	All hadronic	0.58	0.63
	Semi-leptonic	0.38	0.34
	Dileptonic	0.04	0.03
$H \rightarrow b\bar{b}$	ggF	0.49	0.53
	VBF	0.17	0.25
	WH	0.21	0.12
	ZH	0.12	0.10

the production modes could improve the sensitivity of the search.

6.6 Background estimation

6.6.1 Data slices for fitting validation

As previously mentioned, the CR was used for the validation of the QCD background estimation. About 1.2 fb^{-1} of the CR corresponds to the expected statistics in the SR corresponding to 80.5 fb^{-1} . Therefore, the CR and VR were divided into independent 1.2 fb^{-1} data slices which were used to validate the QCD background estimation. The slices were constructed by grouping adjacent data runs (2016 and 2017) until approximately 1.2 fb^{-1} of data was gathered, for a total of about 60 slices.

The left plot in Figure 6.13 shows the signal candidate large-R jet mass for all considered CR slices. The slices have slightly different numbers of events because they were constructed by gathering full runs until the total integrated luminosity was at least as high as 1.2 fb^{-1} . This effect can be seen on the right plot, which shows the total number of events distribution for all considered slices.

QCD background estimation

The primary background sources comes from QCD processes. To find a parametric function that fits the QCD background well, a selection of families of functions was investigated. The functional forms that were found to give a satisfactory description of the QCD process are the following:

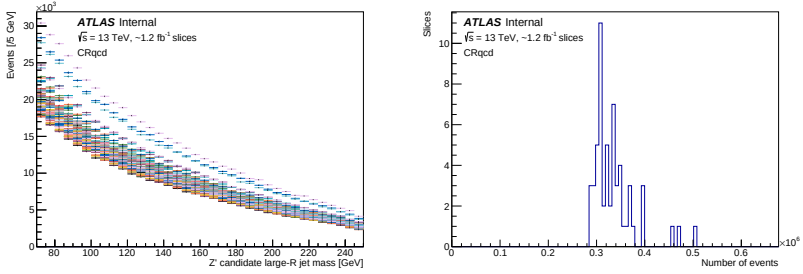


Figure 6.13 – (Left) Signal candidate large-R jet mass distributions in the different CR data slices. (Right) Number of events distribution in CR for all data slices.

- polynomial exponential (nominal)

$$f_n(x|\vec{\theta}) = \theta_0 \exp\left(\sum_{i=1}^n \theta_i x^i\right) \quad , \quad x = \frac{m_J - 150 \text{ GeV}}{80 \text{ GeV}} \quad (6.4)$$

- Formal Laurent series (alternate)

$$f_n(x|\vec{\theta}) = a \sum_{i=0}^n \frac{\theta_i}{x^{i+1}} \quad , \quad a = 10^5, x = \frac{m_J + 90 \text{ GeV}}{160 \text{ GeV}} \quad (6.5)$$

To facilitate convergence during the minimization procedure, the parameterization of the polynomial exponential function maps the independent variable to $x \in [-1, 1]$ for the fit range of $[70, 230]$ GeV, and the parameterization of the Formal Laurent series maps the independent variable to $x \in [1, 2]$. The scaling factor, a , for the Formal Laurent series was not a free parameter; it was empirically chosen to keep the scale of the parameters at $\mathcal{O}(1)$. The nominal function was considered as the polynomial exponential. The Formal Laurent series was used as an additional systematic uncertainty.

The number of parameters of the function were fixed using LH-ratio and F-tests [113]. Results of the tests showed that 5 parameters for the polynomial exponential and 4 parameters for the Formal Laurent series provide an accurate description to the data points.

The fit was validated using the slices mentioned in the previous section. To evaluate the performance of the fit on QCD events, the expected number of events from $V+j$ and top contributions were fixed, in each slice, to the expectation provided by the SM. The fit was repeated on each of the ~ 60 slices. Figure 6.15 shows the $\chi^2/n.d.f.$ distributions for the parametric fit of the data slices in the CR (left) and VR (right). The red lines represent the expected $\chi^2/n.d.f.$ distribution for the given number of degrees of freedom in the fit corresponding to 27 for the nominal fitting function. Within the statistical

precision given by the different data slices, the $\chi^2/n.d.f.$ from the individual fits seem to follow the expected distribution. Similar results were found with the alternate fitting function.

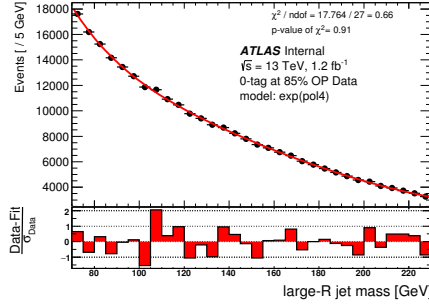


Figure 6.14 – The fit of the 5 parameter polynomial exponential QCD model to 1.2 fb^{-1} of the CR data with the resonant MC templates subtracted. The fit exhibits both a low reduced χ^2 value and a high p -value for the χ^2 indicating a good fit.

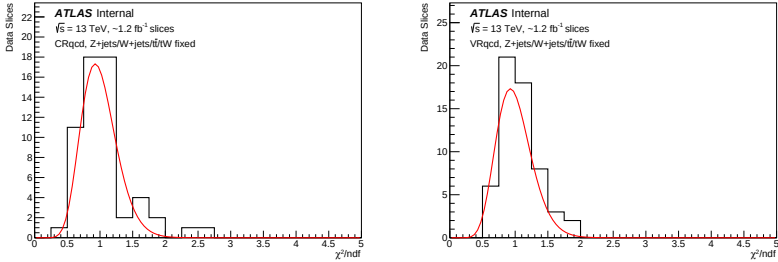
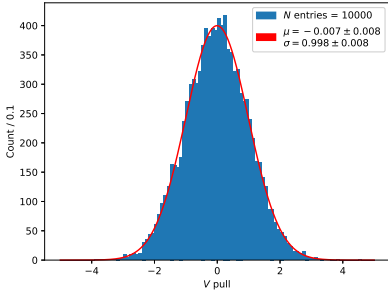


Figure 6.15 – $\chi^2/n.d.f.$ distributions for the nominal parametric fit of the data slices in the CR (left) and the VR (right). Similar results were obtained using the alternate functional form.

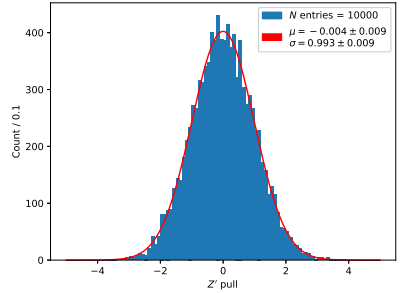
6.6.2 Signal injection tests

Given the choice of parametric model for the QCD background, a bias in the fit signal strengths of any signals can be introduced. To determine the effect of this bias, signal injection tests were performed using a full model comprised of a parameterized QCD model and signal MC templates. The signal templates used were a $V+j$ template constructed from summing the contributions of the $W+j$ MC template and the $Z+j$ MC template with respective k -factors of $k_W = 1.28$ and $k_Z = 1.38$ applied and a Z' signal MC template for a given mass hypothesis of $m_{Z'} \in \{100, 125, 150, 175, 200\} \text{ GeV}$.

For each MC model, the shape was left invariant while the yields (μ_V and $\mu_{Z'}$), which represents their respective signal strengths, were free to float in the fit. The QCD model was Poisson sampled to construct thousands of pseudo-experiments. The parameters used to construct the model for the Poisson sampling were found by fitting the parameterized QCD model to the data with the resonant MC templates subtracted. In each pseudo-experiment generated from the model, $V+j$ and Z' events were injected into the pseudo-data and a full fit was performed. From these fits to the pseudo-data, pull distributions were extracted, where the pull is defined as already discussed in section 5.1.3.1. This process of generating a pseudo-experiment, fitting with the fit model, and then calculating the pull for the signal components was repeated for 10,000 trials. The deviation of the fit Normal distribution's mean from 0 is then an indicator of the bias of the pull given the choice of QCD model. Figure 6.16 shows the pull distribution for the $V+j$ and Z' signals. A gaussian shape is visible with no bias and a width of 1. The pull plot was then repeated for many different μ hypotheses of both the Z' and $V+j$ components. A summary of the results of those tests is shown in Figure 6.17. No significant bias is observed throughout the mass range of the analysis.



(a) Pull distribution for the $V+j$ fit signal strength for injected signal strength $\mu = 1$ for a Z' mass hypothesis of $m_{Z'} = 100$ GeV.

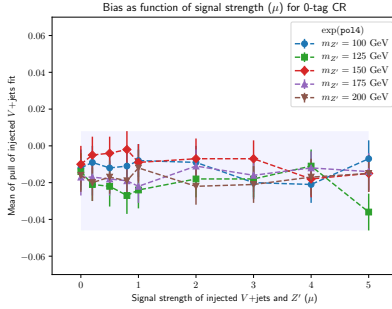


(b) Pull distribution for the Z' fit signal strength for injected signal strength $\mu = 1$ for a Z' mass hypothesis of $m_{Z'} = 100$ GeV.

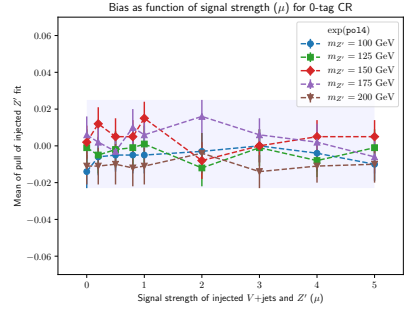
Figure 6.16 – The pull distributions for the fit signal strengths for a) $V+j$ and b) Z' using a full model with a Z' mass hypothesis of $m_{Z'} = 100$ GeV and injected signal strengths of $\mu_V = \mu_{Z'} = \mu = 1$. A Gaussian is fit to the pull distributions with the best fit results for the Gaussian's mean and standard deviation shown on the plot together with their respective uncertainties.

6.6.3 Spurious signal tests

In order to gauge how sensitive the choice of QCD function is to statistical fluctuations faking a possible signal, spurious signal tests were performed. This test tries to fit a



(a) Distribution of the pull mean for the V +jets fit signal strength vs. injected signal strengths for different Z' mass hypotheses.



(b) Distribution of the pull mean for the Z' fit signal strength vs. injected signal strengths for different Z' mass hypotheses.

Figure 6.17 – The distribution of the pull mean for a) V +jet and b) Z' signal strengths vs. the injected signal strength μ for $\mu \in \{0, 0.2, 0.5, 0.8, 1, 2, 3, 4, 5\}$ using a full model with a Z' mass hypothesis $m_{Z'}$ for $m_{Z'} \in \{100, 125, 150, 175, 200\}$ GeV. The lightly shaded rectangular region encloses the extrema of the pull means and their statistical uncertainties, showing that the range of bias on the pulls are within a few percent of the statistical uncertainties on the fit signal strengths. The dashed straight lines are meant only as visual guides, and are not to be treated as linear interpolations between signal strengths.

signal in the data CR slices with no signal injected. In case the QCD function is able to fit non-existent signals in a statistically significant way a systematic uncertainty needs to be introduced to cover that bias. The test was performed using all possible signals the analysis is considering: Z , Higgs boson and Z' signals. Two examples of such fits are shown in Figure 6.18 for spurious signal assumptions of a Z' with $m_{Z'} = 100$ GeV and $m_{Z'} = 200$ GeV. The statistical significance ($\mu_{\text{fit}}/\sigma_{\mu_{\text{fit}}}$, where μ_{fit} was the fitted signal strength and $\sigma_{\mu_{\text{fit}}}$ the corresponding uncertainty) of the fitted signals is 0.01 and -0.2.

The distribution of the pull, which corresponds to $\mu_{\text{fit}}/\sigma_{\mu_{\text{fit}}}$, was produced for different CR slices for the different signal hypotheses. The mean and RMS of these histograms are summarized in table 6.4. Given the statistical precision of the test (RMS), the deviations are compatible with 0. It's also observed that no trend is present in the data, i.e., the deviations do not seem to be dependent on the signal masses.

$\mu_{\text{fit}}/\sigma_{\mu_{\text{fit}}}$	Z	Higgs	Z' (100 GeV)	Z' (125 GeV)	Z' (150 GeV)	Z' (175 GeV)	Z' (200 GeV)
Mean	-0.2	0.16	-0.12	0.28	0.02	-0.38	0.32
RMS	0.82	0.77	0.65	0.71	0.80	0.70	0.87

Table 6.4 – Summary of spurious signal tests in CR slices for different signal hypotheses.

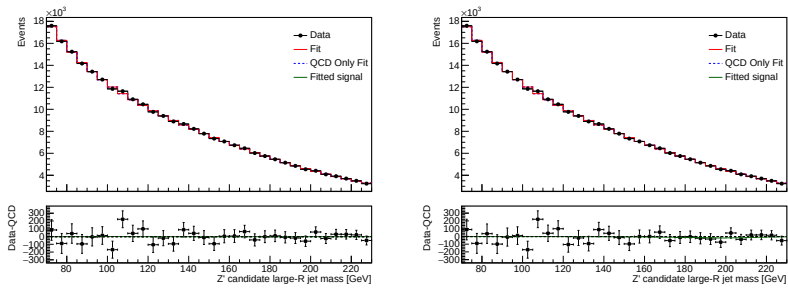


Figure 6.18 – QCD+ Z' signal fit to one CR slice. On the left, with a spurious signal assumption of a Z' with $m_{Z'} = 100$ GeV is used, while on the right, a Z' with $m_{Z'} = 200$ GeV is studied.

6.7 Systematic uncertainties

In the following, sources of systematic uncertainty are discussed. These can be related to experimental calibrations or procedures and to MC modeling of signal and background processes. The uncertainties contribute both to the overall yield and differential shape of the invariant mass distribution.

Given that the the background of this search is overwhelmingly dominated by the contribution from QCD multi-jet processes, which is estimated from data in contrast to contributions from other resonant backgrounds that are estimated using MC simulations, the discussion below is structured as follows:

- Uncertainties on QCD background;
- Uncertainties on resonant backgrounds and signal, further subdivided into:
 - Experimental uncertainties due to calibrations and procedures;
 - Theoretical uncertainties.

6.7.1 Uncertainties on the QCD multi-jet background

As already mentioned, the QCD background is estimated from data through a direct fit procedure. Similarly to the analysis presented in the previous chapter, there are two classes of systematic uncertainties associated with this method: the choice of the function to model the background and the uncertainty on the parameters of the fit. They are discussed in the following.

Uncertainty on the fitting function

The choice of the fitting function is not directly linked to QCD first principles and thus it comes with some arbitrariness. To cope with this, two functions were considered for the fit and the difference between the nominal function and an alternate function was taken as an estimate of the fitting choice uncertainty. The procedure used to evaluate this uncertainty is the same as the one described in Section 5.1.4.

Statistical Uncertainty on the fit

The uncertainty on the fit parameters is due to the finite size of the data set. Separate Nuisance Parameters (NP) were defined for each fit parameter. The variations for a given parameter were defined by setting it to ± 1 , ± 2 and ± 3 -sigma of its statistical uncertainty from the nominal fit, while keeping the other parameters constant. They were then used with a uniform prior in the limit setting procedure.

6.7.2 Uncertainties on resonant backgrounds and signals

In the following, the uncertainties on resonant backgrounds and signal which were simulated using MC techniques are discussed. After addressing experimental uncertainties due to calibrations, the theoretical uncertainties due to signal and background modeling are reviewed.

Large- R jet energy and mass scale and resolution

Systematic uncertainties for large- R jets are related to the variables that quantify the development of hadronic showers, where part of the energy is lost and needs to be corrected a posteriori. These features result in uncertainties on the Jet Energy Scale (JES) and Jet Mass Scale (JMS). The uncertainty on the calibration of the energy and mass scales of large- R jets make use of the R_{trk} approach where kinematic observables measured in the calorimeter are compared to those measured in the tracker and the residual difference between data and MC simulation represents a systematic uncertainty. A total of 4 Nuisance parameters were provided and used in the analysis:

- *Baseline*: base difference between data and PYTHIA8.
- *Modelling*: differences between different simulations, in particular PYTHIA8, HERWIG7 and SHERPA.
- *Tracking*: propagation of the tracking uncertainties used in the evaluation of the R_{trk} procedure.
- *TotalStat*: statistical uncertainty in the sample used for the evaluation of the R_{trk} procedure.

The effect on the estimation of the jet mass due to the finite experimental resolution of the calorimeter systems is named Jet Mass Resolution (JMR) uncertainty. A similar uncertainty affecting the p_T of the large- R jet was found to be negligible and will not be reported. The JMR uncertainty was estimated by smearing the invariant mass of the signal jet.

Figure 6.19 shows the effects of the JES, JMS and JMR for the SHERPA $Z+j$ sample. Similar results were obtained for the $t\bar{t}$ and Z' and Higgs boson signal hypotheses.

6.7.2.1 b -tagging uncertainties

The b -tagging uncertainties were parametrized with separate nuisance parameters for b -, c - and light-jets. In total, a set of 24 NP were provided. Figure 6.20 shows the effect of the three leading b -jet NPs applied to the $H+j$ sample taken as an example. It can be observed that only the overall normalization is shifted and thus the uncertainty was implemented as a normalization factor with the effect of all the different NPs summed in quadrature.

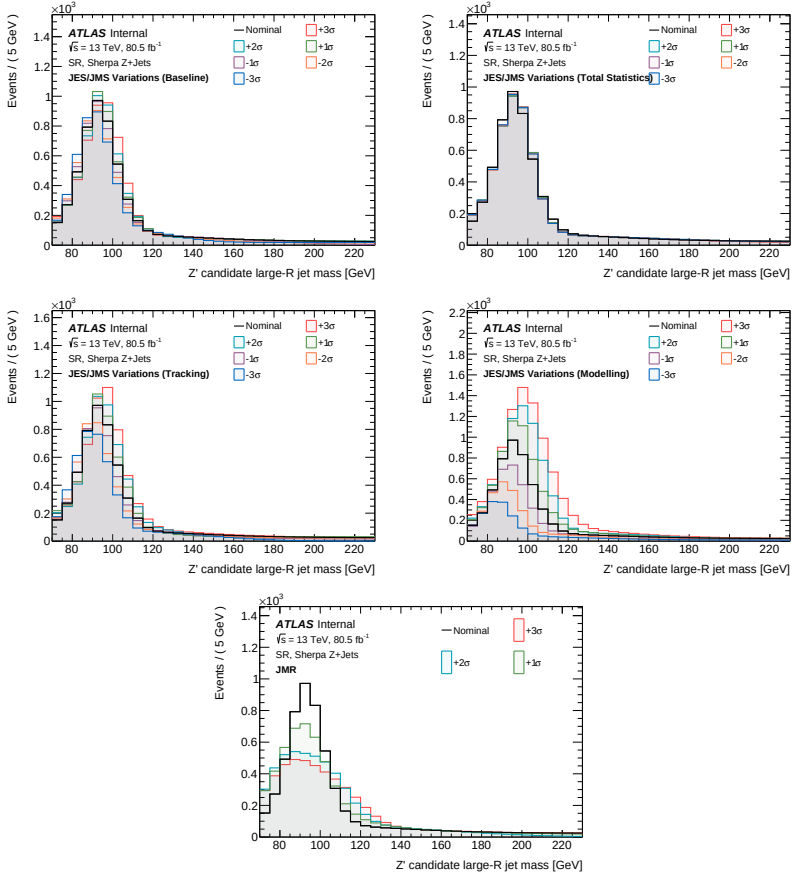


Figure 6.19 – Effects of the large-R jet systematic variations on the $Z+j$ SHERPA templates.

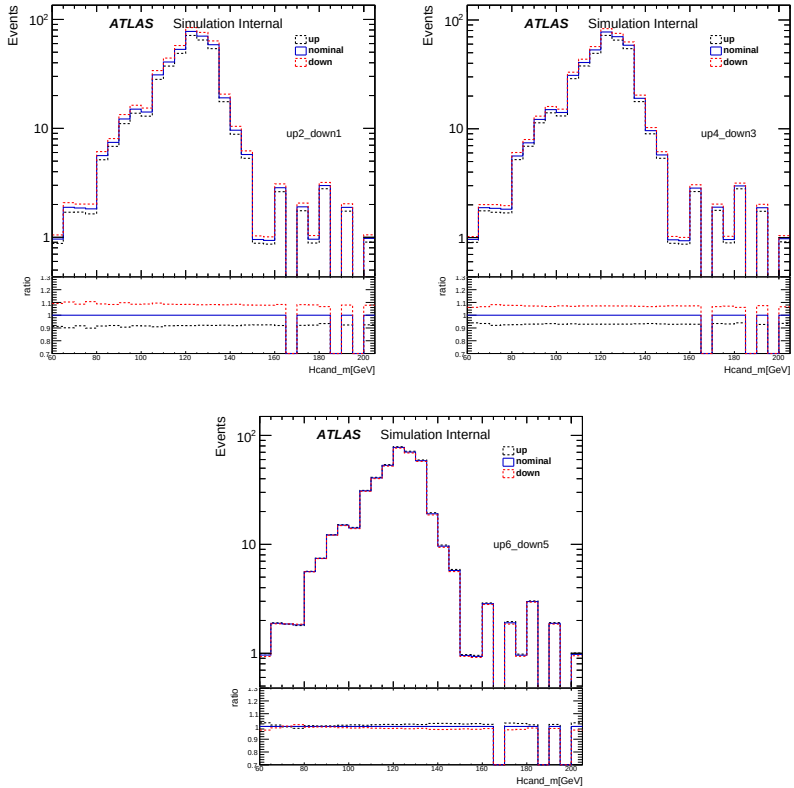


Figure 6.20 – Effects of the systematic variations of the three leading b -tagging NPs on the $H+j$ sample.

6.7.2.2 Luminosity uncertainty

The uncertainty in the integrated luminosity is 2.1% and it is derived using a similar procedure to what described in Section 5.1.4 and it is applied to all processes modeled using MC simulations.

6.7.2.3 Theoretical uncertainties for the signals

V+jets

To account for higher order NLO corrections to $Z/W+j$ processes, an uncertainty of 10 % is taken for electro-weak corrections and an additional uncertainty of 10 % is taken for QCD corrections [114]. This is a conservative approach which also account for PDF and scale variations. The sources of uncertainties are added in quadrature. This relatively large uncertainty is due to the lack of measurements of the differential cross-section of vector bosons at this high p_T regime.

Higgs boson + jets

The NLO correction is not available in ggF when requiring the loop to be resolved with finite top mass effects . An overall theoretical uncertainty of 30% is applied to the ggF $H \rightarrow b\bar{b}$ prediction [109]. The same uncertainty is also applied to the other production mechanisms. This conservative approach also takes into account PDF, renormalization and factorization scale uncertainties.

6.7.2.4 Uncertainty on $V+jets$ modeling

In order to allow for an extra degree of freedom in the shape of the $V+j$ mass peak, an additional nuisance parameter was added to the fit to account for differences seen in the mass shapes between $V+j$ SHERPA (nominal) and HERWIG (alternative) samples. The difference between the fitted signal template shapes is shown in Figure 6.21. The nuisance parameter implemented for this systematic uncertainty has a Gaussian prior, where 0 refers to a template equal to SHERPA, and 1 equal to HERWIG. Values below 0 and above 1 were not allowed as they lead to an unphysical $V+j$ template shape due to extrapolation.

6.7.2.5 Uncertainty on $t\bar{t}$ modeling

A similar approach was implemented to define a modeling uncertainty on the $t\bar{t}$ contribution. An extra nuisance parameter to account for differences seen in the mass shapes between $t\bar{t}$ POWHEG (nominal) and SHERPA (alternative) samples was added. The

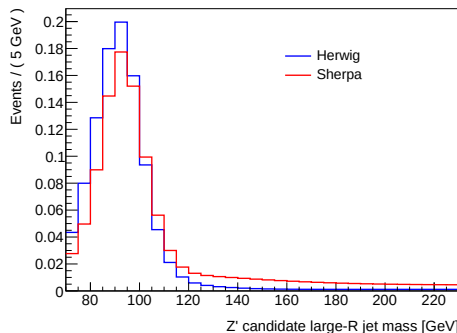


Figure 6.21 – Difference between shapes predicted for the $Z+j$ process from the SHERPA and HERWIG++ generators.

difference between the fitted signal template shapes is shown in figure 6.22. The nuisance parameter related to this systematic uncertainty had values from 0 to 1, where 0 refers to a template equal to POWHEG and 1 equal to SHERPA.

6.8 $t\bar{t}$ background estimation

Boosted $t\bar{t}$ events represent a significant background contribution in the SR, as described in section 6.8. Unfortunately, MC generators used at the time of this thesis were not able to properly predict the $t\bar{t}$ cross section, particularly in such an extreme kinematic phase space, as described in detail elsewhere [115]. For this reason, the $t\bar{t}$ yield in the SR was extracted from data. The scale factor was obtained by fitting the normalization of the $t\bar{t}$ MC template in a $t\bar{t}$ enriched control region (CR $t\bar{t}$ bar). This scale factor was multiplied by the yield of the $t\bar{t}$ MC template normalized according to its cross section in the SR. The scale factor uncertainty was then used as a gaussian prior on the $t\bar{t}$ yield in the SR.

6.8.1 $t\bar{t}$ enriched control region (CR $t\bar{t}$ bar)

The $t\bar{t}$ enriched CR uses the same method of selecting the signal candidate large-R jet as the other regions used in the analysis. As for the CR and the VR, two regions were defined by requiring zero or one b -tags in the two leading track jets of the signal candidate. The configuration with exactly one b -tag is the most natural definition of the $t\bar{t}$ control region, since it exploits the single b -quark in a top decay. This region was used to derive the Scale Factor (SF) used to constrain the $t\bar{t}$ yield in the SR. The alternative selection, referred to as CR $t\bar{t}$ bar0 in the following, was used to validate the extrapolation of the scale factor into the SR.

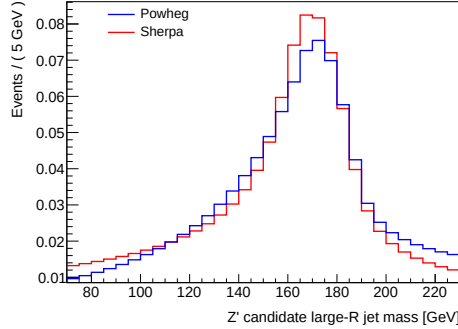


Figure 6.22 – Difference between shapes predicted for the $t\bar{t}$ process from the POWHEG and SHERPA generators.

In addition to the standard event selections, the sample was further purified in top events by requiring the muon from the semi-leptonic decay of the second top quark. The left plot of Figure 6.23 compares the $\Delta\phi(\text{muon, signal})$ distribution between the QCD and $t\bar{t}$ MC samples. The $t\bar{t}$ sample shows the expected back-to-back topology of the muon and a top-like signal candidate large-R jet, while muons in QCD events originate from hadrons decaying in flight and are thus produced close to the signal candidate. Therefore, a cut of $\Delta\phi(\text{muon, signal}) > \frac{2\pi}{3}$ reduced the QCD and $V+j$ contribution to the control region by several orders of magnitude while the $t\bar{t}$ component was reduced by roughly a factor of 3 as expected from $BR(W \rightarrow \mu\nu_{\mu})/BR(W \rightarrow l\nu_l) = \frac{1}{3}$.

To further reduce the QCD multi-jet contamination, a cut on the muon p_T was applied. The right plot of Figure 6.23 compares the muon p_T spectra between the QCD and $t\bar{t}$ MC before the $\Delta\phi(\text{muon, signal})$ selection. Muons from boosted W -boson decays reach higher p_T values compared to the softer QCD initiated muons. A cut of 40 GeV on the muon p_T was applied to eliminate QCD events.

The remaining contamination from $V(ll)+\text{jets}$ and VV events was reduced by requiring an additional b -tagged jet at 77 % b -jet efficiency to be close to the muon with $\Delta R(\text{jet, muon}) < 1.5$.

In summary, the $t\bar{t}$ enriched control region (CR $t\bar{t}$ bar) was defined by the following requirements:

- Signal candidate large-R jet with a single b -tagged VR track-jet;
- One muon that passes a loose isolation criteria, with $p_T > 40$ GeV and $\Delta\phi(\text{muon, signal}) > \frac{2\pi}{3}$ with respect to the signal candidate large-R jet;
- One extra large-R jet with a b -tagged leading VR-track jet with a $\Delta R(\text{jet, muon}) < 1.5$.

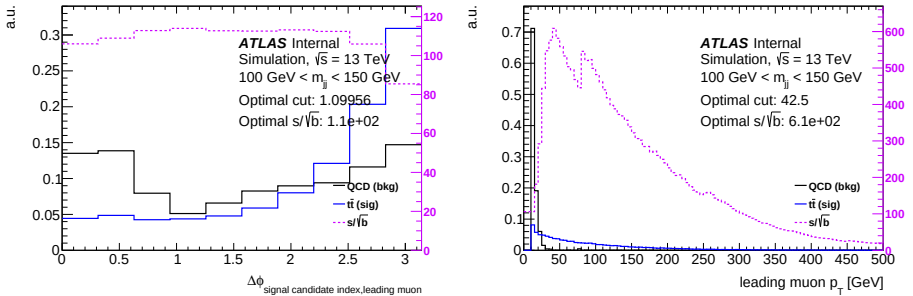


Figure 6.23 – Comparison of the two variables, $\Delta\phi(\text{muon, signal})$ and $\text{muon } p_T$ (right), between QCD multi-jets events and $t\bar{t}$ events. The selection requires exactly one b -tagged track jet in the signal candidate large- R jet. The magenta line shows the $s/\sqrt{b}$ significance at 80.5 fb^{-1} .

Region	scale factor	uncertainty
CRttbar0	0.87	0.12
CRttbar	0.84	0.11

Table 6.5 – The $t\bar{t}$ scale factors and their uncertainties from the two $t\bar{t}$ control regions.

6.8.2 Yield extraction

Finally, the $t\bar{t}$ template MC was fit to the data in the mass region $[70 - 230] \text{ GeV}$. The single top and $W \rightarrow l\nu$ templates were included in the fit, but their normalization was kept constant. The uncertainty was determined by running the Bayesian Analysis Toolkit (see section 6.9.1) with the large- R jet energy scale and resolution variations described in section 6.7.2 as nuisance parameters.

Figures 6.24 and 6.25 show the pre- and post-fit distributions in the two $t\bar{t}$ control regions as well as the pull distributions of the respective fits. The pulls were extracted from the posterior distribution of the NPs as detailed in the next section. The pulls related to the JES and JMR uncertainties are centered at zero, as expected, but more tightly constrained. This is due to the ability of constraining NPs using a signal peak³. A SF of 0.84 ± 0.11 was found for the CRttbar, showing that the MC overestimates the $t\bar{t}$ yield at high transverse momentum, in agreement with other measurements [115]. This factor was used to constrain the $t\bar{t}$ contribution in the final fit to the SR. The SF of the CRttbar0 is shown in Table 6.5 and was found to be consistent with the CRttbar SF.

³In general, these constraints needs to be careful evaluated. At the time of the analysis, these NPs were poorly understood and a constraint of around 20 % using a signal peak was thus allowed.

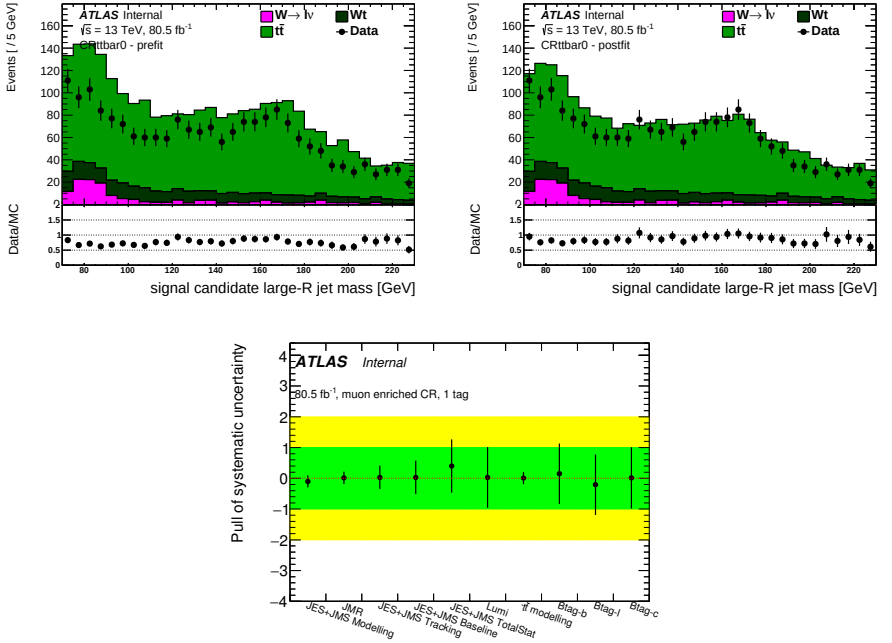


Figure 6.24 – The pre-fit (left) and post-fit (right) data/MC comparison when fitting the CRttbar0. Pull distributions of the nuisance parameters are also shown.

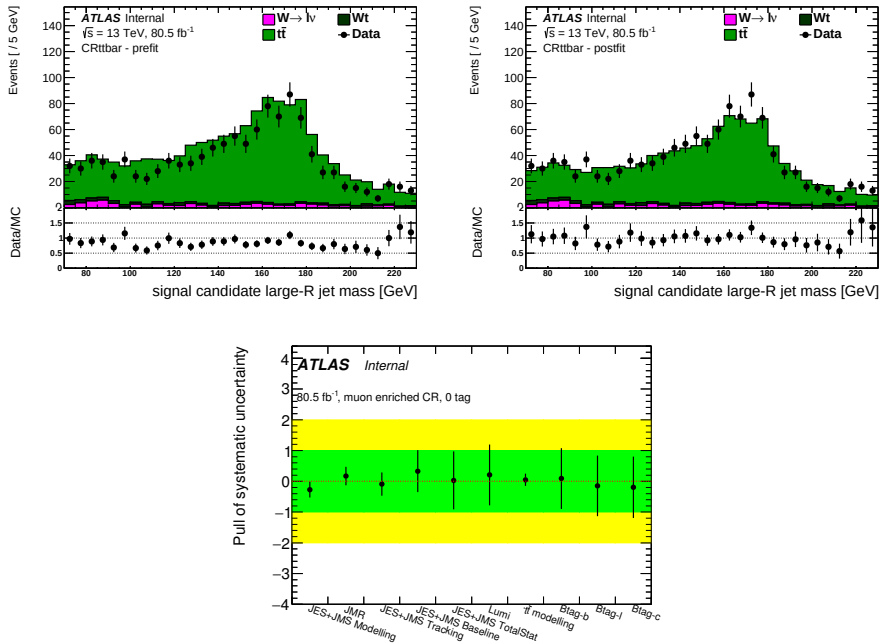


Figure 6.25 – The pre-fit (left) and post-fit (right) data/MC comparison when fitting the CRttbar. Pull distributions of the nuisance parameters are also shown.

6.9 Statistical analysis

This section describes the statistical procedure employed in order to search for SM (W/Z and Higgs bosons) and beyond SM signatures and to quantify their significance or set a 95% Credibility Level (CL) limit on the cross section times acceptance times branching ratio, $\sigma \times A \times BR$.

As discussed in the previous chapter, the first step needed to search for new physics signals is the background-only fit. To properly take into account the Look-elsewhere effect (LEE) effect, the Bump-Hunter (BH) algorithm was used, as already done for the analysis presented in the previous chapter. However, additional complications arise compared to that analysis due to the presence of resonant backgrounds in the invariant mass spectrum. Given that the shapes of $V+j$ and $t\bar{t}$ may be potentially mis-modeled in data and that the BH algorithm only takes into account statistical uncertainties, the background-only fit quality could be reduced by these effects and not by a genuine signal peak originating from new physics beyond the standard model. To cope with this challenge, a first fit was run accounting only for the $V+j$, $t\bar{t}$ and QCD components. The post-fit shapes of the resonant models were then used in the BH fit.

Given no deviation from the background-only model, the limit-setting phase is employed. During the limit-setting phase, a single fit was performed to compute the 95 % exclusion limits of the Z' signals or to measure the W/Z and Higgs boson cross-sections.

This section is organized as follows: Section 6.9.1 describes the Bayesian Analysis Toolkit and the general statistical interpretation of the results, while the search procedure using BumpHunter is described in Section 6.9.2.

6.9.1 Bayesian Analysis Toolkit

The statistical analysis was performed using the Bayesian Analysis Toolkit [116]. The main advantage of the Bayesian interpretation compared to the frequentist one is to access the probability of a parameter of interest given the data. This is done thanks to the Bayes theorem:

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \quad (6.6)$$

where $P(B|A)$ is the conditional probability of event B occurring, given that event A has occurred, $P(A)$ is the probability of event A occurring, and $P(B)$ is the probability of event B occurring. In the case of particle physics experiments, and in particular for searches or cross-section measurements, A is usually the number of events in the SR and B are the data used to perform the measurement. In this view, $P(B|A)$ is the likelihood $L(data|\mu, \theta)$, $P(\mu, \theta)$ is the a priori probability of the parameter of interest (μ) and systematics uncertainties (θ), also called *priors* and $P(B)$ is a normalization factor which is usually complicated to compute analytically. The choice of the *prior* is

the delicate part in Bayesian statistics. In the context of this analysis, a flat probability distribution was used for the Higgs boson, $V+j$ and Z' cross-sections. For what regards the nuisance parameters controlling the systematic uncertainties, a gaussian prior centered at 0 with a width of 1 was chosen. The number of events in the $t\bar{t}$ sample was also constrained using a gaussian prior centered at the number of events extracted in the CRttbar and with a width taken from the related uncertainty from that estimation.

The *posterior* distribution was used to quantify the significance of $V+j$ and to set limits on $H+j$ and Z' models. The form of Bayes Theorem utilized to obtain the posterior distribution, $p(\mu|\text{Data})$, is defined as:

$$p(\mu|\text{Data}) \propto \int \mathcal{L}(\text{Data}|\mu, \theta) \pi(\mu) \prod_i \pi(\theta_i) d\theta, \quad (6.7)$$

the multi-dimensional integral over the nuisance parameters, θ , is referred to as marginalization. This equation can be interpreted as follows: the prior knowledge or belief of the analyser, encoded in the priors $\pi(\mu)$ and $\pi(\theta_i)$, is updated by the outcome of the experiment, encoded in the likelihood $\mathcal{L}(\text{Data}|\mu, \theta)$, in order to obtain the marginalized posterior $p(\mu|\text{Data})$.

In Bayesian marginalization, the parameters of interest, μ , correspond to the normalization of the $V+j$ and $H+j$ signal templates that were extracted simultaneously from a single fit. One nuisance parameter is introduced for each of the systematic uncertainties described in the previous section. A Markov Chain Monte Carlo (MCMC) engine is then used to perform the marginalization over the nuisance parameters. The NPs were treated as correlated between the different signals. This helps in constraining some of the parameters as already observed in the fit in the $t\bar{t}$ control region.

An example of the fit results is shown in Figure 6.26. The Figure depicts the posterior distributions from one of the control slice where a $Z+j$ signal was injected while a Z' signal was not injected but searched for. For the Z' signal, the most probable value in the distribution is around 300 events with a significance from zero of around 0.7σ indicating a small excess compatible with a statistical fluctuation, as expected. The 95 % percentile of that distribution gives the observed exclusion limit at 95 % CL. The $Z+j$ distribution, instead, show a clear peak around the number of injected events, where the mode of the distribution together with its relative shifts define the number of measured events and its uncertainty. Expected limits and cross-sections are found by fixing the number of expected events to the SM prediction (0 for exotic signals). The obtained distributions after marginalization were then used to generate pseudo-experiments. A distribution of re-fitted values was produced, where the mean of that distribution represents the expected value of the parameter of interest and the deviations from the mean define the uncertainty bands of the exclusion limits.

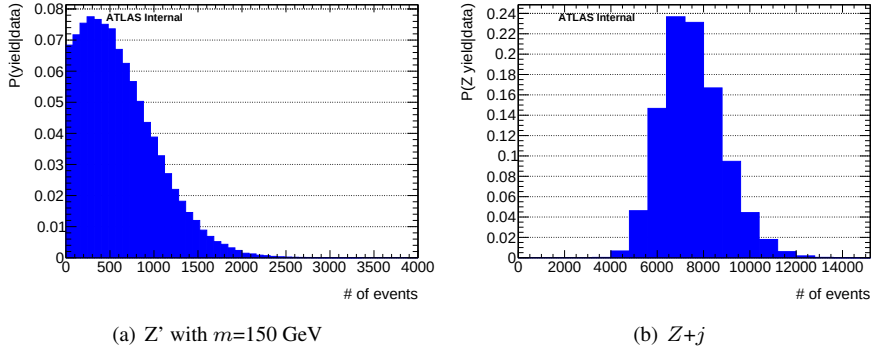


Figure 6.26 – Marginalized posterior distributions from a fit to one of the CR slices for a Z' at 150 GeV and the $Z+j$ processes. No Z' signals were injected whereas 7000 $Z+j$ events were injected for this test. Note the difference in the scale of the x -axis in the two plots.

6.9.2 Search using BumpHunter

The BumpHunter algorithm was used to establish the presence or absence of additional resonances either from $H+j$ or from new physics phenomena. A description of the algorithm was already given in section 5.1.5. It is briefly repeated here to facilitate reading. The algorithm operates on the binned spectrum, comparing the background estimate with the data in mass intervals of varying contiguous bin multiplicities. Starting with a two-bin signal window, the algorithm scans across the entire distribution. For each point in the scan, the significance of the difference between the data and the background is computed. The most significant departure from the smooth spectrum is defined by the set of bins that have the smallest probability of arising from a Poisson background fluctuation. During this procedure, the background model is not changed or refit to the data outside of the excluded region. The LEE is properly taken into account by performing a series of pseudo-experiments drawn from the background estimate to determine the probability that random fluctuations in the background-only hypothesis would create an excess anywhere in the spectrum at least as significant as the one observed.

Given the presence of resonant background processes such as $t\bar{t}$, the BumpHunter algorithm is unable to search for new physics around the peak of the top quark mass. To cope with this, the $t\bar{t}$ yield was constrained with a gaussian term using the scale factor derived from the dedicated CR (see section 6.8.1). Due to the fact that the $V+j$ yield is extracted from the fit itself, exotic signals are searched for in the mass region between 100 to 200 GeV.

6.10 Results

Results are first presented for the search of DM particles. The search for boosted Higgs bosons is then discussed.

Dark matter search

A background-only hypothesis is tested on the invariant mass spectrum of the signal candidate. The effect of the Higgs boson with a SM strength is smaller than the expected uncertainty on the Z' limit and is therefore neglected. The BH algorithm was used to estimate the p -value. Figure 6.27 shows the fit to the data in the SR. The largest deviation from the background was found at around the Higgs boson mass of 125 GeV, although with a small statistical significance. The corresponding global p -value was found to be 0.54 and thus in agreement with the background-only hypothesis.

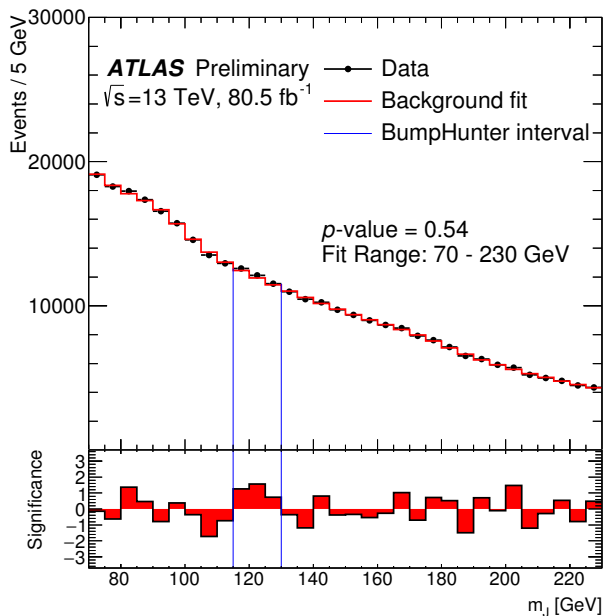


Figure 6.27 – The reconstructed mass distribution m_j with the event reconstruction and selection as described in the text. The solid red line depicts the background prediction, consisting of the non-resonant di-jet, $V+j$ and $t\bar{t}$ processes. The vertical blue lines indicate the most discrepant interval identified by the BH algorithm. Without including systematic uncertainties, the probability that fluctuations of the background model would produce an excess at least as significant as the one observed in the data anywhere in the distribution, the BH p -value is 0.54. The low panel shows the bin-by-bin significance of the difference between the data and the fit, considering only statistical fluctuations [4].

Credibility-level limits at 95% were set on the Z' signals with masses between 100 and 200 GeV. These limits are shown in Figure 6.28, in terms of cross section times acceptance times efficiency. The exclusion limits as a function of the coupling parameter that controls the coupling of the DM mediator to quarks, g_q , can be obtained by scaling the cross-section by g_q^2 and is shown on the right plot of the same Figure. A worsening of the limits in the low and high mass regions is observed. For the mass point at 100 GeV, this is due to the vicinity of the $V+j$ peak, while the presence of the top-peak degrades the limits at high masses. A more detailed description of the effect of the systematic uncertainties on the exclusion limits is given in the next section.

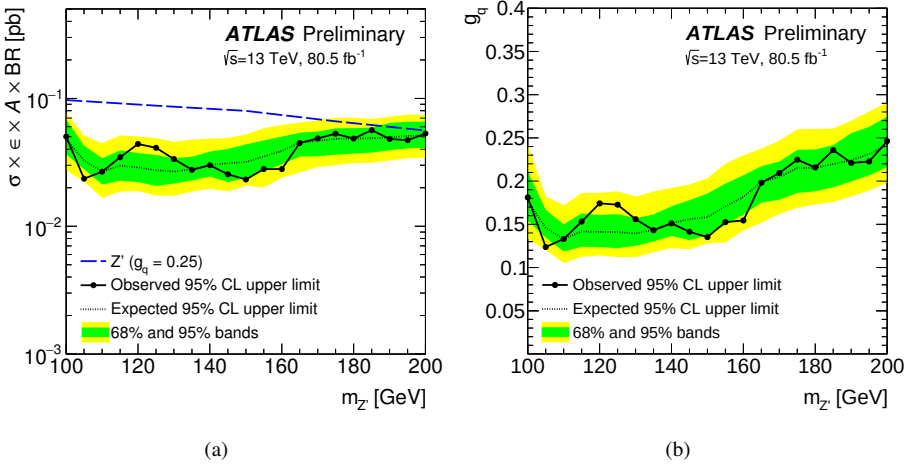


Figure 6.28 – The 95% credibility-level upper limits obtained from the invariant mass distribution on (a) the cross-section times acceptance times branching ratio times efficiency for the DM Z' model and on (b) the g_q parameter that controls the coupling between the DM mediator and SM particles [4].

Boosted Higgs boson search and evidence of $V+j$.

The post-fit invariant mass plot for the Higgs boson search strategy is shown in Figure 6.29. A clear peak corresponding to the $V+j$ process is observed. A peak at 125 GeV is also visible. The data/MC agreement under the top peak shows good compatibility, giving confidence about the validity of the $t\bar{t}$ estimation technique.

The observed signal strength for the $V+j$ process is $\mu_V = 1.5 \pm 0.22(\text{stat.})_{-0.25}^{+0.29}(\text{syst.}) \pm 0.18(\text{th.})$, corresponding to a significance of 5 standard deviation. This is the first evidence at the ATLAS experiment of the yield of vector bosons in final states featuring bottom quarks in the boosted regime. The measurement is dominated by the systematic

uncertainties, mostly due to the low lever-arm of the fit which enhances the correlation between the systematic variation of the $V+j$ template and the parameters used to describe the QCD multi-jet background.

For the $H+j$ process, the observed signal strength is $\mu_H = 5.8 \pm 3.1(\text{stat.}) \pm 1.9(\text{syst.}) \pm 1.7(\text{th.})$, consistent with the background-only hypothesis at 1.6σ . In contrast to the measurement of the $V+j$ process, the extraction of the $H+j$ yield is still statistically limited, and the statistics-only significance is around 2.0σ from the background-only hypothesis. The number of σ expected by the SM was found to be 0.28. The $H+j$ and the $V+j$ components were extracted simultaneously from a single fit, and the corresponding combined credibility levels of μ_V and μ_H are shown in Figure 6.30. As outlined in the plot, the signal strength predicted by the standard model is well contained within the 2σ uncertainty bands. The largest source of systematic uncertainty is the theoretical uncertainty which is due to lack of higher-orders computation of the ggF production mechanism with finite top mass effects.

The marginalized posterior distribution of the nuisance parameters are shown in Figure 6.31. The fit slightly favors the HERWIG template for the $V+j$ process and the Sherpa template for the $t\bar{t}$ process. The JMR and the modeling component of the JMS and JES systematics were constrained up to about 20 % with good compatibility with the results obtained in the fit to the muon enriched control regions where it was shown that these uncertainties can be constrained using resonant signal peaks. The other components of the JES and JMS uncertainties such as *TotalStat* and *Tracking* show non gaussian shapes. This was found to be due to a problematic interpolation of the templates in between the nuisance parameters. However, these uncertainties components have negligible impact on the results and thus can be safely neglected.

The impact of each systematic uncertainty is shown in Table 6.6. This impact is defined as the difference in quadrature between the uncertainty on the signal strength σ computed when all other uncertainties are considered and when they are fixed to their post-fit values. The total systematic uncertainty is then defined as the difference in quadrature between the total uncertainty on μ and the total statistical uncertainty, denoted as $\sqrt{\Delta\sigma^2}$ in the table. The largest impact is due to the JMR, which, despite being constrained on the resonant peaks, is largely correlated or anti-correlated to the parameters of the fit due to the short lever-arm of the fit. This is shown in Figure 6.32 where the correlations between each nuisance parameter of the fit are depicted. Similar conclusions can be drawn for the JES and JMS, and, in particular, for the modeling component which also contributes significantly to the uncertainty on the $V+j$ and $H+j$ signals. Finally, it is worth noticing that the alternative QCD functional form uncertainty becomes relevant for high masses, especially for Z' models at the tail of the invariant mass distribution, where the statistical power of the data is lower and the fit is more sensitive to the choice of the fit function. At high masses, the $t\bar{t}$ scale-factor also plays a significant role, as expected.

		Impact on Signals ($\sqrt{\Delta\sigma^2}/\mu$)			
Source	Type	V+jets	Higgs	Z' (100 GeV)	Z' (175 GeV)
Jet energy and mass scale	Norm. & Shape	15%	14%	23%	18%
Jet mass resolution	Norm. & Shape	20%	17%	30%	20%
$V + j$ modeling	Shape	9%	4%	4%	< 1%
$t\bar{t}$ modeling	Shape	< 1%	1%	< 1%	11%
b -tagging (b)	Normalisation	11%	12%	11%	15%
b -tagging (c)	Normalisation	3%	1%	3%	5%
b -tagging (l)	Normalisation	4%	1%	4%	7%
$t\bar{t}$ scale factor	Normalisation	2%	3%	2%	58%
Luminosity	Normalisation	2%	2%	2%	3%
Alternative QCD function	Norm. & Shape	4%	4%	3%	17%
W/Z and QCD (Theory)	Normalisation	14%	—	—	—
Higgs (Theory)	Normalisation	—	30%	—	—

Table 6.6 – Summary of the impact of the main systematic uncertainties on the uncertainty σ on the measurement of the signal strength μ for the $V+j$, $H+j$ and Z' signals. The most significant systematic uncertainty for each process are outlined [4].

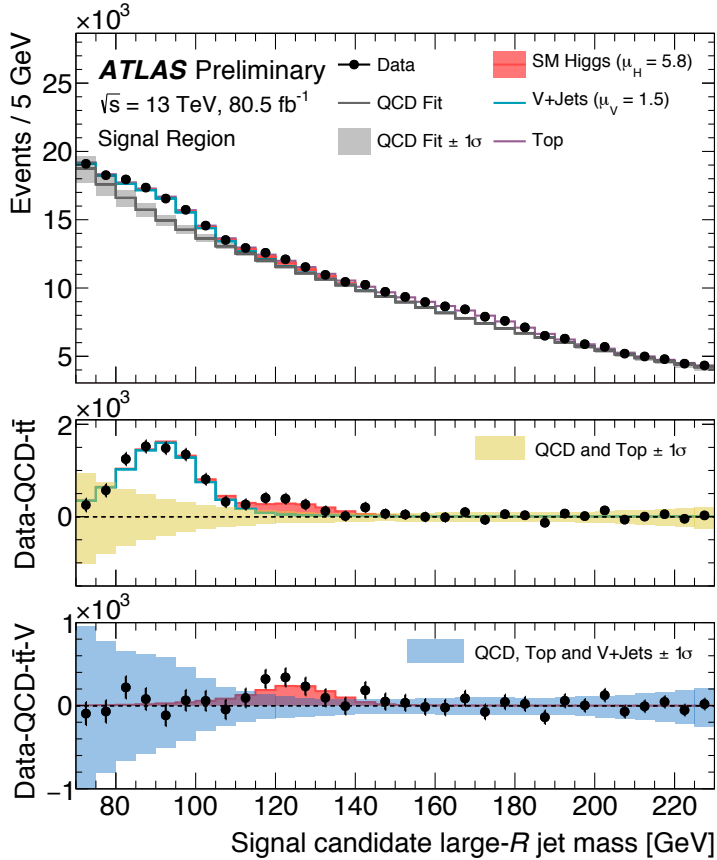


Figure 6.29 – Postfit plot of the SM Higgs boson, $V+j$, $t\bar{t}$ and QCD fit as compared to the data. The middle panel shows the post-fit and data distributions with the QCD and $t\bar{t}$ components subtracted. The lower panel shows the same distributions when also the $V+j$ component is subtracted [4].

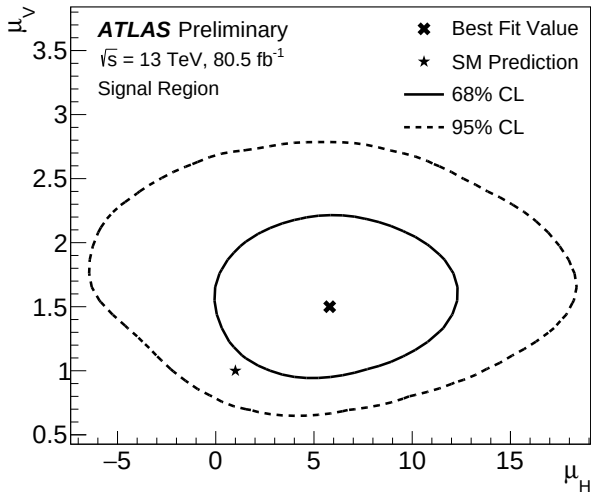


Figure 6.30 – Combined probability distribution of μ_H and μ_V from the SR fit [4].

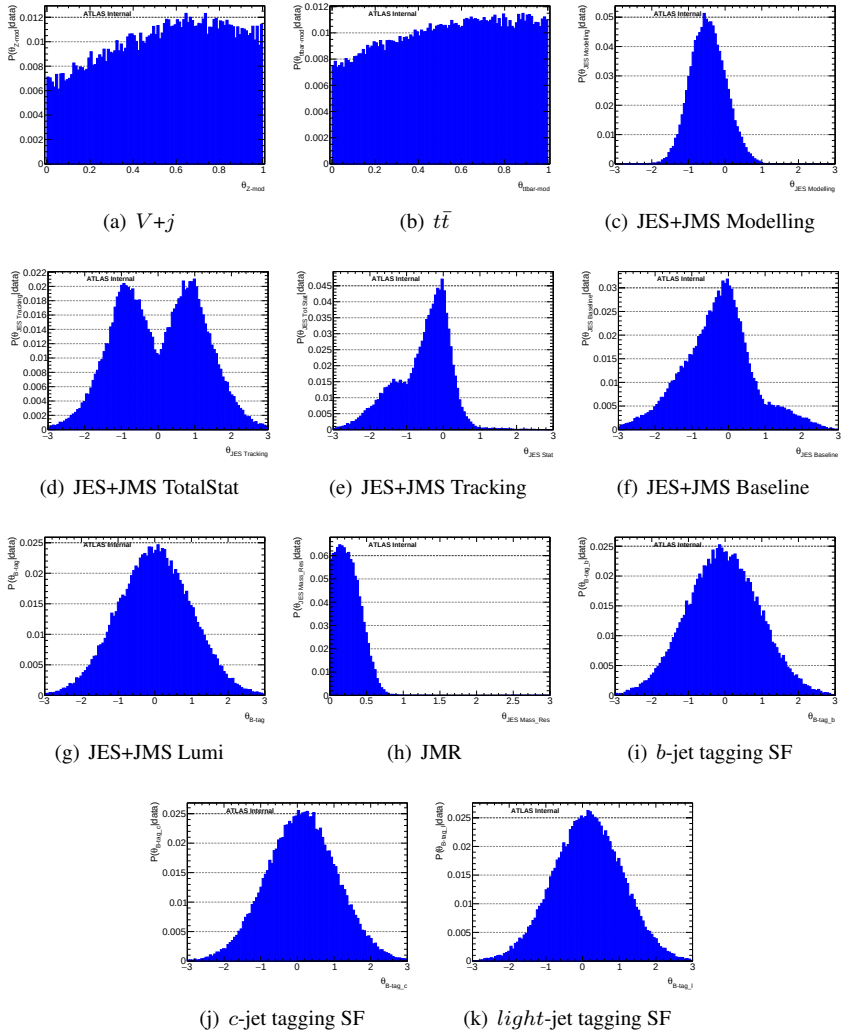


Figure 6.31 – Marginalized posterior of the nuisance parameters used in the fit of the $H+j$ search.

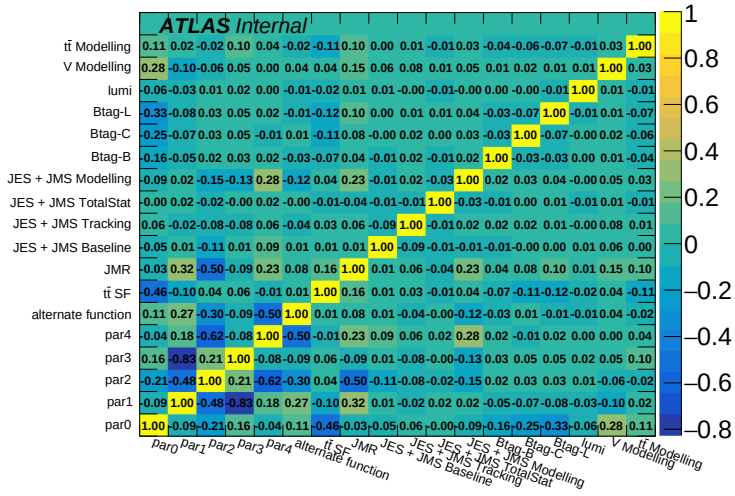


Figure 6.32 – Correlation matrix of the nuisance parameters considered in the fit of the $H+j$ search.

Summary

Two analyses featuring challenging b -tagging conditions have been presented and discussed in this and the previous chapters. A search for heavy resonances decaying to a back-to-back pairs of b -quarks and a search for boosted Higgs bosons decaying into b -quark pairs in a dense environment. The performance of the b -tagging algorithms and their related uncertainties are the essential ingredient for both these analyses. The expected limits of the heavy resonance search were improved by approximately a factor of 2.5 thanks to novel b -tagging algorithms. The search for boosted Higgs bosons provided a measurement at a significance of 5σ for $V+j$ in $b\bar{b}$ final states. The $H+j$ process was also searched for, an excess compatible with the background-only hypothesis with a sensitivity of 1.6σ was observed. The latter measurement is currently limited by the statistical uncertainty. At the HL-LHC, where the integrated luminosity will be increased to 3000 fb^{-1} , analyses looking at differential measurements of the Higgs boson transverse momentum will become one of the leading measurements of HEP experiments. As already mentioned, the differential cross-section of the Higgs boson not only probe the Yukawa coupling at the highest energy regime accessible at the LHC but it also serves as a tool to search for new physics. The luminosity reach at the HL-LHC will enable measurements of these distributions. However, this high luminosity poses unique experimental challenges. For example, the detectors will be exposed to unprecedented levels of radiation damage. The pixel layers of the ATLAS tracking detector, in particular, will have to sustain the largest amount of radiation due to its vicinity to the interaction point. In the following chapters, the impact of radiation damage on silicon detectors will be introduced and a new pixel technology based on the CMOS manufacturing process will be presented along with its characterization at radiation levels expected at the HL-LHC.

Principles of silicon detectors

Silicon detectors have found a broad field of applications during the last decades as particle detectors. The first experiments which used a silicon-based tracker were the CERN's NA11 and NA32 [117]. Since then silicon detectors have been widely used in high energy physics experiments. Thanks to their high granularity, fast time response, radiation-hard properties and relatively low-cost, they are ideal candidates to build large tracking detectors in multi-purpose experiments. In this chapter the detection mechanisms used in semi-conductor detectors will be outlined with emphasis on their ability to cope with the unique environment provided by the LHC and its upgrade, the HL-LHC.

7.1 Semi-conductor detectors

The dynamics of free charge carriers in semi-conductors are modeled by means of forbidden bands in the energy domain. The periodic structure of the crystal lattice allows to describe the electrons of the silicon atoms in a band structure with forbidden zones, the so called band-gaps. A schematic representation of the energy bands is shown in figure 7.1. The valence band is defined as the highest accessible electron energy range at a temperature at absolute zero. Similarly, the conduction band is the lowest unfilled band at 0 K [118]. If an electron in the valence band acquires an energy greater than the height of the band-gap, it passes to the conduction band where it is free to move through the lattice. The missing electron in the valence band is modeled as an effective particle with positive charge, referred to as *hole*. Semi-conductor detectors exploit the band structure of the material by collecting the electron-hole (e - h) pairs produced by the

interaction with a traversing particle through ionization. The minimal amount of energy to create an electron-hole pair is however larger than the band-gap of the silicon, as it is $\epsilon = 3.6 \text{ eV}$ [119].

The Fermi-Dirac statistics is used to describe the density of electrons and holes:

$$n_i = \frac{g_i}{1 + e^{\frac{E_f - \mu}{kT}}} \quad (7.1)$$

where g_i is the degeneracy factor of the energy state, μ is the Fermi-Dirac quasi-energy and E_f is the fermi energy, the highest occupied energy level at zero temperature.

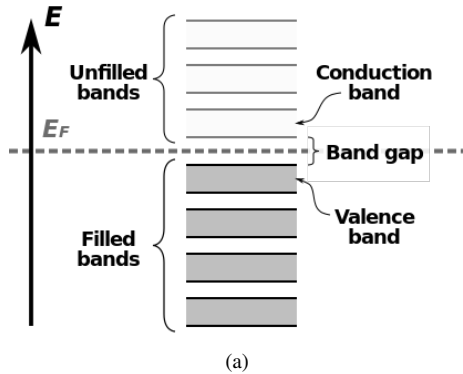


Figure 7.1 – Semiconductor band structure at zero temperature where no thermal excitation is present. The valence band is the last filled energy range and the conduction band is the first unfilled energy range. The band-gap is the difference between the two bands, in this region no free carriers are present.

It is possible to implant impurities in the device in order to change its electrical properties. These are atoms from the third and fifth group, usually boron and phosphorus. The latter, usually referred as donors, introduce valence electrons. While the former, called acceptors, introduces holes. Silicon doped with donors is called *n*-material. Similarly, silicon doped with acceptors is called *p*-material. When a *p*-doped semiconductor and a *n*-doped one are put into contact, a *pn*-junction is formed. The concentration difference of the free charge carriers leads to diffusion between the interface. The majority of charge carriers from one side diffuse into the other doped side where recombination occurs thus creating a region depleted of free-carriers, the depletion zone. Due to the leftover acceptor and donor ions implants, the depleted region is electrically charged. The remaining electric field (referred as built-in electric field) counteracts further diffusing carriers so that an equilibrium is reached. The length of the depleted region can be tuned using an external biasing voltage. In particular, when the negative terminal is connected to the *p*-material, as shown in figure 7.2, the holes and electrons are pulled away from the depletion zone. In such conditions the junc-

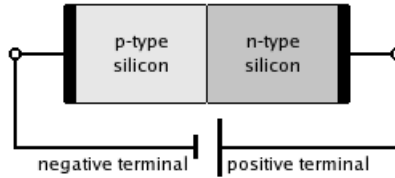
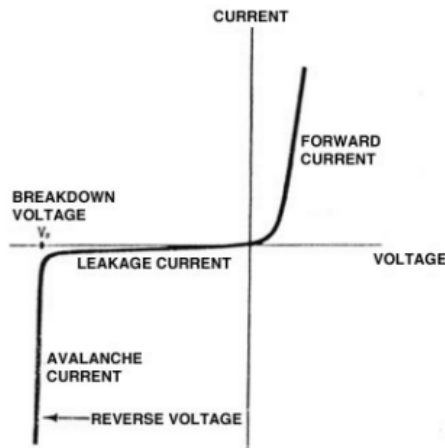


Figure 7.2 – A reversed biased diode.

tion is reversely biased and the width of the depletion increases. The maximum voltage that the silicon can tolerate while keeping the current across the diode low is called the breakdown voltage. If instead the voltage is supplied with opposite polarity, such that it exceeds the built-in potential, a net flux of current is favored. The typical current-voltage (IV) characteristic for a diode is depicted in Figure 7.3.



(a)

Figure 7.3 – A typical diode IV characteristic. Three main region are present as a function of the applied voltage. If the polarity of the external voltage opposes the built-in potential, a electric current through the pn-junction is observed (forward current). For negative bias voltage the depletion region acts as an insulator, however charge carriers can be thermally activated contributing to the leakage current. When the reverse bias voltage exceeds the breakdown voltage, an abrupt increment of the reverse current is observed.

It can be shown that the solution of the Poisson equation under the assumption that donors and acceptors are completely ionized is given by [20]:

$$W(V) = x_p + x_n = \sqrt{\frac{\epsilon_0 \epsilon_{Si}}{e} \left(\frac{1}{N_A} + \frac{1}{N_D} \right) (V + V_{bi})} \quad (7.2)$$

where:

- W is the width of the depletion zone
- N_A and N_D are the acceptor and donor concentrations. These values are linked to the resistivity of the material through the relation: $\rho = \frac{1}{q(\mu_n n + \mu_p p)}$ where ρ is the resistivity, $\mu_{n/p}$ the electrons and holes mobility. In the case of heavily doped material $N_{A(D)} \approx p(n)$ such that the previous relations can be simplified to: $d \propto \sqrt{\rho V}$
- V_{bi} is the built-in voltage and represents the voltage which is intrinsically formed at the pn-junction without an external biasing voltage.

The $e-h$ pairs created by the interaction of a traversing particle can be easily collected when produced within the depleted region. It is therefore desirable to operate the detector with the largest depletion depth possible. This is achieved by increasing the biasing voltage in reverse mode while keeping it below breakdown. The optimal voltage working point for a stable operation of the detector is therefore a compromise between a large depletion zone and the breakdown voltage. Such a point of operation depends heavily on the choice of technology and it is one of the most important parameters in the operation of silicon detectors.

A pixel sensor is, in summary, a reversely biased pn -diode with a highly segmented cathode or anode. A schematic cross-section outlining the main feature of a single pixel detector is shown in Figure 7.4.

7.2 Signal generation

7.2.1 Particle interaction with matter

Charged particles moving through matter interact with the electrons in the material. The mean energy loss due to ionization (also called stopping power) is given by the Bethe-Bloch formula [120]:

$$\left\langle -\frac{dE}{dx} \right\rangle \frac{1}{\rho} = K z^2 \frac{Z}{A} \Phi(\beta) (1 + \nu) \quad (7.3)$$

$$\Phi(\beta) = \frac{1}{\beta^2} \left(\frac{1}{2} \ln \frac{2m_e c^2 \beta^2 \gamma^2 T_{max}}{I^2} - \beta^2 - \frac{\delta}{2} \right) \quad (7.4)$$

Where:

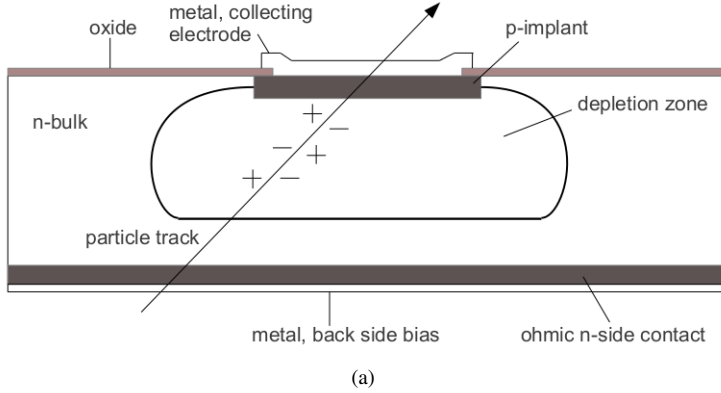


Figure 7.4 – Schematic cross section of a pixel detector. In this example the pn-junction is formed by an n-doped substrate and a heavy p-doped layer. The generated signal is collected through the p-layer. The bias voltage is applied at the backside metal contact. A heavy n-doped layer is needed to form an ohmic contact with the metal avoiding a direct metal-semiconductor contact. The oxide is needed to insulate the silicon.

- K is a fundamental constant equal to $4\pi N_A r_e^2 m_e c^2$
- z : charge of the traversing particle
- ρ : mass density of the absorbing medium
- δ : density correction due to the polarization of the atoms by the electric field of the traversing particle
- $\beta = v/c$: velocity of the traversing particle and $\gamma = \frac{1}{\sqrt{1-\beta^2}}$
- I : mean excitation energy
- T_{max} : maximum energy transfer possible in a single collision
- ν : higher order correction $\mathcal{O}(z^3, z^4, \dots)$

The previous equation results from a calculation to the lowest non-vanishing order of the Born approximation in the interaction between the incident particle and the atomic electrons. It describes the mean rate energy of energy loss in the region $0.1 \lesssim \beta\gamma \lesssim 1000$ with an accuracy of a few percent. At low energy of the traversing particle (for copper $\beta\gamma \sim 0.3$), i.e. at particle velocities comparable to those of outer atomic electrons, higher-order corrections become significant. At high energies (for copper $\beta\gamma \sim 100$) radiative corrections which result from the multiple virtual emission of photons by the incident particle become significant [20], at even higher energy ($\beta\gamma \sim 1000$)

they represent the dominant process in the energy loss mechanism. Figure 7.6 shows the stopping power as a function of $\beta\gamma$. As evident from the figure, the function is characterized by broad minima. In most practical cases the incident particles have a mean energy loss close to those minima and are therefore called minimum-ionizing particles or briefly "mip" [20].

The energy loss of a particle passing through matter is subject to statistical fluctuations. For a sensor of moderate thicknesses the energy loss probability distribution is described by the Landau-Vavilov distribution [121, 122]. The Bethe-Bloch equation describes the mean of such a distribution. However, due to its long tail the mean differs from the most-probable value. The latter can be expressed as:

$$\Delta_p = \xi \left[\ln \frac{2mc^2\beta^2\gamma^2}{I} + \ln \frac{\xi}{I} + j + \beta^2 - \delta \right] \quad (7.5)$$

where $\xi = K/2 \langle Z/A \rangle x/\beta^2$, x is the detector thickness and j is a unitless constant $j = 0.20$ [119]. The Landau-Vavilov distribution is shown in figure 7.6 for different thickness of the material. The tail of the distribution is due to the so called δ -electrons, where the incident particle transfers enough energy such that the electron itself produces secondary ionization. In reality, because of the finite resolution of the detector, the collected electrons distribution is a convolution of a Landau-Vavilov and a Gaussian.

7.2.2 The Ramo theorem

The instantaneous charge Q induced at the collecting electrode by the movement of the charge carriers is given by the Shockley-Ramo theorem:

$$Q_k = \sum_{n=1} q_i \phi_k(\vec{r}_{i_f}) - \sum_{n=1} q_i \phi_k(\vec{r}_{i_0}) \quad (7.6)$$

Where $\vec{r}_{i_0}$ and $\vec{r}_{i_f}$ are the initial and final position of the carrier, $\phi_k(\vec{r}_{i_f})$ is the "weighting potential" (also called *Ramo* potential) obtained by raising the electrode under consideration to unit potential, setting all others to zero, and solving the Poisson equation [119]. The theorem is based on the concept that current induced in the electrode is due to the instantaneous change of electrostatic flux lines which end on the electrode. The previous equation can be integrated to get: $i = qE_w v$, where v is the instantaneous velocity of the carriers and E_w the component of the "weighting electric field" in the direction of v . Given that the velocity of the carriers is directly proportional to the induced current, it is important to discuss the transport mechanism of free carriers in silicon to understand how it influences the collected signal.

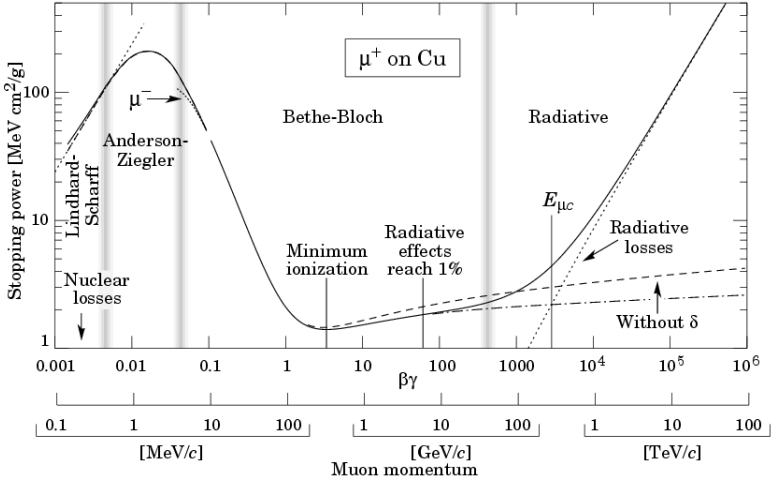


Figure 7.5 – Stopping power for a muon in copper as a function of $\beta\gamma = p/Mc$ [20].

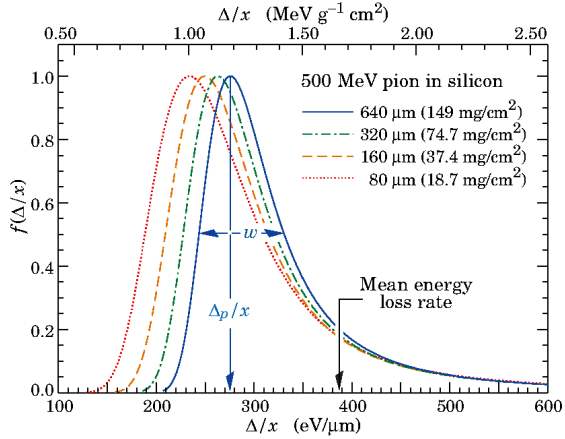


Figure 7.6 – Landau energy loss distribution for different thicknesses of the detector [20].

Charge transport

Two main effects characterize the charge transport: diffusion and drift. The first one is characterized by the random thermal motion of free carriers which implies a net movement from a high concentration region to a low concentration one. This effect can be quantified by the following relations:

$$J_{n,diff} = -D_n \Delta n \quad ; \quad J_{p,diff} = D_p \Delta p \quad (7.7)$$

where $J_{n/p,diff}$ is the diffusive current density, n and p are the electron and hole concentration and $D_{n/p}$ the diffusion constant related to the mobilities via the Einstein relation $D_{n/p} = \mu_{n/p} kT/e$.

The drift component is described by the Drude model [119]. According to this model charge carriers in the presence of an electric field are accelerated between two random collisions. The drift current per unit areas is therefore defined as: $J_{n/p,drift} = \mu_{n/p} q n/p E$. The average direction of motion is given by the electric field direction, the related average drift velocity is given by [119]:

$$v_n = -\mu_n E \quad ; \quad v_p = -\mu_p E \quad (7.8)$$

where the mobility is defined as $\mu_{n/p} = \frac{q\tau}{m_{n/p}}$ with τ being the characteristic time between two collisions and $m_{n/p}$ the effective mass of the electrons and holes respectively [118]. This linear relation breaks for high values of the electric field when the acquired velocity is comparable with the thermal velocity of the carriers ($\sim 10^5 m/s$). As the acceleration increases, the number of collision becomes higher leading to a saturation of the drift velocity. This effect is also known as "mobility degradation" [119].

In summary, the total carrier density is given by the sum of the drift and the diffusion component: $J_{n/p} = J_{n/p,drift} + J_{n/p,diffusion}$. In chapter 8 the effect of both components on the induced signal of the detector will be discussed in detail, using test-beam data and finite-element simulation.

7.3 Signal Processing

The signal induced at the electrode must be amplified and digitized to be transmitted to the data-acquisition system. In the most popular versions of silicon detectors these operations usually take place in a dedicated read-out chip hosting the full Front-End (FE) electronics. The FE chip is usually finely segmented to match the size of the pixel in the sensor and directly connect to it via bump-bonding. The pixel detectors built following this design are referred as *hybrid* pixels and are currently the most common type of sensors used in multi-purpose experiments. A more innovative design which integrates the FE chip within the collecting silicon sensor is called a monolithic, active, pixel sensor and it is one of the research subject of this thesis. While the main features of the two approaches will be described in detail in the next session, the general principle of signal processing will be described in the following.

The electronic circuitry of a sensor is typically composed by an analog signal processing stage and a digital logic. In a simplified description, the analog logic is made of three main parts: a pre-amplifier, a feedback circuit and a discriminator.

The current induced by the e-h pair is amplified using an inverting amplifier which converts an input charge Q_{in} to a voltage. Figure 7.7 shows the basic principles of a charge-sensitive amplifier. The capacitance C_f is one of the fundamental parameters of the FE design. In the ideal condition of infinite gain, the output voltage is: $v_o = -Q_{in}/C_f$. In reality the gain is finite and a residual voltage, due to the internal and detector capacitances, remains at the input. This residual voltage affects the charge sharing between pixels and reduces the output voltage of the amplifier. The effective impedance of the amplifier needs therefore to be significantly larger than the detector capacitance. However, the noise produced at the amplifier is usually the dominant source of noise in the FE [119]. The feedback capacitance needs to be tuned carefully to maximize the rejection of these noise sources. The choice of C_f is therefore a compromise between many parameters such as gain, noise contributions, time response and low power consumption. Typical values of a standard pixel detector are around 30 fF with a gain of 100.

A feedback circuit is required to reset the feedback capacitor of the charge sensitive amplifier to avoid pile-up of pulses and to reduce the leakage current, especially after irradiation. This is achieved by either adding a resistor or a constant current source in parallel to C_f . The slope of the discharge function can be tuned via the feedback circuit thanks to global and/or local Digital to Analog Converters (DACs).

Finally, the signal arrives at the discriminator which is used to compare the signal amplitude to a threshold setting. The threshold is directly correlated with the minimum amount of charge needed to fire the corresponding pixel and, therefore, to its efficiency. The value of the threshold needs to be set as low as possible while keeping a good sepa-

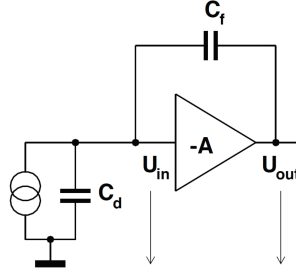


Figure 7.7 – Simplified representation of a charge sensitive amplifier. The silicon sensor is represented with a current source in parallel with the overall detector capacitance C_d . Figure adopted from [119].

ration between signal and noise. It can be controlled by dedicated DACs both globally, which set the overall threshold to be used at sensor level, and locally to fine tune possible mis-matches pixel-by-pixel which are mostly due to production inaccuracies. The discriminator information is also used to store the input charge released in the detector. The time that the signal remains above threshold is proportional to the height of the signal and thus proportional to the input charge. This quantity, referred to as Time-Over-Threshold (ToT), represents an effective measurement of the collected charge and therefore of the energy deposited by the traversing particle. Since the rising and falling edges of the signal depends on multiple FE parameters, a dedicated ToT calibration is needed to convert the ToT value into a more physical quantity such as the input charge.

One of the sources of degradation in the time response of the detector is the correlation between the height of the signal and the characteristic rise time of the pulse as shown in Figure 7.8, this effect is referred to as time-walk. Given the large variety of sources which can lead to different signal height, such as charge sharing, crossing angles, diffusions and more, the effect of the time-walk is effectively a smearing in the time response of the detector.

7.4 Radiation damages

The energy loss in silicon detectors can be split into Non-Ionizing Energy Loss (NIEL) and ionizing energy loss. The former displaces crystal atoms forming defects in the crystal lattice. Particle traversing silicon detector deteriorate its lattice through hadronic interactions introducing electrically active defects. Through these defects, electrons in the conduction band or holes in the valence band can be trapped and eventually recombine. In contrast to the NIEL which affects the bulk of the device, the ionizing energy loss alters mostly the silicon-dielectric interface. The e - h generated in the dielectric drift, via tunneling, to the interface where they attract electrons which can eventually

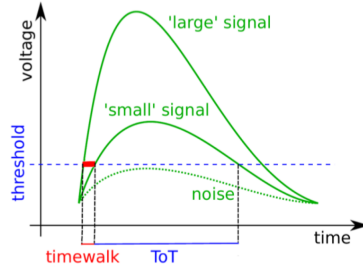


Figure 7.8 – Schematic view of the time-walk effect.

alter the performance of the pixel detector.

These damages modify the principal characteristic of silicon detectors, such as leakage current and maximum depletion voltage, and thus they represent, together with the degradation of the FE electronics, one of the most important effect in the operations of tracking detectors at the LHC.

7.4.1 Non-Ionizing damages

Hadrons traversing the silicon bulk interact via the strong force displacing the atoms and thus altering the crystal lattice of the silicon. Defects in the bulk of the sensor are modeled by introducing energy levels in the forbidden band-gap. Through these defects, electrons in the conduction band or holes in the valence band can be trapped and eventually recombine. NIEL is defined as the amount of energy released into the material by an incident particle which not due to ionization. Different particles have different effectiveness in releasing NIEL, therefore to compare irradiation the damage is normalized to the NIEL of a 1 MeV neutron. The induced defects can drastically change the macroscopic properties of the material, where the main effects due to the NIEL are:

- Space charge inversion
- Increase of the leakage current
- Modification of the full depletion potential

As radiation induces electrically active defects, the doping of the material is altered. It is therefore useful to define an effective doping concentration N_{eff} . Due to the fact that N_{eff} changes with the fluence, thus affecting the depletion region, the bias voltage must be increased during the lifetime of the experiment for most of the standard planar

pixel sensors used at the LHC experiments [119]. N_{eff} can be determined by inverting equation 7.2:

$$|N_{\text{eff}}| = \frac{2\epsilon_0\epsilon_s V_{\text{depl}}}{et^2} \quad (7.9)$$

Where V_{depl} is the bias voltage needed to reach full depletion and t is the thickness of the sensor. It has been shown [119] that starting from an n -doped material N_{eff} decreases until it changes sign, which occurs when it is dominated by the acceptor-like defects as shown in figure 7.9. This mechanism is known as *space charge sign inversion*.

Since the traps act as generation-recombination centers the thermal activation of an electron-hole pair is more frequent and therefore the generation lifetime τ_g ¹ decreases resulting in an increase of the leakage current density in the bulk. Its variation can be parametrized as follows:

$$\Delta J = \alpha \phi \quad (7.10)$$

With J being the leakage current density and α the *current related damage rate* which depends on the initial resistivity of the silicon. Therefore, the leakage current increases linearly with the fluence ϕ as shown in Figure 7.10. This effect can be mitigated by cooling down the sensor so that the thermal activation through shallow traps is reduced.

The evolution of N_{eff} with the fluence is modeled using a phenomenological model, the so-called Hamburg-model [123]. The Hamburg model provides accurate predictions of pixel properties after irradiation and it plays a crucial role in the construction and operation of trackers using high-resistivity silicon detectors such as the one currently installed in the ATLAS detector.

With the advancement of new silicon sensor technologies based on low resistivity substrates, such as the HV-CMOS technology, a novel effect, not yet described by the Hamburg model was observed. First seen in TCT² and laboratory measurements [124] and later in test-beam experiments, the *Acceptor removal mechanism* corresponds to an increase of depletion depth with irradiation. This observation is interpreted as an effective decrease of the number of acceptor in p -type silicon bulk sensors and it was found to depend on the initial resistivity of the substrate, such that for a high-resistivity sensor it becomes negligible as shown in Figure 7.11. The mechanism describing the dependence of acceptor removal rate on the initial resistivity is yet to be understood.

During the course of this thesis, some of the first evidences for the *Acceptor removal mechanism* were observed in test-beam experiments. These studies will be reported in details in section 8.3.1.2.

¹characteristic time between two pairs creation

²The Transient current technique is an experimental technique used to study the collection properties of silicon detectors.

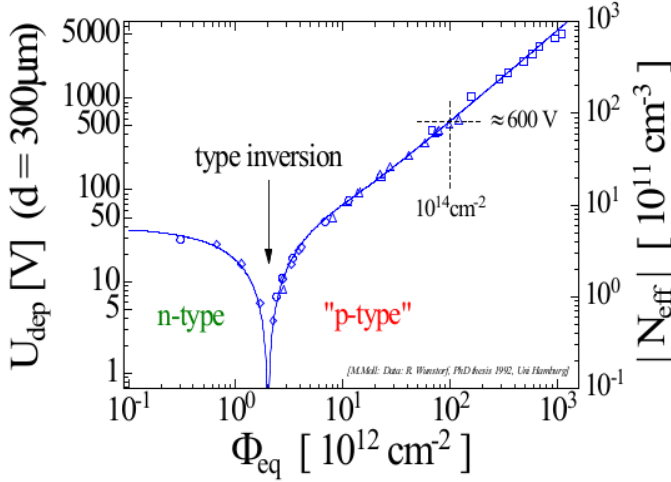


Figure 7.9 – Change of the full depletion voltage of a 300 μm -thick silicon sensor and its absolute doping versus the normalized fluence [125].

7.4.2 Ionizing damages

In contrast to the NIEL which affects the bulk of the device, the ionizing energy loss affects mostly the silicon-dielectric region. The dose of ionizing energy loss radiation damage is usually expressed in Rad, which represent $6.24 \times 10^{10} \text{ MeV}$ of ionizing energy deposition per kilogram of material. An ionizing particle creates electron-hole pairs in the oxide layer. Since the electrons have high mobility in the oxide ($\mu_{n,oxide} = 20 \text{ cm}^2/(\text{Vs})$) they are quickly collected. Holes, instead, have a very low mobility ($\mu_{p,oxide} = 2 \times 10^{-5} \text{ cm}^2/(\text{Vs})$) because of the large number of shallow hole traps present in the oxide lattice. Holes tunnel from one trap to the other in the direction of the electric fields until they reach the oxide/silicon interface where, due to impurities at the oxide surface, a large number of deep hole traps are present. This positive charged layer in the SiO_2 attracts free electron carriers in the bulk, where in the case of p -doped silicon, an inversion layer is formed which can eventually short two neighboring n -doped pixel implants. In order to avoid this effect, three techniques have been developed: an heavy p -doped region can be implanted in between the implants, which is called $p\text{-stop}$. Alternatively, one can form a light p -doped region which extends up to the all inter-pixel length, the so-called $p\text{-spray}$ or a mixture of the two which makes use of both $p\text{-stop}$ and $p\text{-spray}$ can be implemented. A detailed discussion on this topic is out of the scope of this thesis, but the effect of the p -implant on the charge collection properties of HV-CMOS devices is discussed in chapter 8.

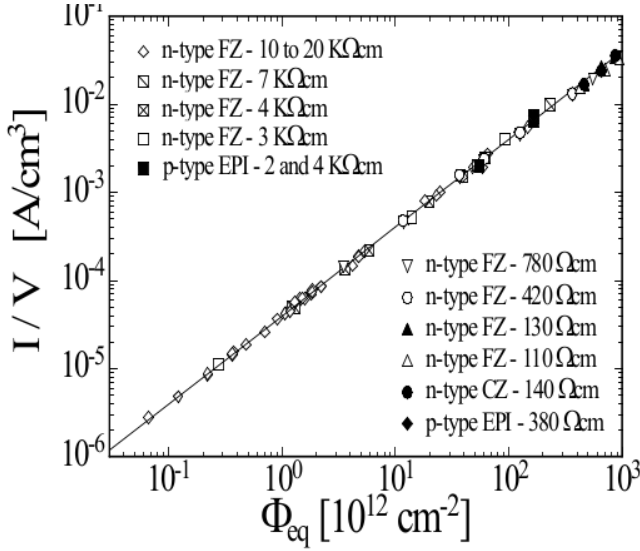


Figure 7.10 – Current related damage rate fitted with experimental data [123].

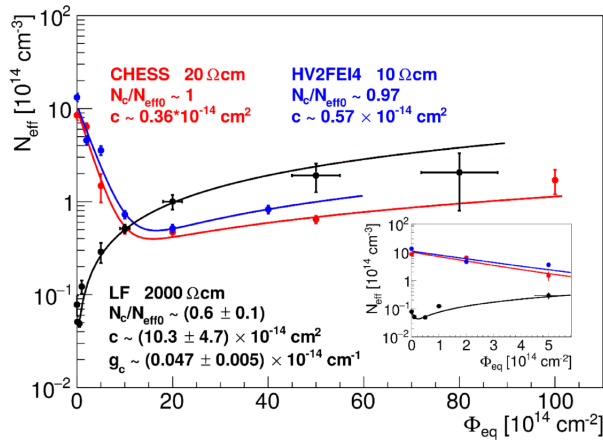


Figure 7.11 – Effective doping concentration as a function of radiation fluency for three devices with different initial resistivity [124].

Developments towards a monolithic sensor for the HL-LHC

The High-Voltage CMOS (HV-CMOS) technology was originally used to design electronic chips that drive automotive or industrial devices. It is suited for a wide variety of applications including smart sensors, sensor interface devices, building controls and LED lighting control. Thanks to the commercially available manufacturing processes that allows for the implementation of low-cost and low material budget detectors, tracking systems built in HV-CMOS technology are an interesting options for large scale detectors. Many HEP collaborations such as ALICE, CLIC and MU3e are planning to use this technology.

The LHC poses unique challenges in term of radiation hardness and timing resolution for a pixel detector. During the HL-LHC, a total integrated luminosity of around 3000 fb^{-1} will be collected by ATLAS and CMS throughout the HL-LHC data-taking period. The radiation damage related to this increase of integrated luminosity requires upgrades to the experiments. In particular, the inner tracking detectors will have to be replaced. A large area of extremely radiation-tolerant silicon detectors will need to be installed. The new full-silicon based tracking detector of the ATLAS experiments at the HL-LHC is called ITk. HV-CMOS pixel sensors are a promising candidate for the outermost pixel layers of the ITk, where the expected fluence is up to $1 \cdot 10^{15} \text{ n}_{eq}/\text{cm}^2$. Assessing the performance of these detectors at this high radiation and high rate environment is one of the subjects of this thesis.

The chapter is organized as follows: first a detailed description of the HV-CMOS technology will be given, then results from laboratory measurement, test-beam mea-

surement and TCAD simulations will be discussed.

8.1 The HV-CMOS technology as a particle detector

The operating principle of the HV-CMOS sensor is based on a multi-layered structure used to isolate the bias voltage and the transistors used to process the signal on-chip. A schematic figure of the overall HV-CMOS sensor design is shown in Figure 8.1. The sensor are made of a thin p -type silicon bulk which contains a deep n -well hosting the in-pixel electronics. The deep n -well acts both as collecting electrode and substrate of the transistors, where such a device is referred to as a "smart" diode. For the HV-CMOS pixel sensors considered for this thesis, the typical resistivity of the bulk is $\sim 10 \Omega cm$, a factor of 100 lower compared to the typical sensors currently used by ATLAS and CMS¹. The high-voltage is applied from the top of the device through a p -implant. The sensor is operated with a bias voltage of the order of 80 V, while breakdown occurs at around 100 V. The corresponding depletion depth is around $10 \mu m$.

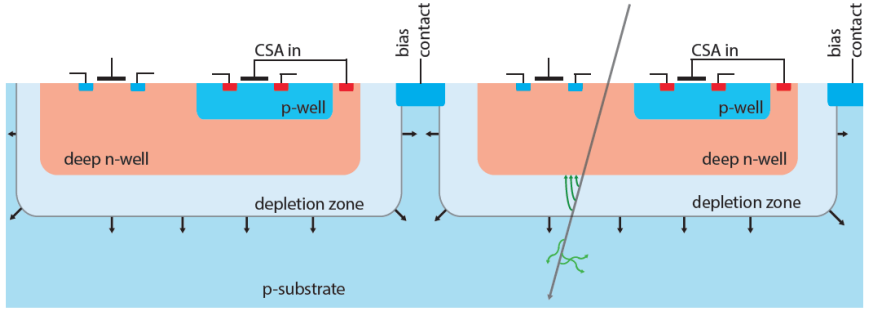
A mip passing through the silicon releases around $80 e^-/\mu m$; assuming a collection efficiency of the drift charges of 100%, around $800 e^-$ would be collected. This value is sensibly lower compared to the typical threshold of hybrid pixels sensors which is around $5000 e^-$. The CMOS production process allows for an in-pixel amplification stage which is used to amplify the collected signal to a suitable amplitude for either a discriminator or a direct read-out chip. HV-CMOS sensors hosting full read-out electronics are called monolithic sensors. When the HV-CMOS sensor is instead coupled, after the amplification stage, to a dedicated front-end chip through a layer of glue, the assembly is referred to as Capacitively Coupled Pixel Detector (CCPD).

This thesis focuses mostly on the study of CCPDs which are an interesting option by themselves, but they also serve as proxy to asses the feasibility of monolithic pixel sensors in a high-rate and high-radiation environment. The reason for this is that CCPDs and monolithic assemblies share the same design in terms of sensor substrate and, therefore, they also share the same charge collection mechanism. The thin depletion zone allows for very fast charge collection that, in turn, leads to a low sensitivity to charge trapping. Since charge trapping is the main reason for sensor degradation by non-ionizing radiation, a high hardness can therefore be expected. In addition, deep sub-micron CMOS technology is designed to be resistant to ionizing radiation, and therefore high radiation hardness of the electronics is also expected [127].

The main advantages of using CMOS pixels as part of the ITk are the following:

- On-chip signal amplification makes it possible to use AC-coupling to the readout chip. Instead of the expensive bump-bonding process, the sensor chip can be sim-

¹CMOS sensors designed with high-resistivity substrate are also possible (also called HR-CMOS pixel detector), as described elsewhere [126].



(a)

Figure 8.1 – Illustrative representation showing two neighbouring HV-CMOS pixels. For each pixel a deep n -well (in light red) is implemented in the p -substrate (in light blue) and hosts the NMOS transistors. PMOS transistors are imbedded in the p -well (in bright blue) which is isolated from the bulk by the deep n -well. p -implants provide a biasing ring around individual pixels. An ionizing particle traversing vertically the detector is schematically represented with its charge deposition collected by drift in the depleted zone towards the deep n -well and by diffusion in the deep bulk.

ply glued to the FE-I4 chip, as in the case of CCPDs. Alternatively, the CMOS pixel itself can host the full read-out electronics as in the case of monolithic sensors.

- The size of hybrid pixels is mostly constrained by the minimum size needed to form the bump-bonding. Since no bump-bonding is needed in CMOS sensors, the pixel size can be made smaller. Smaller pixel size leads to smaller input capacitance, better position resolution and higher granularity. The latter is particularly important for tracking algorithms at the HL-LHC due to the high pile-up environment.
- The HV-CMOS process is a standard electronic production process and is therefore cheap and widely available.

For these reasons, the HV-CMOS technology is an interesting and promising candidate for tracking detectors at LHC experiments.

8.1.1 h18CCPD_{v4} prototypes

Several CCPD prototypes have been investigated during the course of this thesis. For simplicity only the last, more advanced version will be discussed here.

CCPDv4 are HV-CMOS prototypes built in AMS 18nm technology [128]. The sensor is glued on top of the front-end chip, the FE-I4, used to read-out the IBL pixels. Figure 8.2 shows the overall CCPDv4 assembly. CCPDv4 prototypes have a total size of $\approx 2.4 \times 2.9 \text{ mm}^2$ and were manufactured with a resistivity of $20 \Omega\text{cm}$. The prototypes under consideration feature four different pixel flavors, mostly differing by the on-sensor electronic design. The *Stime* pixels in particular have been studied for this thesis. Each *Stime* pixel has a size of $33 \times 123 \mu\text{m}$ and contains an amplifier and a discriminator together with a 4-bit in-pixel tune DAC, thus allowing for a per-pixel threshold tuning as schematically shown in Figure 8.3.

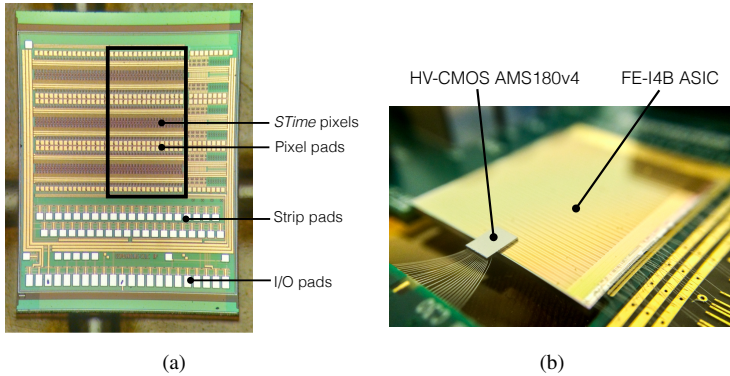


Figure 8.2 – Left: Photograph of the CCPDv4 sensor used in this study with the sub-matrix of *Stime* pixels marked. Right: Assembly of FE-I4 pixel readout chip to a HV-CMOS CCPDv4 sensor via capacitive coupling [8].

To match the FE-I4 pixel size of $50 \times 250 \mu\text{m}$, the HV-CMOS pixels are grouped together in bunches of three, forming two $100 \times 125 \mu\text{m}$ *macro*-pixels as shown in Figure 8.4. In order to identify the sub-pixels, the ToT of each of the pixels connected to the same FE-I4 was fixed. However, this feature was not used during beam-test and thus the reconstruction was performed on the *macro*-pixel. The CCPDv4 sensors were glued to the FE-I4 chip using a non conductive epoxy glue with a flip-chip bonder at the University of Geneva.

8.1.2 H35 full-size demonstrator prototypes

In order to show the viability of the HV-CMOS technology for full-sized production, a large-scale pixel sensor prototype has been produced, the H35DEMO. The H35DEMO is produced in H35 350 nm technology with a total size of $24.4 \times 18.5 \text{ mm}$ and a pixel pitch of $250 \times 50 \mu\text{m}$ to match one-to-one the FE-I4 pixels. The demonstrator is divided into four independent matrices: two monolithic matrices with integrated read-out built in either CMOS or NMOS circuitry and two analog matrices containing only

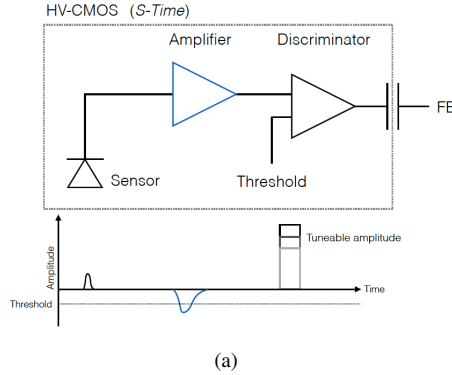


Figure 8.3 – Schematic representation of the in-chip electronics. The sensor is shown as a diode connected to a charge-sensitive amplifier followed by a discriminator with a tunable threshold. The output signal is then capacitively connected to the FE-I4.

a per-pixel amplifier. The analog matrices provide an amplified signal which is then capacitively coupled to a FE-I4 chip. Within each analog matrix there are different sub-matrices with dedicated variations of the on-pixel electronic as shown in Figure 8.5. The main differences between the matrices are the transistor technology used for the analog circuitry (linear transistor or enclosed layout, or simply ELT), different design of the bias electrode with or without an additional Deep P-Well (DPTUB) as illustrated in figure 8.6 and finally different gains of the in-pixel amplifier. Table 8.1 summarizes the main differences among the analog matrices.

Table 8.1 – Sub-matrix flavors in H35DEMO analog sensors [9].

	Matrix analog 1	Matrix analog 2
sub-matrix 1	Extra DPTUB and ELT	Extra DPTUB, high gain
sub-matrix 2	Without DPTUB and ELT	Without DPTUB, high gain
sub-matrix 3	Without DPTUB and linear transistor	Without DPTUB, low gain

The pixel design of the H35DEMO features a segmented deep- n well. The central n -well hosts additional p - and n -implants used to build the CMOS circuitry while screening the HV. The bias voltage is applied from the top of the sensor similarly to the CCPdv4 prototypes. H35Demo samples were glued at the University of Geneva using an *Accura* flip-chip machine. Figure 8.7 shows the details of the gluing process.

Several prototypes corresponding to different resistivities were produced for testing purposes. Nominal resistivities of: 20, 80, 200 and 1000 Ωcm were studied in simulation and laboratory measurements for this thesis.

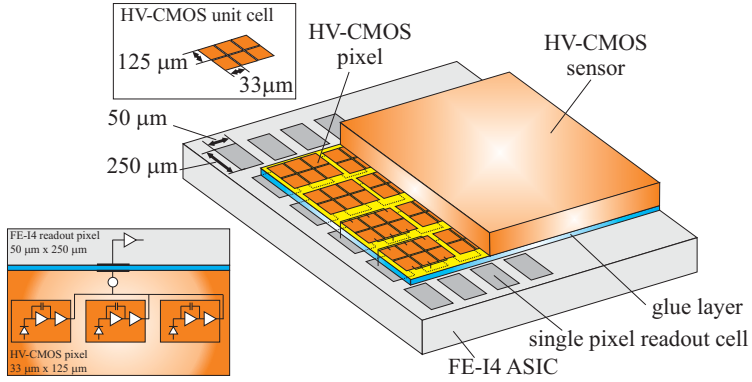


Figure 8.4 – Schematic representation of the HV-CMOS to FE-I4 connections. The bottom-left panel insert shows how three HV-CMOS pixels (forming the so-called *macro-pixel*) are capacitively coupled to a single FE-I4 readout pixel [8].

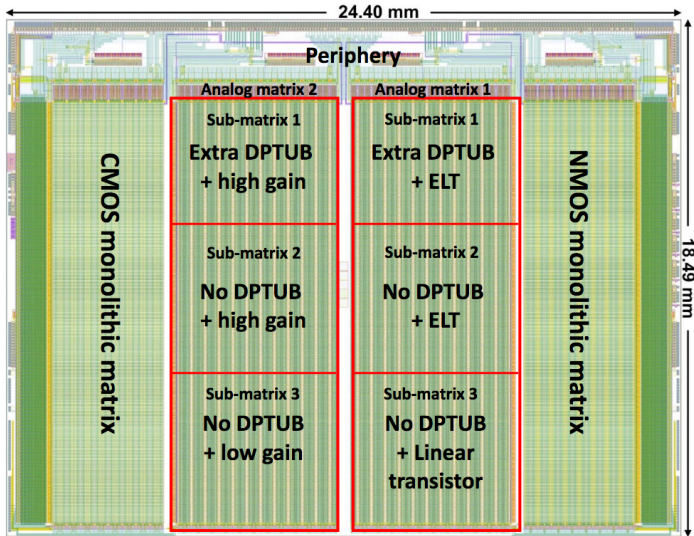


Figure 8.5 – The H35DEMO demonstrator sensor with its sub-matrices. The monolithic matrices are located at the left and right. The two CCPD matrices are located in the middle and feature three pixel flavors [9].

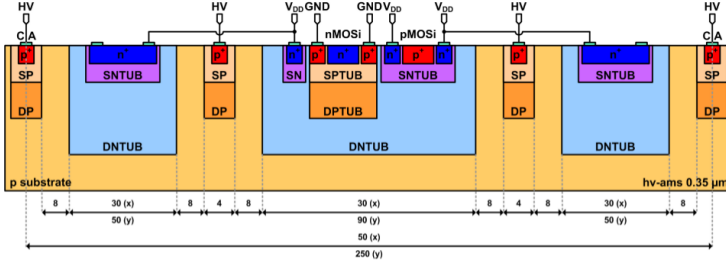


Figure 8.6 – Schematic representation of a pixel of the H35Demo [129] outlining the layered structure of the p - and n -well used to build the on-pixel circuitry.

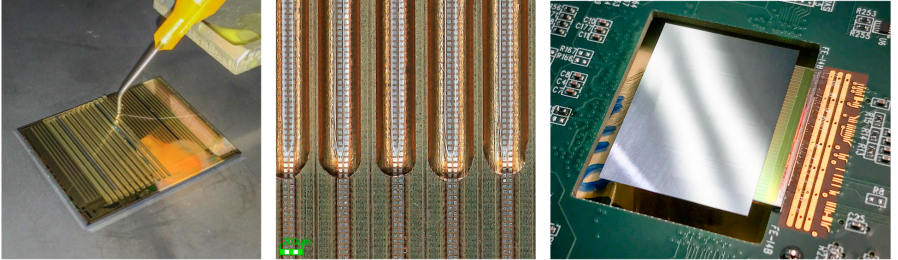


Figure 8.7 – Left) Deposition of epoxy on the H35DEMO matrix. Middle) glue (partially) deposited on double pixel column. Right) 100 μm thin H35DEMO-FE-I4 assembly on PCB [129].

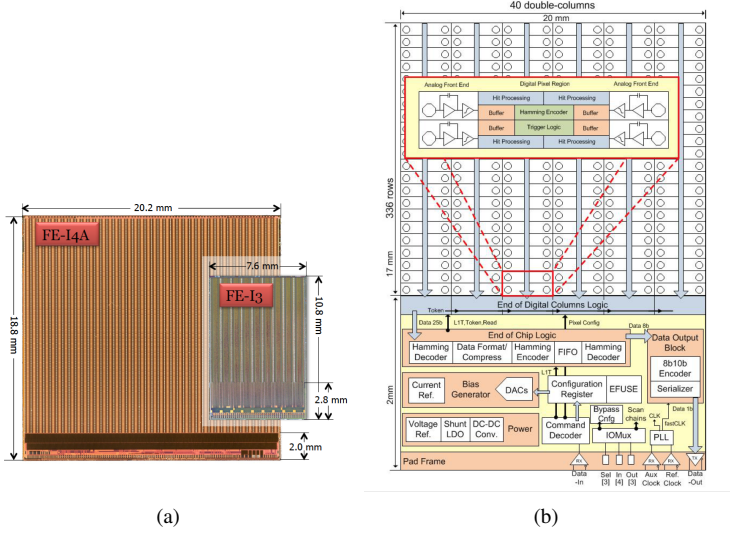


Figure 8.8 – Left: Picture of the FE-I4, the previous version of the chip, the FE-I3, is shown for comparison. Right: Sketch of the organization of FE-I4 [130].

8.1.3 The FE-I4 chip

The operating condition of the IBL have necessitated the development of a new front-end read-out chip, called the FE-I4. The FE-I4 consists of an array of 26880 pixels, 80 in the beam direction and 336 in the azimuthal one. The FE-I4 has a pixel matrix architecture that is different from the previous read-out chip, the FE-I3 (used in the ATLAS pixel detector) which is characterized by a column drain readout followed by peripheral data storage and trigger logic. Figure 8.8 shows the two read-out chips. For the FE-I4, the data storage is made locally at the pixel level until triggering and subsequent propagation of the trigger inside the pixel array. Each pixel consists of an independent analog section, amplifying the collected charge from the sensor. In the analog section, hits are discriminated at the level of a tunable comparator with an adjustable threshold, and charge is translated to Time over Threshold (ToT). The 26880 pixel array is organized in columns of analog pixels, where each pair of analog columns is tied to a shared digital double-column unit centered between them. Inside the double-column, 4 analog pixels communicate to a single digital region as shown in figure 3.2. When a trigger is issued, ToT buffers are sent to the periphery and associated to the bunch-crossing corresponding to the specific trigger. More technical details can be found elsewhere [130].

8.2 The testing equipment

8.2.1 The test system: Caribou

A flexible and efficient test system for laboratory characterization and beam-test measurements is essential for a large R&D program such as the one being pursued by the ATLAS CMOS collaboration. A modular test system was developed in collaboration with BNL. CariBou (Control And Readout Itk BOard) is a modular test system for silicon sensor R&D, initially designed and developed for CCPDs but adaptable to different sensors [131].

The block diagram of the overall system is shown in Figure 8.9.

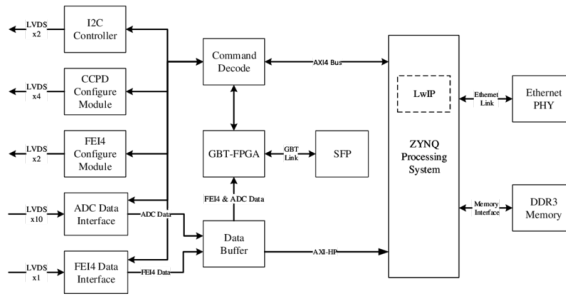


Figure 8.9 – Block diagram of the read-out system [131].

The Front-End assembly is composed by the CaR (Control and Readout) board and the FE chip board as shown in Figure 8.10. The first is designed to provide configuration and readout to the device under test and it controls the pulse injections, power supplies, bias voltages, and hosts the analog input channels of the ADC. The latter is specific to the device-under-test where, in the case of CCPDs, both the HV-CMOS sensor and the FE-I4 are wire-bonded to the FE chip board.

The core of the firmware is the central interface board, which is based on the Xilinx ZC706 FPGA development board. It controls bias voltages, pulse generators, and power rails on the CaR Board and configures FE and HV-CMOS sensor with the commands issued by the PC workstation. The data from the readout board are also decoded and sent to the PC through a Gigabit Ethernet link for off-line analysis [131]. Figure 8.11 shows the overall Caribou system during data-taking in a beam test at the CERN SPS.

The tuning of the CCPD is a critical task during detector operation in test-beam experiments. Due to construction differences, the effective threshold of each pixel can differ with respect to the global value provided by the CaR board leading to a potential pixel-by-pixel threshold mismatch. Given the relatively low value of the threshold used in HV-CMOS sensors, a good homogeneity of the effective threshold is crucial to

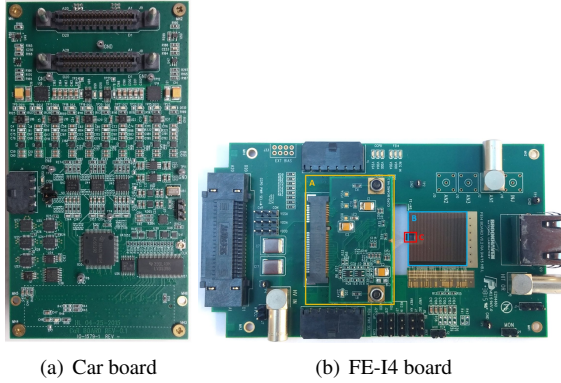


Figure 8.10 – Pictures showing the car board and the FE chip board [131].

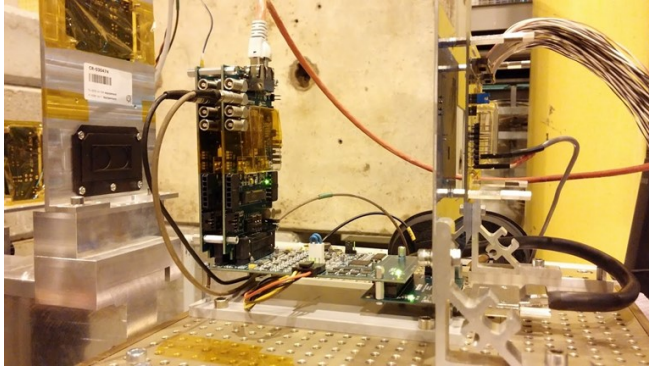


Figure 8.11 – Picture of the CariBou read-out system during test-beam operation at the CERN SPS facility.

achieve an overall high detection efficiency and low noise rate, especially after irradiation. This is possible thanks to a fine-tuning procedure of the local TDAC value of the in-pixel discriminator. The CCPD $v4$ prototypes were tuned using the pulse injection provided by the Car board. A known charge signal is injected several times into the in-pixel preamplifier and the percentage of signal over threshold is computed. The injected charge is changed until the rate over threshold reaches 100 %. Given the statistical nature of the thermal noise in the sensor and electronic noise in the circuitry, an S-curve is obtained. The curve is fitted with an error function, the extracted σ defines the level of noise in the detector and the extracted μ defines its effective threshold. This procedure is then repeated for several TDAC values. Results for an un-irradiated CCPD $v4$ prototype are shown in Figure 8.12. A linear fit is then run between the scanned TDAC values to find optimal TDAC working point corresponding to the target μ value. As shown in the

Figure, an overall threshold RMS of around $25 e^-$ is found after the tuning procedure. This narrow distribution indicates that the global threshold can be lowered avoiding otherwise noisy pixel outliers. An equivalent noise charge (ENC) can be extracted from the σ of the fit, where an average value of around 40 electrons was found for the DUT, as described here [131]. Such a low ENC value gives confidence about the validity of the tuning procedure thus ensuring homogeneous performance of the CCPDv4 prototype. Similar results were found for pixels irradiated up to $1 \cdot 10^{15} N_{eq}/cm^2$, which is a relevant value for the outer layer of the ITk.

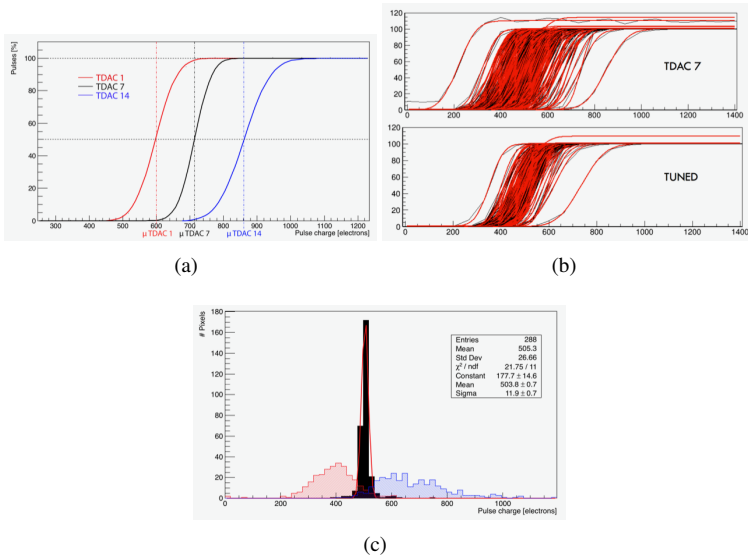


Figure 8.12 – a) Results of the injection scan with different TDAC values. b) The results of the fit with an error function for the *Stime* pixels matrix before and after tuning. c) Effective threshold distribution for a TDAC globally set to unity (red), to 14 (blue) and after tuning (black) [131].

8.2.2 The FE-I4 Telescope

For a complete R&D program towards the validation of a new detector technology, it is essential to evaluate the sensor response to real particles. Beam-test experiments using charged particle tracking telescopes are a well-established method for detector characterization. For this purpose, the University of Geneva ATLAS group has designed and produced a tracking telescope (referred here as the "FE-I4 telescope"). The FE-I4 Telescope has been successfully used in several test-beam campaigns at the CERN SPS and at the Fermilab test beam facilities. The overall FE-I4 Telescope is shown in Figure 8.13.

It is composed of two arms, each hosting three planar pixel sensors based on the FE-I4 chip with pixel pitch of $250 \times 50 \mu\text{m}$ mounted on an aluminium frame. As the pixels are not squared, the middle planes are rotated by 90° to ensure comparable pointing resolution in the two directions orthogonal to the beam axis. A modular PCB adapter-board, glued to the backside of the sensor, provides powering to the FE-I4 chips as well as noise filtering circuitry for an efficient tuning of the sensor and a smooth data-taking. A Device Under Test (DUT) box is placed in between the telescope's arms, it is positioned by means of two micrometer stages along the X and Y directions [6]. The high irradiation level of the DUT necessitates a cooling system to reduce the thermal noise induced by shallow traps in the bulk of the sensor. For this reason, the baseplate hosting the DUT can be cooled down to -50°C by an external chiller. To avoid condensation cold nitrogen gas is flushed into the box and temperature and humidity sensors are used to monitor the thermal condition of the box during operation.

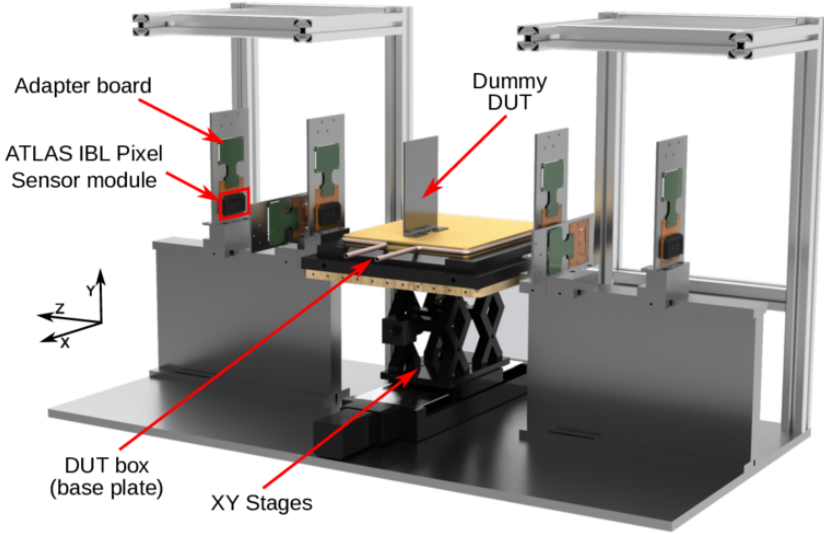


Figure 8.13 – View of FE-I4 telescope showing the two telescope arms holding the planes assembly, the DUT box, a dummy DUT and the two linear stages [6].

The voltages needed to operate the telescope planes and the DUT are provided by a set of High- and Low-voltage power supplies mounted on a MPOD mini-crate. In order to remotely control the power supplies, the chiller and the linear stages, as well as to monitor the humidity sensor, a Detector Control System (DCS) based on LabView has been developed and successfully employed during test-beam data-taking.

The Data Acquisition system (DAQ) is based on a High Speed I/O board and the Re-

configurable Cluster Elements (RCEs) [132]. These components have been originally developed for the characterization and qualification of the FE-I4 modules. The HSIO is a general purpose readout board based on a Xilinx Virtex-4 FPGA. It relays commands from the RCEs and manages the data collected by the sensor. It also provides a global clock to all detectors and issues triggers to the telescope planes and DUTs. The RCE is a computational unit which is responsible for the configuration of the HSIO. Technical details about the DAQ components can be found elsewhere [6, 132]. In order to control the DAQ system, a dedicated PC running the ATLAS trigger and Data Acquisition framework was employed. The DAQ system can read-out a total of 8 FE-I4 in parallel, allowing for simultaneous data-taking of up to two DUTs. A schematic view, summarizing the overall DAQ system of the Telescope, is shown in Figure 8.14.

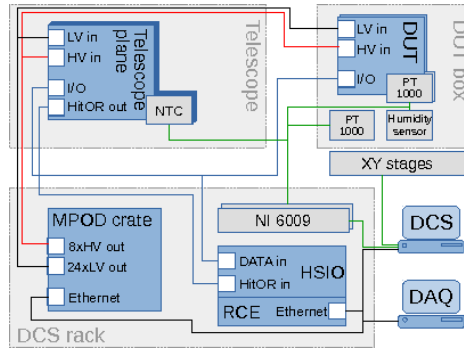


Figure 8.14 – Schematic view of the telescope setup [6].

The trigger system is based on the self-triggering functionality of the FE-I4 modules. During standard operation the first and last telescope planes are used in coincidence (within 25 ns^2) to generate a trigger signal which is then directly delivered to the DAQ system. The triggering FE-I4 chips were configured to output signals only for a subset of pixels thus allowing a definition of a region-of-interest trigger. This feature was particularly useful during the data-taking of the CCPD prototypes. Given their small dimensions compared to an FE-I4 module, an high rate of DUT data has been achieved by reducing the acceptance of the telescope planes around the DUT. In order to fully characterized the DUT in term of its timing performance, a window of 16 BC was read out consecutively after each trigger. The telescope planes, instead, were read out within a time window of 4 BC to reduce the data transfer load to the readout system. An excellent trigger rate of 6 kHz was reached with two measured devices. On-line reconstruction was integrated into the readout software. More than 60 million events were collected in the 2015 and 2016 test-beam campaign, allowing for a complete characterization of several HV-CMOS prototypes.

²25 ns corresponds to one LHC Bunch-Crossing (BC).

8.2.3 The offline reconstruction software

The offline reconstruction software was originally based on the Judith framework [133]. During the course of this thesis the software has been significantly changed with respect to its original version. The improvements in CPU performance and general user flexibility led to a new product, named *Proteus* [5] which is now used by the ATLAS test-beam group. Proteus is nowadays still being constantly improved, a detailed description of its evolution is out of the scope of this thesis. In the following sections the reconstruction algorithms and their performance using the FE-I4 Telescope at the time of the data-analysis carried out for this thesis will be presented.

8.2.3.1 Clustering algorithm

When a particle crosses a silicon detector, a single or multiple pixels may fire. This depends on the particle crossing point, the angle of the beam, rotation of the sensors and charge collection properties of the detector as schematically shown in Figure 8.15.

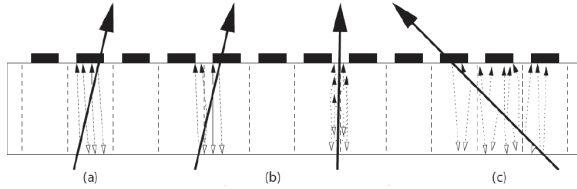


Figure 8.15 – Schematic view of different particles traversing a silicon detector and the related charge collection mechanism which may lead to multiple pixel being fired. One, two and three for a), b) and c) respectively. [119].

A clustering algorithm groups together a set of activated neighbouring pixels that are assumed to originate from a single particle traversing the telescope plane or DUT. The cluster is formed by iteratively grouping seed pixels. Each pixel hit in the event for a given telescope plane is considered as a seed, neighbouring hits are searched for without allowing for holes in between hits. The procedure is then repeated for each clustered hit until no neighbours are found. This process is performed for all hits in the silicon plane, excluding hits already associated to a cluster.

In case a cluster is found, a method to reconstruct its position is needed. The digital clustering algorithm simply takes the barycenter of the hits forming the cluster:

$$(u, v)_{digital} = \frac{1}{N} \sum_i^N (u_i, v_i) \quad (8.1)$$

where u and v are two orthogonal directions along the pixel pitches when the system of reference is chosen as the detector plane itself, this is the so-called local system

of reference. N is the number of hits grouped into the cluster. A more refined algorithm considers also the ToT associated with the hits assuming a linear behaviour of the collected charges in-between pixels:

$$(u, v)_{analog} = \frac{1}{Q_{tot}} \sum_i^N Q_i \cdot (u_i, v_i) \quad (8.2)$$

Q_i is the ToT of the single hit and Q_{tot} is the scalar sum of the ToT of each of the hits composing the cluster. The assumption of linearity is often a strong one and it is largely broken when the electric field in between pixels is highly non linear as in the case of HV-CMOS pixels, as discussed in Section 8.4. For these cases a more realistic description is needed. In principle the electric field profile could be extracted using finite-element analysis simulation and used to predict the cluster position. However, it is found [134] that a good approximation can be reached assuming a sigmoid function with a variable parameter σ which is estimated directly with a fit to the test-beam data. This procedure is known as η correction and was not yet implemented into the reconstruction software at the time of the results of this thesis. The digital clustering was used for the CCPD prototypes since the ToT information of the macro-pixel was not available as discussed in section 8.1.1. The analog clustering, instead, was used for the telescope planes.

The cluster size is the number of neighbouring pixels with a signal above threshold and is one of the key distribution as it is directly related to the charge sharing properties of the sensor. The Cluster Size (CS) distributions is shown in figure 8.16 for one of the telescope planes. Around 80 % of the time a single hit cluster is reconstructed, the remaining 20 % of clusters contain more than one pixel. The geometrical information of the cluster shape is also shown in Figure 8.16. An asymmetric cluster geometry is observed for $CS = 2$, which is attributed to the rectangular shape of the FE-I4 pixels leading to a larger charge sharing area along the short pixel direction. Aside from geometrical effects, few events, labeled with an asterisk in the plot, show large cluster size with neighbours hits along a single direction. These are due to δ -electrons traversing several pixels in the bulk of the sensor. To avoid possible biases in the determination of the cluster position, these clusters were excluded during reconstruction.

8.2.3.2 Tracking algorithm

Tracking algorithms are usually divided into 2 steps: pattern recognition and track fitting. Pattern recognition algorithms aim at identifying the clusters associated to the candidate track hypothesis, and are also called track finding algorithms. Once the clusters are found, a fit is performed to obtain the optimal track parameters. Track finding algorithms have to cope with a large combinatorial background and are usually the most time and CPU intensive tasks of the reconstruction chain. In general, many different

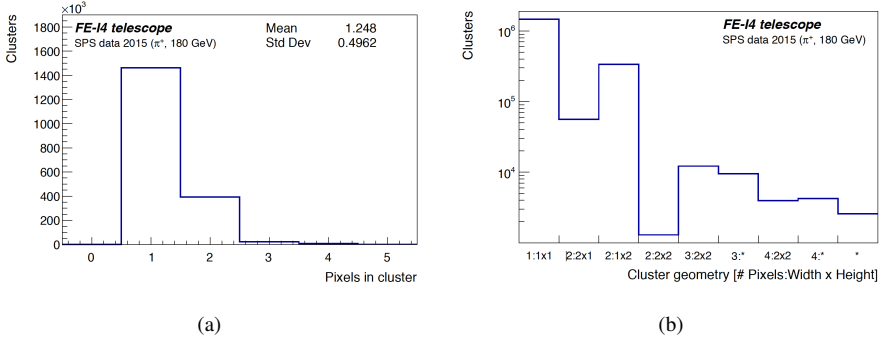


Figure 8.16 – a) Cluster size distribution for the third telescope plane. b) Geometrical shapes of the reconstructed clusters. Shapes not explicitly listed in the plot are labeled with an asterisk [6].

algorithms exists in high-energy physics experiments and in particular for test-beam reconstruction. The choice of the best algorithm to use depends mainly on the condition of the telescope. Given the very low noise rate FE-I4 chips and the short triggering window used during data-taking, the combinatorial background arising from noise hits and hits originating from events overlapping in time is low. For this reason, a simple but effective track finding algorithm was employed.

The starting point of the tracking algorithm is a seed cluster in the first telescope plane facing the beam axis. Clusters on consecutive planes are searched for within a given solid angle defined with respect to the seed cluster. Initially it is assumed that the track is parallel to the telescope's longitudinal direction, then this assumption is iteratively corrected as new clusters are associated to the track. In case multiple candidate clusters are found, the track bifurcates and further candidate cluster searches continue. The reconstructed tracks are ordered in $|\chi^2/n.d.f. - 1|$ and the first track is selected. Clusters belonging to the reconstructed track are excluded from further searches. The procedure is repeated in case multiple seed clusters are found.

The high energy of the particle in the SPS and Fermilab test-beam allow one to safely neglect multiple scattering contributions to the fitting, therefore the candidate set of clusters are fitted with a straight-line. Figure 8.17 show a schematic summary of the tracking algorithm.

To improve the quality of the reconstructed tracks, only tracks with a cluster in all six telescope planes were used. A quality cut of $\chi^2/n.d.f. < 2$ was implemented to avoid high intensity bursts of the beam, nuclear interaction producing showers in the telescope planes and multiple scattering at high angles. The fraction of reconstructed tracks normalized to the number of trigger was found to be $\sim 96\%$, out of which 93

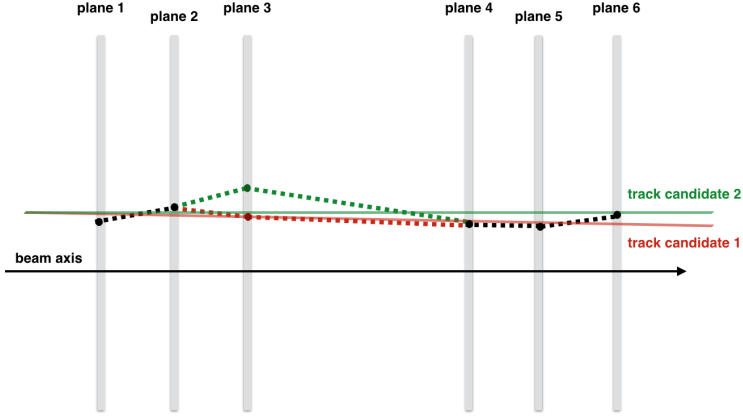


Figure 8.17 – Schematic representation of the tracking algorithm. The clusters are shown in black. The cluster in the first telescope plane is used as seed for the tracking algorithm. The track bifurcates due to two candidate clusters, shown with dashed lines in red and green in the figure. Two straight-line fits are performed and the one with $\chi^2/n.d.f$ closest to 1 is chosen.

% were single tracks event, 2 % double-track events and the remaining 1% had three or more tracks. Tracking and trigger performance of the telescope are summarized in Table 8.2. Thanks to the self-triggering of the FE-I4 telescope it is possible to define a fiducial active pixel area in the telescope planes around the DUT. This is particularly useful in the case of small prototypes such as the CCPD v_4 .

Table 8.2 – Tracking and trigger rates with and without the ROI during a test-beam for one of the CCPD v_4 prototypes.

ROI trigger	Trigger rate [kHz]	Fraction of in-DUT tracks
no	6.3	~ 70 %
yes	6.0	~ 2 %

One of the main figures-of-merit in test-beam analysis are the residuals, defined as the difference of the track position at the plane of interest and the cluster used to form the track in that plane:

$$Res_u = u_{track}(z = plane) - u_{cluster}; Res_v = v_{track}(z = plane) - v_{cluster} \quad (8.3)$$

Where u and v are coordinates in the local system of reference of the plane. Since the track itself depends on the cluster being used in the computation, residuals are usually shown unbiased, i.e. the cluster on that plane of interest is excluded from the fitting procedure. Unbiased residual distributions for one of the telescope planes are shown in Figure 8.18. The mean in both directions is centered at zero showing no biases from the alignment of the sensor. The RMS of the distribution is a measure of the resolution of the sensor. In the case of a single-hit cluster and assuming a flat beam profile within the cluster, its resolution is computed as:

$$\sigma = \sqrt{\frac{\int_{-p/2}^{p/2} f(x)x^2 dx}{\int_{-p/2}^{p/2} f(x) dx}} = \sqrt{\frac{\int_{-p/2}^{p/2} x^2 dx}{\int_{-p/2}^{p/2} dx}} = \frac{p}{\sqrt{12}} \quad (8.4)$$

p is the pitch of the sensor along one of the two coordinates u or v . As shown in the plot, the calculated values are larger than those obtained from the residuals distribution. In particular, the residuals along the shorter pitch indicates a larger deviation. This is attributed to the charge sharing effect, which for a telescope sensor is asymmetric in the two directions due to the rectangular shape of the pixel, as discussed in the previous Section.

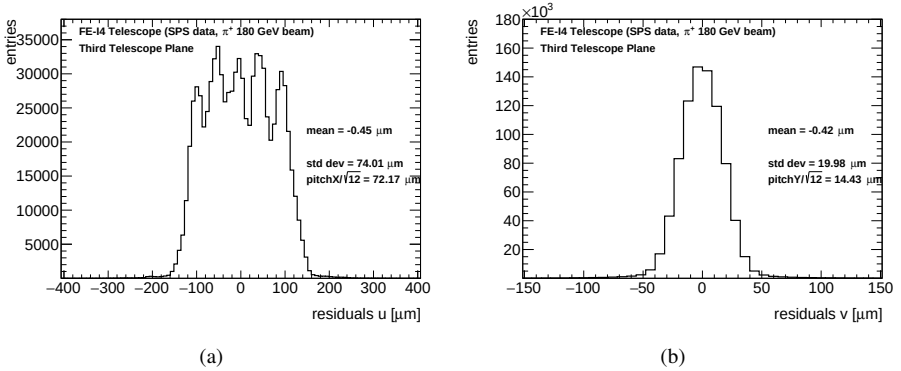
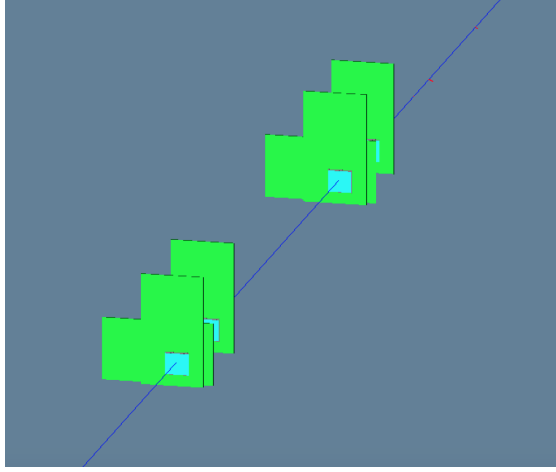


Figure 8.18 – Unbiased residuals for the third telescope plane during a test-beam campaign at the CERN SPS.

The residuals along the u direction clearly show a five peak structure. To determine the reason for this effect, simulations have been run using the Allpix software [135], a Geant4-based [52] simulation package specialized for test-beam setups. Figure 8.19 shows an event-display of the simulation.

The geometry used in simulation emulates a typical run of the FE-I4 Telescope where the two middle-planes are rotated by 90° . All planes were perfectly aligned to each other and the beam was simulated with no inclination. π^+ at 180 GeV were sim-



(a)

Figure 8.19 – Overall layout of the simulated FE-I4-Telescope using Allpix. A 180 GeV π^+ traversing the six telescope planes is shown in blue.

ulated to reproduce the test-beam condition. The charge collection mechanism in the sensor are simulated using a simplified model, which only considers if the sum of the energy released in the pixel is greater than a threshold, thus not including charge sharing effects. Figure 8.20 shows the residuals distribution along the X axis³. The distribution shows five peaks equally spaced by $50 \mu m$. This feature comes from the geometry arrangement of the telescope and the rectangular shape of its pixels. The rotated planes increase the granularity of generated clusters by $pitch_x/pitch_y = 5$ in the X direction, which allows one to distinguish between tracks with a resolution of $50 \mu m$ as shown in the right panel of Figure 8.20. In reality, due to charge sharing and mis-alignment of the detectors, the five peaks are broad and have different heights. In conclusion, this effect only affects the shape of the residuals, which are generally assumed to be flat.

8.2.3.3 Alignment procedure

A typical tracking system instrumented with pixel detectors usually reaches a pointing resolution of the order of $10 \mu m$. The system is therefore sensible to small offsets and rotations of the sensors which are not appreciable on-site during its assembly. Figure 8.21 shows a schematic example of a sensor misalignment. The algorithm which corrects for these effects using the tracking system itself is called Alignment algorithm.

³Since no mis-alignment was simulated, the local and the global coordinate frame are identical and the u coordinate is replaced with the X coordinate in the plot.

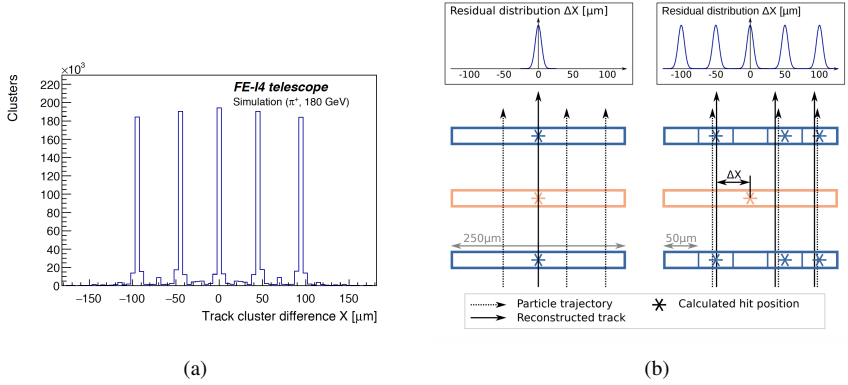


Figure 8.20 – a) Unbiased residual distribution from the simulated model of the FE-I4 Telescope. Five peaks, spaced by 50 μm are clearly visible. b) Schematic description of the origin of the peaked structures. The blue boxes show the pixels of the telescope planes while the orange boxes represent the pixel of the DUT [6].

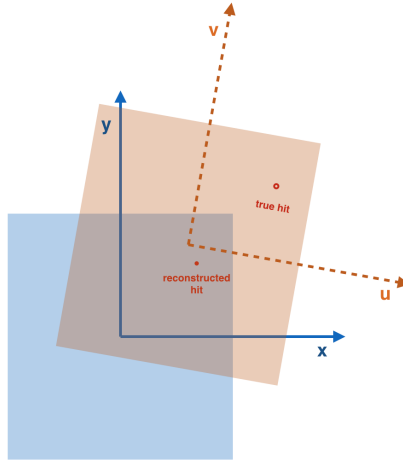


Figure 8.21 – Schematic figure of a sensor misalignment. The reconstructed plane position without alignment corrections is shown in blue. The true position of the sensor is shown in light red. The axis in the two cases correspond to the global and local system of reference respectively.

The alignment algorithm chosen for the reconstruction of the FE-I4 Telescope data is divided into 2 parts:

- **Coarse alignment:** The first step of the algorithm corrects for any offset along the X and Y directions without using reconstructed tracks. The first plane of the telescope is taken as a reference and the difference between cluster positions of neighbouring planes are computed. The algorithm assumes a beam perpendicular to the telescope planes, this assumption is revised in the subsequently alignment step. Given a perfectly aligned telescope, the position of the clusters in different planes should match 1:1. Figure 8.22 shows the distributions of the plane-to-plane differences along the X- and Y-axis for the third and the fourth telescope planes. A gaussian is fitted to the distributions and the extracted mean is used to shift the planes along the two directions.

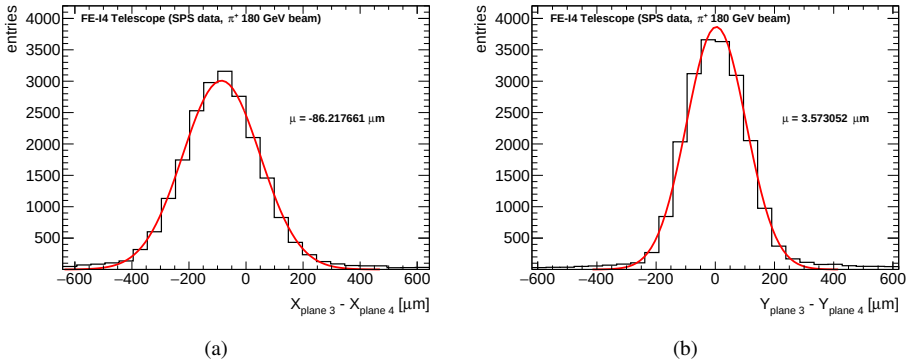


Figure 8.22 – Plane-to-plane cluster position differences. The resulting distribution is fitted along both directions and offsets are corrected using the mean of fitted gaussian distribution. The mean of the distributions is used to correct the offsets in the first step of the alignment procedure, the coarse-alignment.

- **Fine alignment:** The second step uses the tracks to correct for residual misalignments along X and Y as well as for rotation of the planes along the longitudinal axis of the Telescope. This correction is derived from the distribution of the unbiased residuals. The sensor on each plane is divided in slices along the X-axis and the unbiased residuals distributions along the Y-axis is computed as shown in Figure 8.23. The distribution in each slice is fitted with a Gaussian function, with each mean value providing a mean displacement of the Y-residuals per slice. A linear fit of the obtained Gaussian means is used to correct the rotation and offsets. Examples of the plots used during the fine alignment procedure are shown in Figure 8.24.

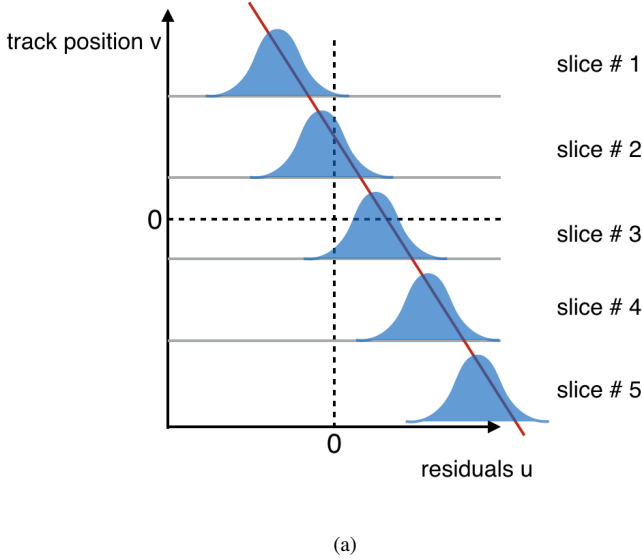


Figure 8.23 – Schematic figure of the fine alignment procedure. Each sensor is divided into slices, residuals are computed for each slice and fitted with a gaussian. The mean of the gaussian is then fitted with a straight line to extract the rotation around the beam-line and leftover offset corrections from the coarse alignment.

Since the tracks themselves depend on the misalignments being corrected by the algorithm, the procedure is iterative. Figure 8.25 shows the applied corrections as a function of the number of iterations until convergence is reached. The reduced χ^2 distribution of the tracks is also shown for different number of iterations in Figure 8.26. The distribution is sharper for high iteration multiplicities and the most probable value converges towards one as expected.

8.2.3.4 Pointing resolution

The pointing resolution of the telescope is defined as the track uncertainty at the DUT position. Given the linear fit used to form the track, the pointing resolution was estimated using the track linear-fit error propagation.

$$\sigma_{(x,y)}(z) = o_{(x,y)}^2 + z^2 s_{(x,y)}(z) + 2z C_{x,y}(z) \quad (8.5)$$

where $o_{(x,y)}$ is the uncertainty on the first telescope plane, $s_{(x,y)}$ is the uncertainty on the slope and $C_{x,y}$ is the covariance matrix of the fit for x and y . Given the geometry of the Telescope and the pixel granularity, the telescope resolution was estimated to be

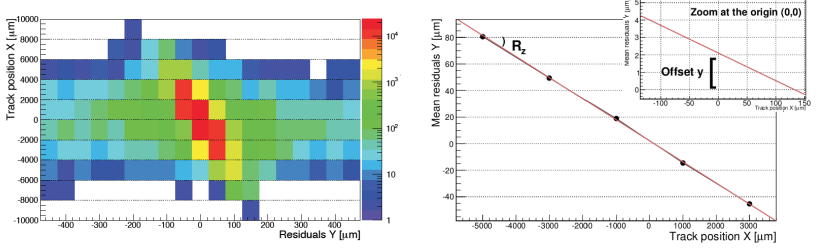


Figure 8.24 – Left) Unbiased Residual along the Y direction as a function of the track X-coordinate position at the DUT. The mean value of each Gaussian fit for the slices and its linear fit in red are shown on the right.

$\sigma_X = 11.7 \mu m$ and $\sigma_Y = 8.3 \mu m$. This computation neglects effects from multiple scattering and charge sharing properties of the pixels at the telescope's plane. The first degrades the pointing resolution at the DUT while the latter improves it, as already discussed in the previous section. The high energy reached at the CERN SPS of 180 GeV for a π^+ beam makes the multiple scattering contribution a sub-leading effect. This can be seen by comparing the RMS of the residuals distribution of the Telescope plane with the pixel resolution (see previous section): $\sigma_{RMS}/\sigma_{pixel} < 1$ for both directions x and y , giving confidence about the validity of the statement. Therefore, the computed resolution of the telescope is merely an upper limit.

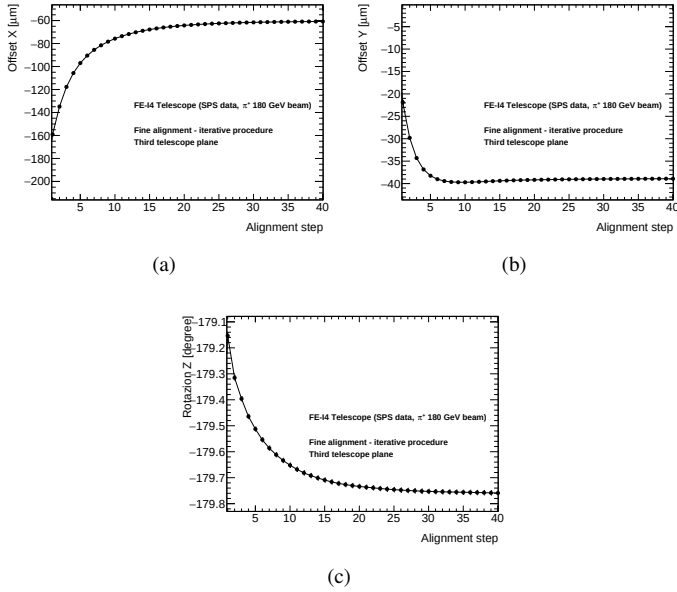


Figure 8.25 – Results of the fine alignment procedure. The offset along X (a), along Y (b) and the rotation along the beam axis (c) are shown as a function of the number of iterations. The curves show the convergence for all these parameters.

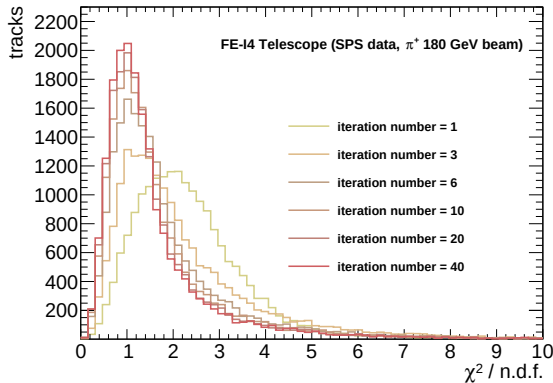


Figure 8.26 – Reduced χ^2 distribution for different iteration of the fine alignment procedure.

8.3 Test-beam results

Test-beam measurements aim to characterize the performance of the DUT in terms of its efficiency and timing properties. This is achieved by comparing the position of the tracks at the DUT and the cluster position at the DUT for a given trigger. For these studies, a pixel detector is considered to be efficient if the interpolated track position is located within an ellipse centered around the measured cluster with the semi-axis being one and half times the pitch of the *macro* pixel as shown in Figure 8.27. The ellipse is chosen to cope with rectangular pixel and it is defined as follows:

$$d = \sqrt{\left(\frac{x_{track} - x_{cluster}}{p_x/2}\right)^2 + \left(\frac{y_{track} - y_{cluster}}{p_y/2}\right)^2} \quad (8.6)$$

The per-pixel efficiency is thus defined as $\frac{N_{matched}}{N_{tot}}$ where $N_{matched}$ is the number of matched clusters-to-tracks and N_{tot} is the total number of reconstructed tracks passing through it. Inefficient events are taken into account as events in which no hit were measured at the DUT, when a valid track interpolation to the DUT was found.

In the following, results in terms of timing and efficiency of un-irradiated and irradiated CCPDv4 will be presented and results of un-irradiated CCPD full-size demonstrators will also be discussed.

8.3.1 Characterization of the h18 prototypes

During the 2015/16/17 test-beam campaigns several CCPD prototypes were tested. The first sample characterized was un-irradiated and it showed an efficiency of 99 % within 3 BC. Given these promising results, R&D efforts were conducted towards a characterization of irradiated prototypes with protons and neutrons up to $5 \cdot 10^{15} n_{eq}/cm^2$. The performance achieved by the irradiated samples were excellent, showing high efficiency and fast collection. In view of these results, a full-size demonstrator has also been produced and tested at the Fermilab test-beam facility and at the CERN SPS. Results will be presented in detail in the following sections.

8.3.1.1 Non-irradiated samples

Un-irradiated CCPDv4 samples were tested in the 2015 test-beam at the CERN SPS using the FE-I4 Telescope. In order to perform a voltage-to-charge calibration of the threshold value of the on-pixel pre-amplifier, a ^{55}Fe source was used. Assuming 3.65 eV as the ionization potential for silicon, a conversion factor of $8.6e^-/mV$ was found by using the K_α peak of ^{55}Fe . The sensor was then tuned using the Caribou setup. The threshold distribution obtained after tuning resulted in a mean of $607 e^-$ and a Gaussian width of $73 e^-$ [7].

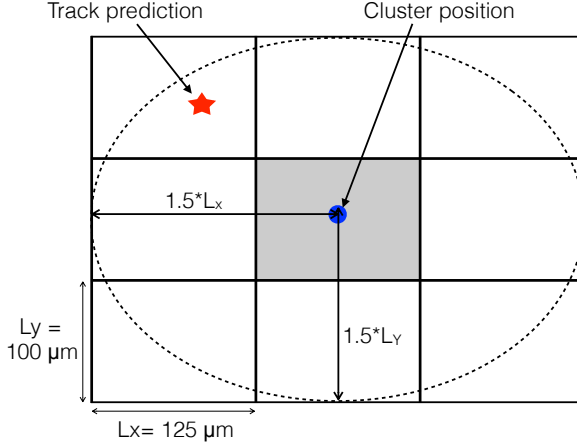


Figure 8.27 – Search area used to calculate the efficiency. Each $125\ \mu\text{m} \times 100\ \mu\text{m}$ macro-pixel (shown in gray) is formed by three single HV-CMOS pixels [7].

The cluster size distribution is shown in Figure 8.28. Since it is directly related to collection properties of the detector, it represents an effective measurement of charge sharing and it is therefore one of the key distributions used to characterize silicon detectors. The events with single-pixel clusters were recorded in $\sim 78\%$ of triggered events while clusters formed by two pixels were observed in $\sim 20\%$ of the cases. The remaining 1% of the clusters featured three or more hits and can safely be neglected in the following discussion.

Residuals distributions are shown in Figure 8.29. The RMS of the distributions are in reasonable agreement with the expected intrinsic resolutions of the macro-pixel in the case of single hit in cluster: $\sigma_X = 125/\sqrt{12} = 36.1\ \mu\text{m}$ and $\sigma_Y = 100/\sqrt{12} = 28.9\ \mu\text{m}$.

Figure 8.30 shows the timing distribution, in bins of $25\ \text{ns}$, for different cluster sizes. Among the possible mechanisms leading to signal leakage into neighboring pixels (e.g. cross-talk, diffusion of charge carriers, δ -electrons), diffusion is the dominant one for the prototype under test. Slow carriers diffusing into the non-depleted region of the bulk of the detector generate a slowly raising and faint signal, prone to time-walk effects. A long tail corresponding to slow collected signal is observed for all cluster sizes. The timing distribution of clusters of size one, instead, shows a narrower distribution giving evidence of signal collected by drift. The long tail is therefore due to the clusters of size two as shown in Figure 8.30. By separating the timing distribution with fastest and slowest hits, it becomes evident that the diffused charge in large multiplicity clusters (charge sharing) leads to the long tail. The timing distribution of clusters of size one is

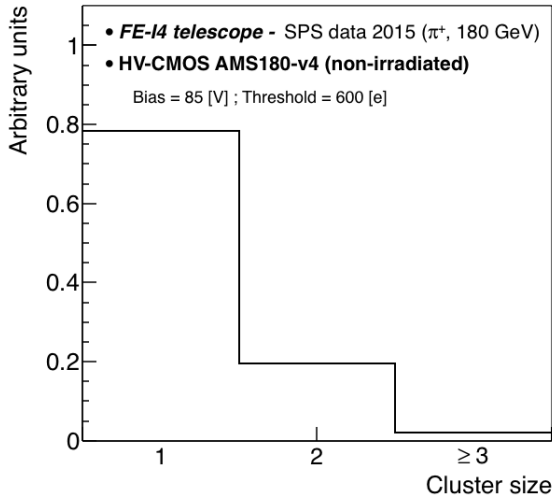


Figure 8.28 – Cluster size distribution under nominal operation conditions. The distribution is normalized to unity.

very similar to that of the fastest hit of the two-pixel clusters since both are collected by drift.

As discussed in section 8.1.1 the *STime* pixels have a fixed pixel ToT information used to map the sub-pixels to the *macro*-pixel thus preventing a quantitative estimation of the collected charge. A direct measurement of time-walk cannot be performed using *STime* pixels. To further study this effect, the *Analog* sub-pixel matrix of the CCPDv4 prototype was used. The main difference between the two pixel flavors is that the *Analog* pixel matrix does not feature a discriminator on-chip thus allowing for more accurate study of time-walk effects. As shown in Figure 8.31, there is a clear dependence between the timing and signal amplitude, which is due to time-walk for this HV-CMOS prototypes. As the electronics on-chip between *STime* and *Analog* pixels differs only by the presence of the discriminator, it is reasonable to deduct the the same time-walk effect in *STime* pixels. The *Analog* pixel matrix was only used to corroborate the previous statement and in the following only results related to the *STime* pixels will be further discussed.

In order to focus on the properties of the charge collected by drift, and to limit the effects of the known time-walk present in this version of the HV-CMOS sensor, only results for the fastest hit are shown in the following.

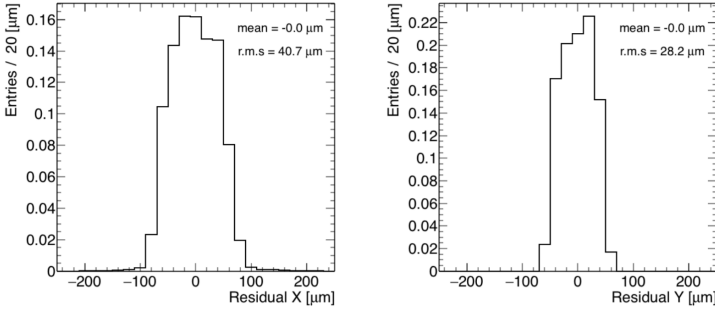


Figure 8.29 – Residuals distribution in the X and Y direction.

The detection efficiency of the non-irradiated sensor under test at a bias voltage of 85 V is shown in Figure 8.32. An homogenous efficiency above 99 % is observed for all pixels. The average efficiency of the sensor was found to be: $\bar{\epsilon} = 99.7\%$. To avoid edge-effects due to the finite resolution of the telescope, the outermost columns and row were excluded from the computation of the average efficiency.

Using the resolution of the telescope it was possible to study in-pixel efficiency maps. To increase the available statistics of the plot, all tracks in the fiducial (excluding outermost columns and rows) pixel-matrix were merged into a single pixel. Figure 8.33 shows the in-pixel efficiency of a *macro*-pixel and the relative contributions to the efficiency of different cluster sizes. The overall in-pixel efficiency shows a very homogeneous distribution indicating that, on average at 80 V and $600 e^-$, no inefficient regions are identified in the sensor. Since charge sharing is improbable when a single hit is found in the cluster, the in-pixel efficiency for $CS=1$ shows a region of high efficiency in the central region of the pixel. Events with a cluster size of two, instead, contribute mainly to the edge regions, as expected from charge sharing between neighboring pixels. The less common events in which the cluster contains three or more pixels are localized at the four corner regions.

The efficiency as a function of the global discriminator threshold is shown in Figure 8.34 for a bias voltage of 80 V. At low threshold values, the noise of the sensor dominates degrading its performance. At high values, instead, the signal is cropped resulting in low efficiency. In between of these two regions, a stable plateau is observed with efficiency above $\bar{\epsilon} > 99\%$ for a threshold of 385 and $690 e^-$.

The efficiency as a function of the sensor bias voltage is shown in figure 8.35 for a threshold of $600 e^-$. The average efficiency is larger than 99 % for all the tested bias voltages. It is noticeable that the HV-CMOS prototype shows high efficiency even at low bias voltage. In this regime, charge is collected by diffusion and thanks to the in-pixel pre-amplifier an high efficiency is achieved⁴. At higher HV values the efficiency

⁴The large uncertainty at 10 V is due to the fact that during that run, the ROI trigger was not set, thus

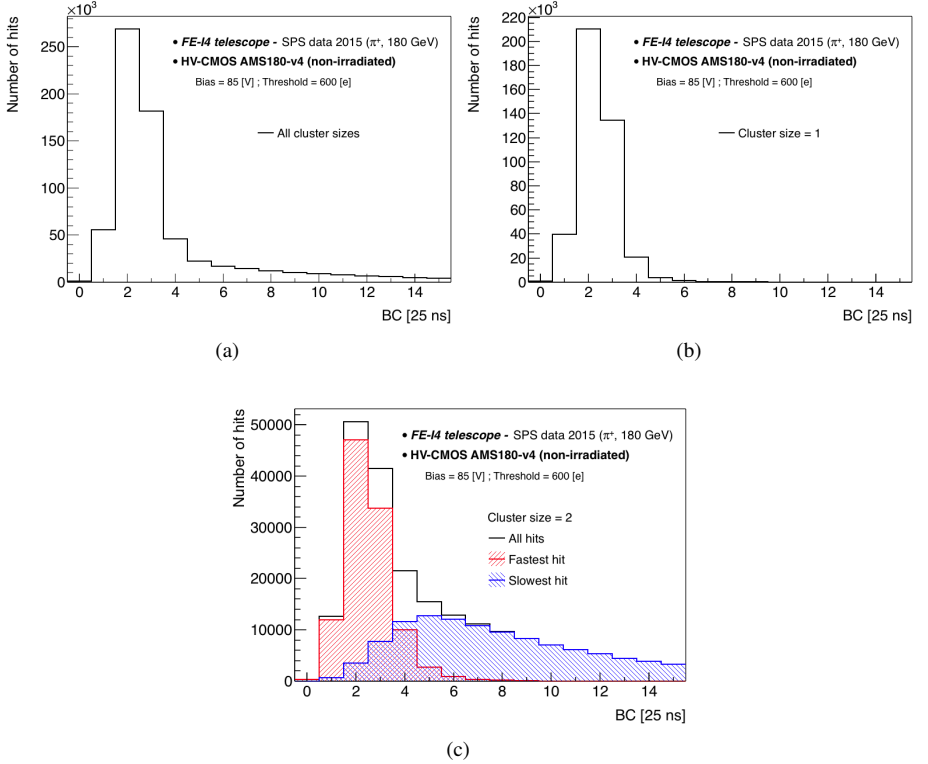


Figure 8.30 – Timing distribution of the DUT hits in 25 ns bins for (a) all cluster sizes , (b) cluster size one and (c) cluster size two. In (a), all pixels are shown. In (c), the distribution of the measured time of each of the two pixels in the cluster is shown.

increases following an approximately linear function. This is due to the fact that the electric field in between pixels is not saturated leading to un-depleted regions in the bulk of the sensor where charge is mostly collected by diffusion. As shown in Figure 8.35, the efficiency at the border of the sensor is slightly reduced. This happens mostly along the y -axis where the *macro*-pixel is composed of 3 sub-pixels, among which the released charge is shared.

In order to characterize the timing properties of the DUT, the efficiency was computed in each time-bin used for the readout, as shown in Figure 8.36. For increasing bias voltages, the charge is mostly collected by drift, the efficiency increases and the timing response of the sensor is faster. The right plot of Figure 8.36 shows the cumu-
reducing the number of collected events at the DUT.

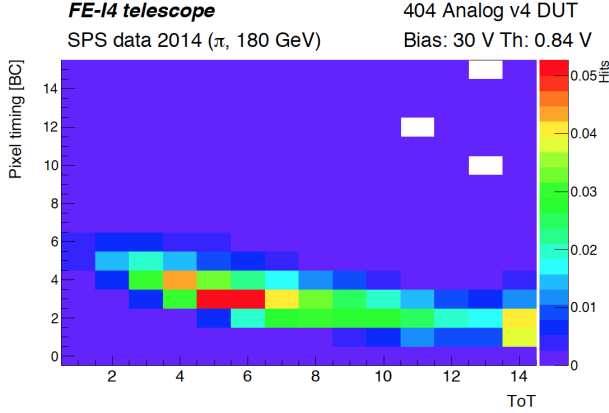


Figure 8.31 – Normalised distributions of the pixel timing versus ToT for *Analog* pixels.

lative efficiency for different time-bins. The distribution was computed with respect to the consecutive maxima also shown in Figure 8.36. At 85 V, 90 % of the signal is collected within 3 BC. To further investigate the source of the slowest component, in-pixel efficiency distribution are produced in different time-bins as shown in Figure 8.37 for an bias voltage of 20 V to enhance features related to the diffusion component. A clear pattern is revealed: as the collection time becomes slower, the efficiency shifts towards the edge of the pixel, giving evidence, once more, for a slow diffusion component and related time-walk effects. A similar effect is observed for a HV = 80 V, closer to the optimal working point of the detector, as shown in Figure 8.38 where the average in-pixel timing map is outlined.

In summary, the un-irradiated CCPDv4 prototypes show high efficiency, and a promising timing response of 90 % within 3 BC. This is not yet sufficient to be operated in a HL-LHC experiment and further developments are ongoing. However, these results demonstrate the feasibility of such technology in a high-rate environment.

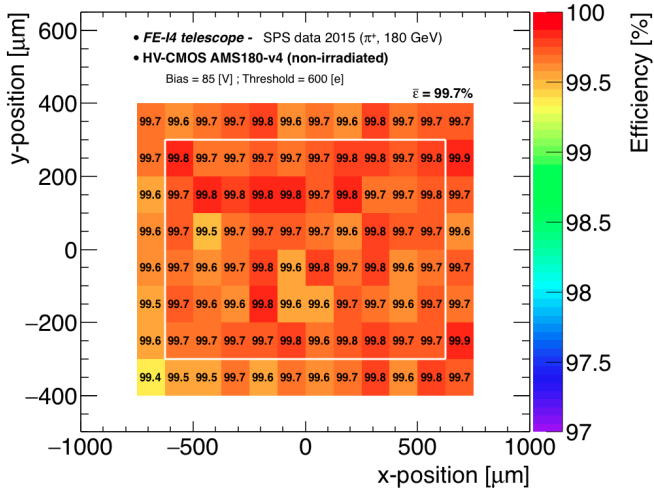


Figure 8.32 – Efficiency map for the non-irradiated sample under test. To avoid edge-effects, the average sensor efficiency is computed only for the pixels inside the white box.

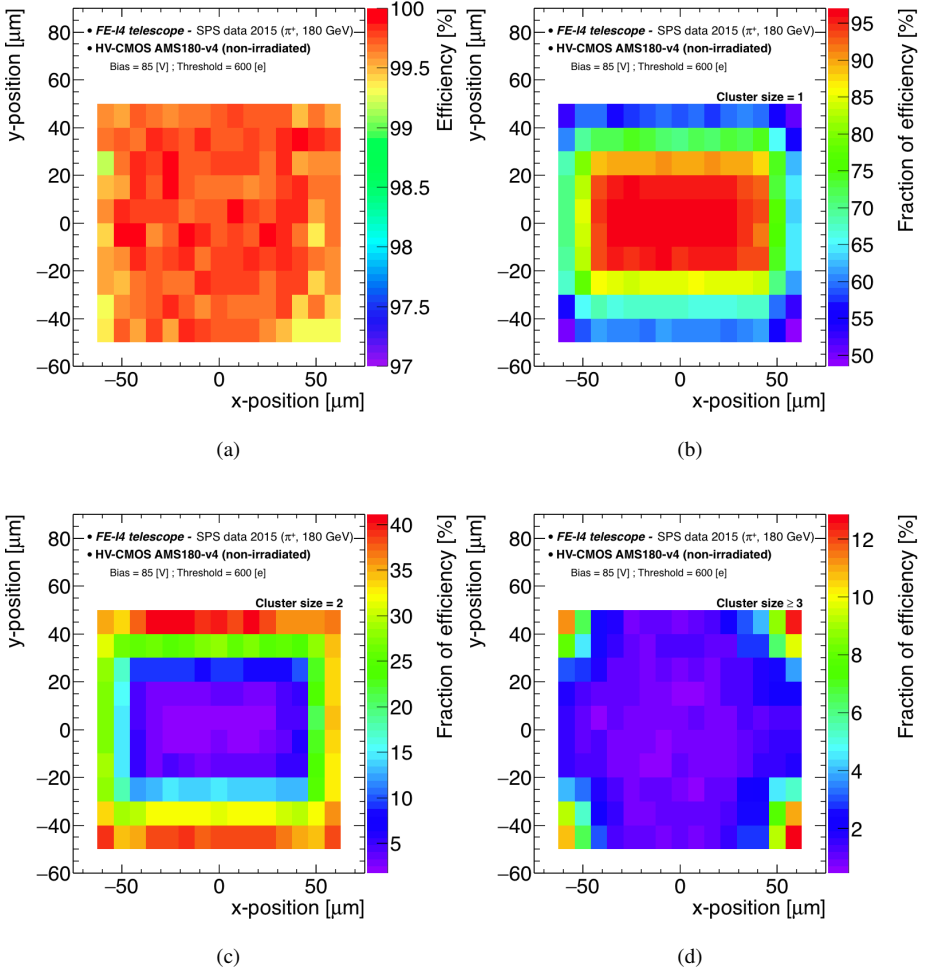


Figure 8.33 – Efficiency of a *macro*-pixel corresponding to three single HV-CMOS pixels connected to a FE-I4B readout cell. (b-d) Relative contributions to the distribution shown in (a) from pixel clusters of different sizes [7].

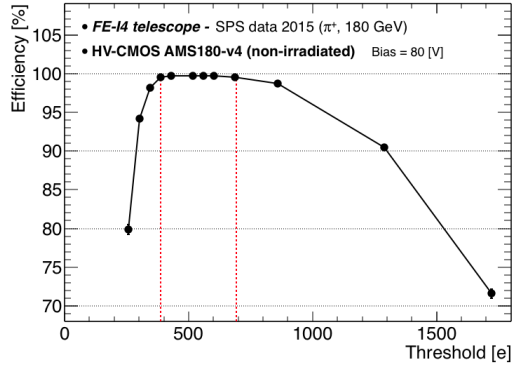


Figure 8.34 – Average efficiency as a function of the global threshold. The red lines outline the regions with $\bar{\epsilon}$ above 99 % [7].

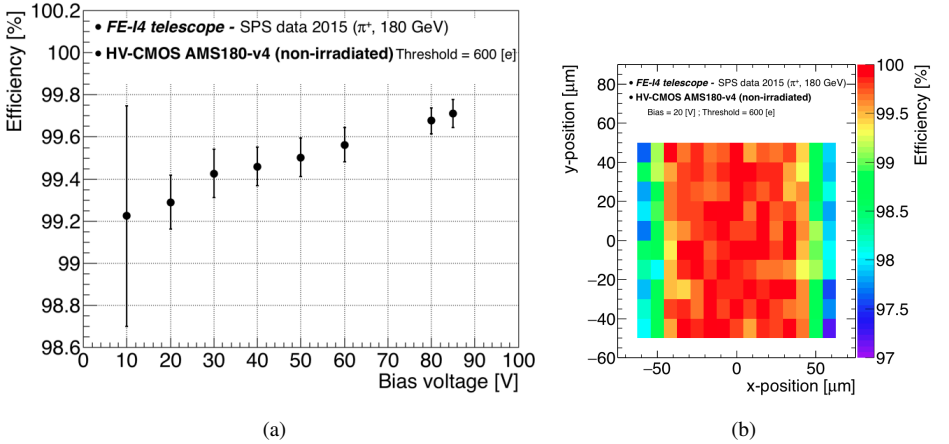


Figure 8.35 – a) Efficiency for different biasing voltage. During the data-taking at HV = 10 V, the ROI trigger was not used leading to lower statistics at the DUT and thus large statistical uncertainty. b) In-pixel efficiency distribution for a bias voltage of 20 V [7].

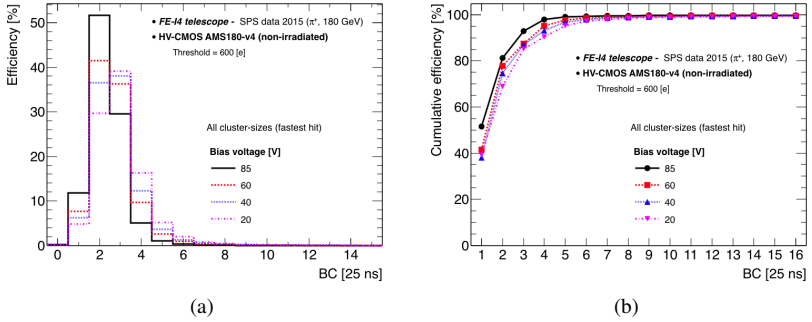


Figure 8.36 – a) Efficiency and (b) cumulative efficiency in bins of 25 ns for different sensor bias voltages. For cluster sizes of two or more, only the fastest hit is shown. The first data point shown in (b) corresponds to the maxima of the distributions shown in (a) [7]

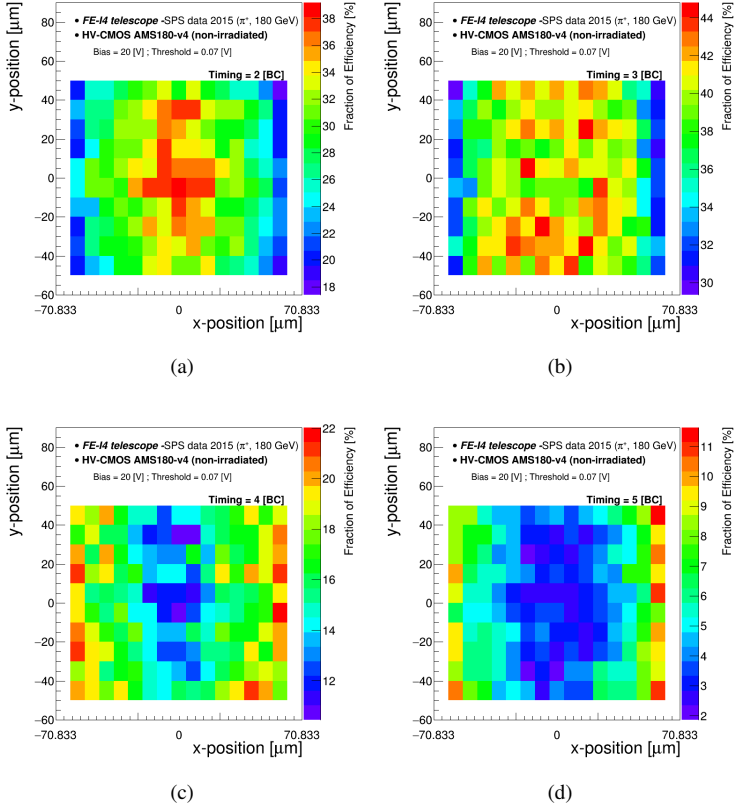


Figure 8.37 – In-pixel efficiency for different time-bins. The threshold quoted in the plot is equivalent to $600 e^-$.

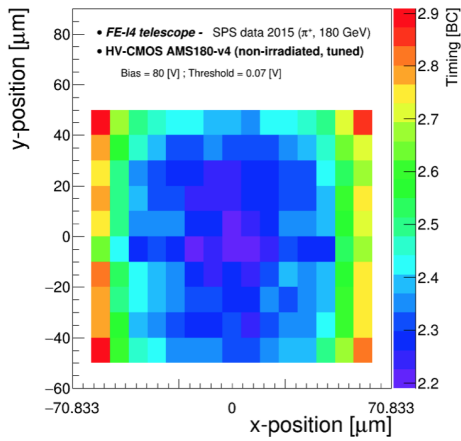


Figure 8.38 – In-pixel timing map showing the mean timing of the cluster as depending on the track position [7].

8.3.1.2 Neutron and proton irradiated samples

Radiation damage in silicon pixels is one of the main challenges in the development of tracking detectors for LHC experiments. In order to study the response of the HV-CMOS sensors at an irradiation level foreseen for HL-LHC, a set of irradiated samples were produced. The samples were irradiated using reactor neutrons in Ljubljana and 18 MeV protons at the Bern cyclotron to fluences between $1 \cdot 10^{14}$ and $5 \cdot 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$. The irradiation steps were chosen to emulate the lifetime of an outer layer of the tracking detector at the HL-LHC, without considering any replacement of the stave. The samples were kept at a temperature of around -15°C during data-taking to reduce the noise of the irradiated DUTs. Finally, the calibration factor between deposited charge and threshold voltage of $\sim 8.6 \text{ e}^-/\text{mV}$ obtained from the un-irradiated sensor (see previous section) is still valid for irradiated ones, however, as it was not re-measured, the thresholds are given in mV throughout this section.

To characterize edge-effects due to the finite resolution of the telescope, a more detailed study was performed by looking at the in-pixel efficiency for the outermost pixel column as shown in Figure 8.39 for the sensor irradiated at $10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$. A uniform distribution up to around $10 \mu\text{m}$ from the edges of the sensor is observed. This is compatible with the telescope resolution described in section 8.2.3.4 and can be explained by particles passing outside the active pixel sensor area that are wrongly associated with the edge of the DUT after reconstruction. To veto these tracks, a fiducial area extending up to 3σ away from the edge of the sensor is used in the subsequent analysis.

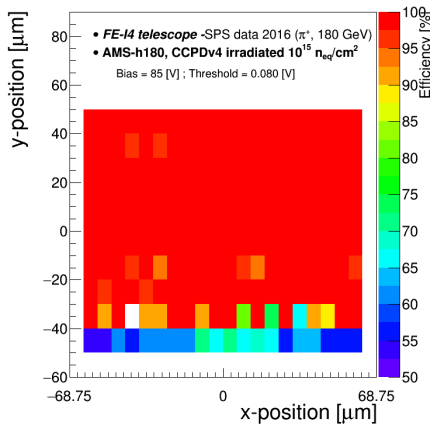


Figure 8.39 – In-pixel efficiency distribution for the lower row of the sample. A decrease of efficiency is observed at the edge.

Residual distributions are shown in Figure 8.40. The distributions in both directions are centered at zero, indicating that a good alignment was obtained. The RMS, as already observed in the analysis of non-irradiated samples, are compatible with the theoretical single-pixel resolution. Table 8.3 shows the cluster sizes for the different irradiated samples. The diffusion component observed in the non-irradiated samples is suppressed due to the introduction of shallow traps due to radiation damage which reduces the charge sharing effect and, in turn, the cluster sizes. The large majority of clusters have a size of one for all of the irradiated samples.

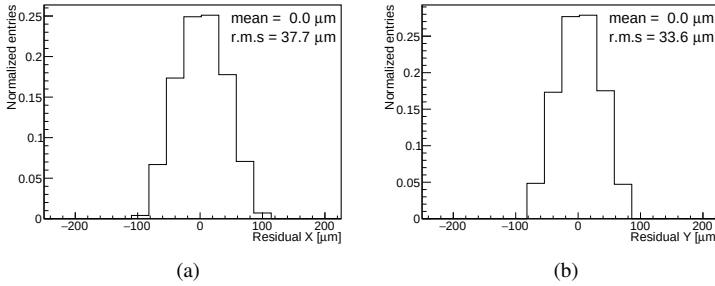


Figure 8.40 – Normalised residual distributions of the DUT irradiated at $1 \cdot 10^{15} n_{eq}/cm^2$ along the x (a) and y (b) directions [8].

Table 8.3 – Cluster size fractions for different fluences [8].

Fluence [n_{eq}/cm^2]	0	$1.3 \cdot 10^{14}$	$5 \cdot 10^{14}$	$1 \cdot 10^{15}$	$5 \cdot 10^{15}$
CS = 1	0.783	0.970	0.958	0.978	0.961
CS = 2	0.196	0.028	0.038	0.020	0.034
CS ≥ 3	0.020	0.002	0.004	0.002	0.004

An average efficiency of 99.7% was measured showing a flat distribution at both sample- and pixel-level as shown in Figure 8.41. Given the large number of DUTs, the efficiency distributions are presented by means of histograms. Figure 8.42 shows the efficiency histograms for samples at different irradiated doses outlined in the plot. Average efficiencies of 98.1, 99.7, 99.7 and 97.6% are found for samples irradiated at $1.3 \cdot 10^{14}$, $5 \cdot 10^{14}$, $1 \cdot 10^{15}$ and $5 \cdot 10^{15} n_{eq}/cm^2$ respectively. It can be noted that for the sample irradiated at the highest fluence of $5 \cdot 10^{15} n_{eq}/cm^2$ there are outlier pixels, most probably originating from deteriorated circuits due to the rather high irradiation. It is also worth mentioning that this fluence is five times larger than the expected maximum fluence of the outermost pixel layers of the ITk.

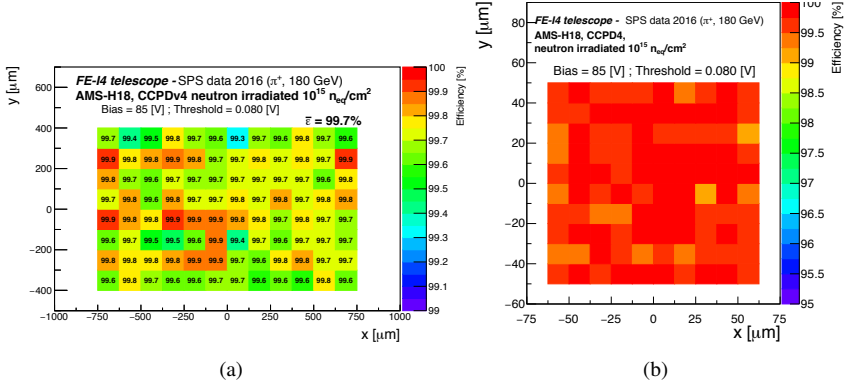


Figure 8.41 – a) Hit efficiency map for CCPDv4 neutron-irradiated with $1 \cdot 10^{15} \text{ N}_{\text{eq}}/\text{cm}^2$ b) Sub-pixel hit efficiency map overlaid from all central pixels. No significant efficiency loss is visible in any region of the pixel [8].

Bias-voltage and threshold scans were conducted to characterize the working conditions of the DUTs. The results are shown in Figure 8.43 and 8.44. For the bias voltage scan, a plateau is reached after about 40 V for most of the irradiated sensors, in particular the very low and very high fluences profit from going to the highest possible bias voltages of about 85 V. This is due to the fact that the HV-CMOS sensor, contrarily to planar devices, are not operated at full depletion depth. The thin depletion zone of HV-CMOS sensors keeps increasing for higher value of the biasing voltage thus improving the collection efficiency. For the middle fluences, the extension of the depleted region is already large enough thanks to the acceptor removal effect (see section 7.4) to not require the highest possible bias voltages. The sample irradiated at $5 \cdot 10^{14}$ was found to be noisier than the other samples at 85 V, as visible from the decrease of efficiency at that HV value. For the sample irradiated at the lowest fluence of $1.3 \cdot 10^{14}$ and at intermediate biasing voltage, a decrease of efficiency with respect to the two sensors irradiated at $5 \cdot 10^{14}$ and $1 \cdot 10^{15}$ is observed. This trend is in line with earlier measurements [124] that observed an initial reduction of collected charge due to the loss of diffusing charge carriers not yet mitigated by the increase of the depleted region due to the acceptor removal effect. For the largest irradiation level, an increase of efficiency is observed for high HV values as outlined in the plot. This is attributed to charge multiplication effects: the high electric field combined with the high-density of traps generated by the radiation damage can lead to charge multiplication due to impact ionization when sufficiently high voltage is applied to the sensors, a more detailed description of which can be found elsewhere [136].

With regard to the threshold scans, it can be seen that at very high thresholds there

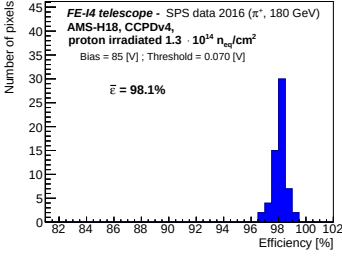
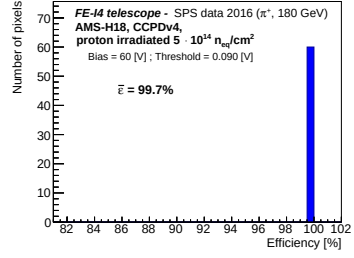
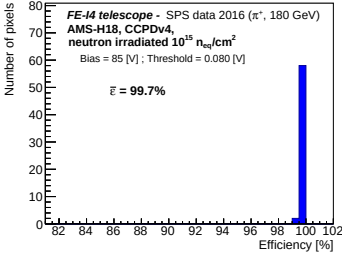
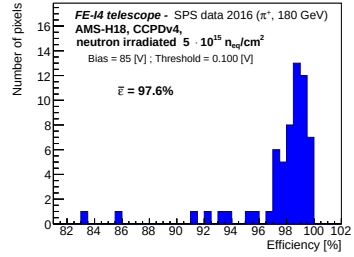
(a) Hit efficiency histogram for $1.3 \cdot 10^{14} n_{eq}$.(b) Hit efficiency histogram for $5 \cdot 10^{14} n_{eq}$.(c) Hit efficiency histogram for $1 \cdot 10^{15} n_{eq}$.(d) Hit efficiency histogram for $5 \cdot 10^{15} n_{eq}$.

Figure 8.42 – Hit efficiency histograms for different fluences of protons (upper row) and neutrons (lower row) [8].

is a loss of efficiency due to low charge signals not being detected. This effect is barely visible for the sample irradiated at $5 \cdot 10^{15} n_{eq}/cm^2$, as already observed from the bias scan, which is presumably due to the higher depletion depth present at this irradiation level. For low threshold settings, the noise dominates, leading to the busy configuration of the discriminators which may be unable to detect particles. At intermediate threshold values, a stable plateau is observed which is more prominent for the intermediate fluences, while for $1.3 \cdot 10^{14}$ and $5 \cdot 10^{15} n_{eq}/cm^2$ the lack of signal due to small depletion depth or increased trapping reduces the plateau region.

These results are very promising and demonstrates the capability of HV-CMOS sensor to collect particles with high efficiency up to irradiation levels foreseen for the ITk. The following discussion will be focus on their performance in term of timing properties.

One of the upgrades made for the analysis of irradiated samples is the implementation of a Clock-Phase Veto (CPV) to improve the time distribution of the DUT due to the sampling of the clock cycle of 25 ns of the FE-I4. During ATLAS operation, the FE-I4 is synchronized to the bunch crossings of the LHC beam. Particles collide in a narrow

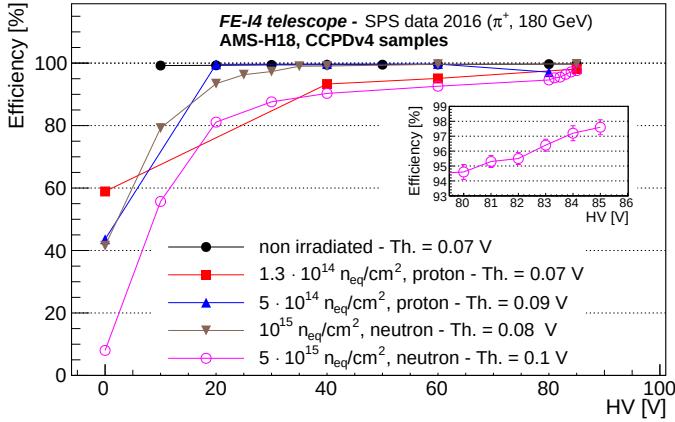


Figure 8.43 – Average hit efficiency as a function of bias voltage [8].

time window with respect to the rising edge of the FE clock. However, the beam-line of the CERN SPS does not provide a bunched structure thus the time of arrival of the particle and the FE clock are asynchronous [8]. This leads to an artificial smearing of the timing distribution at the DUT. In order to reduce this effect, a CPV was implemented, where only particles that are detected in an interval of 6.4 ns of the FE clock-phase are accepted as depicted schematically in Figure 8.45. The effect of the veto for a telescope plane is also shown in Figure 8.45. Thanks to the CPV, the remaining timing delays at the DUT are mostly decoupled from telescope effects and are likely to be caused by either slow charge collection, slow rise time of the amplifiers in the on-pixel circuits or by time-walk [8].

The timing distribution of the four DUTs is shown in Figure 8.46. Most of the events are collected in one timing bin and 95% of the charge is collected within three BCs for the four tested fluences. The effect of acceptor removal is also visible as the collection time gradually improves for higher fluences due to the increase of electric field causing faster collection. At the highest irradiation level of $5 \cdot 10^{15} n_{eq}/cm^2$, a degradation in the time resolution is observed most likely due to the lower signal collected and the higher threshold, both leading to a more pronounced time-walk effect.

The time distribution is also shown for different biasing voltages for the sample irradiated at $1 \cdot 10^{15} n_{eq}/cm^2$. For low HV, the small depleted region leads to a slow collection time. As the HV increases, the electric field extends further into the bulk of the sensor thus improving the time resolution significantly. To further investigate the timing properties of the sensor, the in-pixel mean timing map is shown in Figure 8.47. Similar to the case of un-irradiated sensors, the charge is collected faster in the central

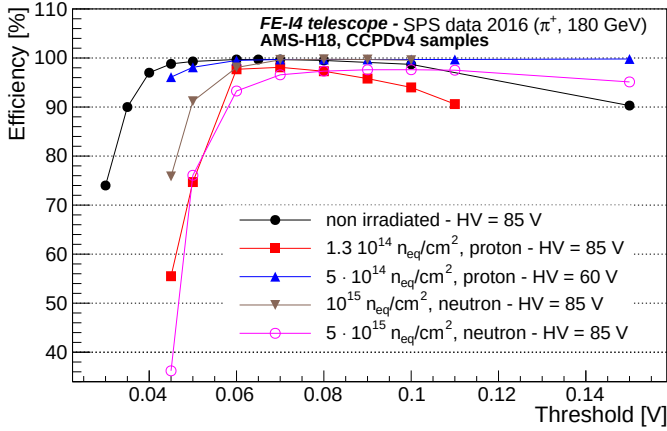


Figure 8.44 – Average hit efficiency as a function of threshold voltage [8].

region, while events at the edges of the pixel are slower on average, as already observed in un-irradiated devices (see previous section). The HV-CMOS sensors are biased from the top side leading to regions of low electric field strength behind the biasing electrode placed in between pixels. This effect was studied with TCAD simulations and will be discussed in detail in Section 8.4.

These results give strong evidence for the radiation tolerance of HV-CMOS sensors and their suitability as sensors for use in large-area silicon-based tracking detectors at high-radiation and high-rate environment.

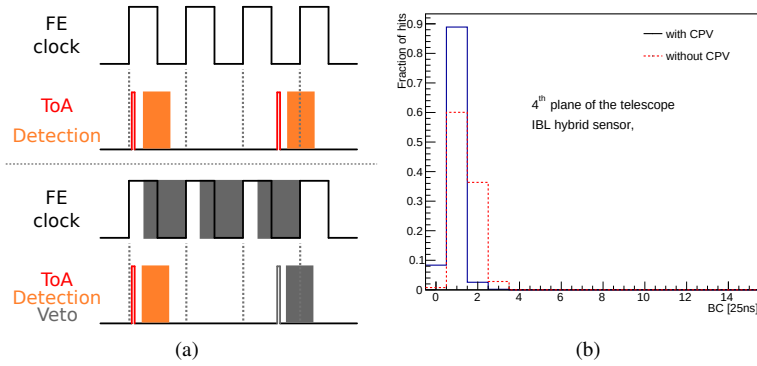


Figure 8.45 – a) Schematic of the Clock-Phase Veto. Triggers from particles arriving late in the FE-I4 clock cycle are discarded, emulating a bunched particle beam. b) Timing distribution of a planar sensor of the *telescope plane* with and without Clock-Phase Veto [8].

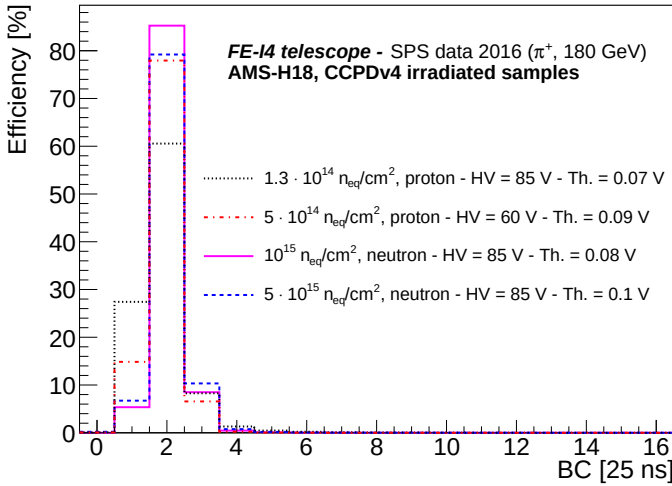


Figure 8.46 – Timing distributions for the four irradiated CCPDv4 samples at the operational bias voltages [8].

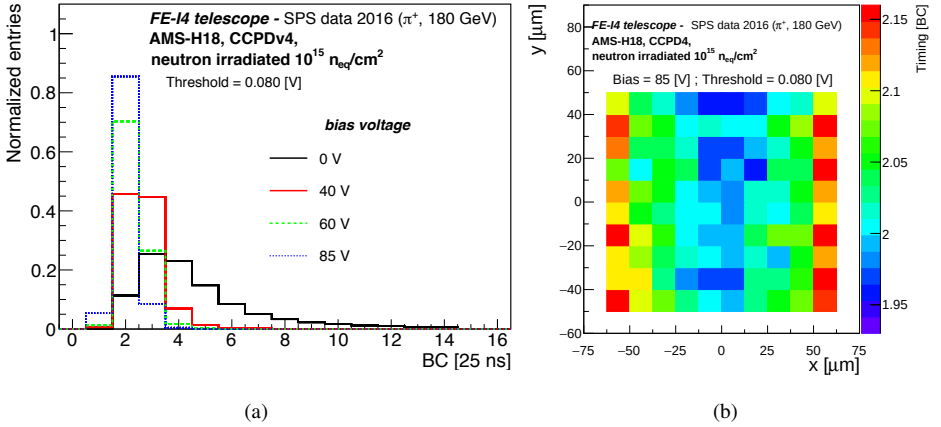


Figure 8.47 – a) Timing for a CCPDv4 sensor for four values of the bias voltage. b) In-pixel timing map showing the mean timing of the event as depending on the track position inside the pixel [8].

8.3.2 Characterization of the H35 full demonstrator

In view of the promising results obtained from the CCPD $v4$ prototypes, a full-size demonstrator was tested at the CERN SPS and Fermilab MTest facilities. In order to investigate the impact of substrate resistivity on the detection efficiency and time resolution, samples with four different resistivities of 20, 80, 200 and 1000 Ω cm were produced by the foundry, assembled and finally tested using the FE-I4-Telescope. The sensors were capacitively coupled to the FE-I4 chip at the University of Geneva using a semi-automatic *Accupra* 100 flip-chip bonder. The gluing process showed good uniformity over the demonstrator surface thus ensuring an homogenous coupling capacitance in between the sensor and the FE-I4 chip. The breakdown voltage was measured, for most resistivities, to be around 170 V, as discussed in detail here [9]. One of the major differences with respect to the prototypes is the pixel size that was increased to $250 \times 50 \mu\text{m}$ to match the FE-I4 pixel size. Because of this, no sub-pixel encoding is needed and the discriminator on the HV-CMOS sensor was removed such that the amplifier output is directly AC coupled to the FE-I4, allowing for a direct ToT measurement.

The H35 HV-CMOS demonstrator features several sub-pixel matrices. For these measurements only the Analog1 and Analog2 (see section 8.1.2) were tested. A summary of the test-beam data-taking conditions used for this analysis are detailed in Table 8.4.

Table 8.4 – Summary of measurements performed on the H35DEMO prototypes in test beam. Note that the FE-I4 threshold is the signal being transferred by the capacitive injection from the H35DEMO, not the charge generated on the sensor [9].

Resistivity [Ω cm]	Matrix	High-Voltage [V]	Threshold [ke^-]
20	Analog 1	0-160	1.5, 2
80	Analog 1	0-160	2.5, 3, 4
200	Analog 2	0-140	2, 2.5, 3, 4
1000	Analog 1	0-160	1.5, 2, 2.5, 3

The cluster-size distribution for different resistivities and biasing voltages is shown in Figure 8.48. Most of the clusters are composed of a single pixel, which is due to the large size of the pixel compared to the previous prototypes. The effect of the HV is more important for higher resistivities, in particular for 1000 Ωcm where a competing effect in the charge collection mechanism is visible. Since the bias is applied from the n -well located at the top of the sensor, when the depletion depth becomes larger than the distance between the collecting and biasing electrode, electric dispersion occurs in between them. This leads to a region in the deep bulk of weak electric field strength which, in turn, leads to an increase of cluster-sizes for intermediate voltages. This effect

will be described in more details in the next section using TCAD simulations.

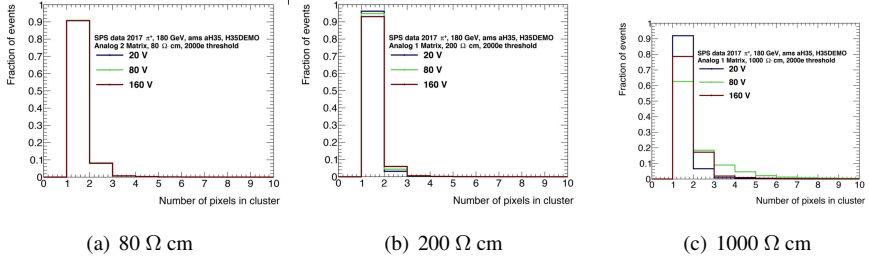


Figure 8.48 – Cluster size versus bias voltage and different substrate resistivity for a 2000 e^- threshold [9]

As most clusters were formed of a single pixel, the spatial resolution is determined primarily by the pixel size. Residual distributions are depicted in Figure 8.49. The noise, being uncorrelated with the traversing particle, is estimated with a straight line fit. The non-gaussian tail of the distributions can be explained by δ -electrons and cross-talk due to capacitive coupling between a pixel pad and its neighbours. Given the large sample size of the detector, the beam illumination is not uniform resulting in the tilt observed at the tail of the residual plots. This effects were not visible with CCPD v_4 due to the small size of the prototypes.

The efficiency map and the bias scan for different resistivities and threshold are shown in Figure 8.50 for the Analog1 matrix, sub-matrix 2 (similar results are obtained for the different sub-matrices). The homogeneous behaviour obtained from the efficiency map confirms the good level of gluing uniformity. Across the active pixel matrix, a single defective pixel is observed. The efficiency varies as a function of the resistivity of the sample as expected. Since $d \sim \sqrt{\rho V}$, the higher the resistivity, the smaller the bias voltage needed to obtain a given detection efficiency. All samples tested show an efficiency of 99% confirming the already promising results obtained with small prototypes.

The timing distribution is also studied as shown in Figure 8.51 for the second high-gain matrix. Only a faint dependency with the biasing voltage and resistivity is obtained with most of the charge collected in 2 BC. Since the collection time is proportional to the velocity of the carriers, which is expected to vary for different biasing and resistivity conditions, it is reasonable to deduct that the timing resolution is limited by jitter⁵ of the pre-amplifier rather than from the charge collection mechanism in the bulk of the

⁵Jitter is defined as a smearing of time resolution due to different noise sources.

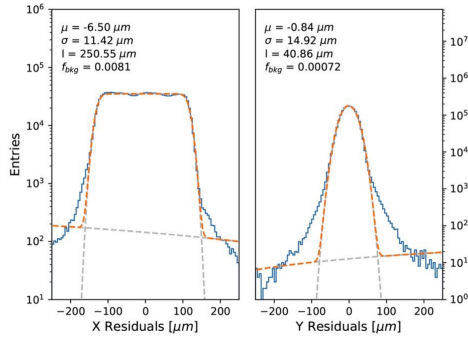


Figure 8.49 – Residuals distribution. The fit of a gaussian convoluted with a box function (orange) is shown. The background is estimated with a straight line fit from the tails of the distributions [9].

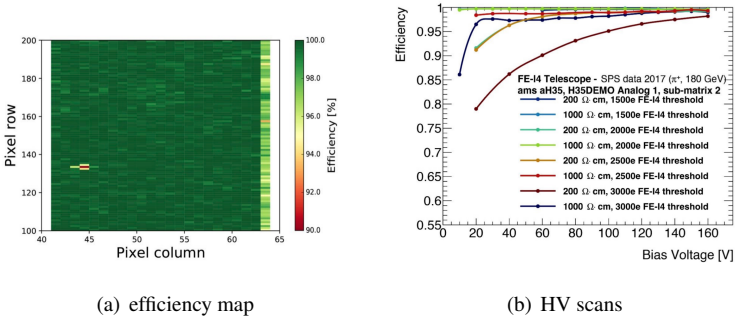


Figure 8.50 – a) Efficiency maps for the Analog matrix 1. The decrease of efficiency of the last columns is due to the proximity with the pixels of the neighbouring matrices, which can collect some of the charge at the edge of the matrix due to charge sharing. A single defective pixel is also present in the matrix. b) Bias scan for different resistivities and threshold for the Analog 1 matrix, sub-matrix two [9].

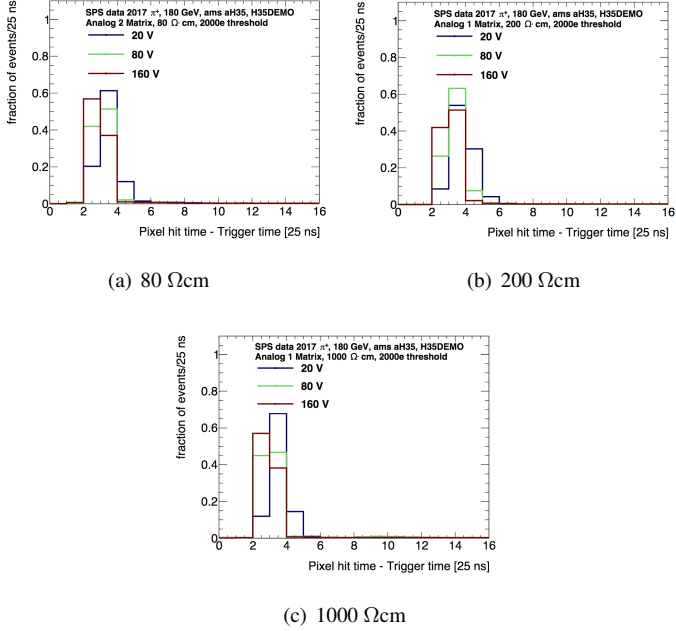


Figure 8.51 – Timing distribution for different resistivities [9].

detector.

To summarize, results of the H35DEMO confirmed the high detection efficiency measured from the small size prototypes. The time distribution showed evidence of jitter in the in-pixel amplifiers. In the next version of the sample, upgrades to the electronics are expected to further improve the timing resolution.

8.4 Investigation of charge collection properties of CMOS sensors using TCAD simulations.

Technology Computer-Assisted Design (TCAD) is a finite element simulator which allows one to find approximate solution to a system of coupled partial differential equations. Finite element simulation is based on variational techniques that locally simplify a complex system of differential equations into a linear system that can then be solved by simple linear algebra methods. The approximation is carried out by sub-dividing the surface or volume of the silicon under analysis into rectangular, triangular, prismatic or pyramidal sub-elements, small enough that the solution is polynomial in each meshing

element. The interested reader can find a more detailed description of finite element simulations elsewhere [137].

TCAD simulations are widely used in high-energy physics experiment to simulate many different aspects of semiconductor devices, ranging from the fabrication process to the charge collection mechanism. In the following, results of the the electrical characteristics by means of TCAD simulation of the H35Demo will be discussed.

8.5 The model layout

To accurately emulate a silicon device, TCAD simulation packages offers the possibility to either simulate the full production process of the sensor or to use a simplified structure based on analytic functions to define the doping profiles. In order to perform a simulation of the full production process it would be necessary to have access to many construction parameters such as annealing time, temperature, and much more. Usually foundries do not make those parameters publicly available, thus reducing the accuracy of the simulation. As a consequence, analytic functions were used to describe the doping profile.

A simulated pixel structure of the H35Demo is shown in Figure 8.52 while the doping profile on the biasing deep n -well is shown in Figure 8.53. To emulate the pixel cell of the H35Demo, the pixel is divided into 3 sub-pixels. The basic pixel-structure has been described in details in section 8.1.2. The central deep n -well hosts a shallow n -well and p -well. The three sub-pixels are connected to a common read-out. The bias electrodes are located at the top of the shallow p -layers in between two sub-pixels.

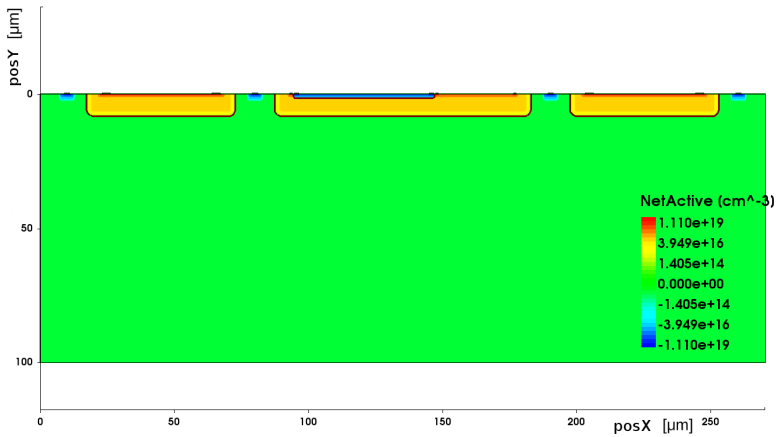
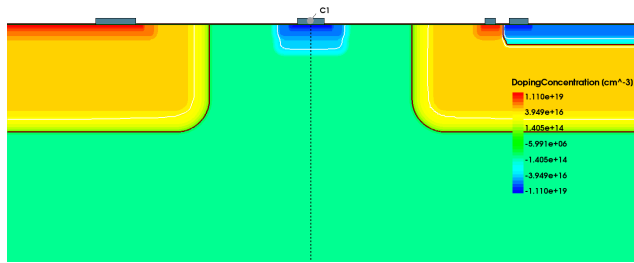
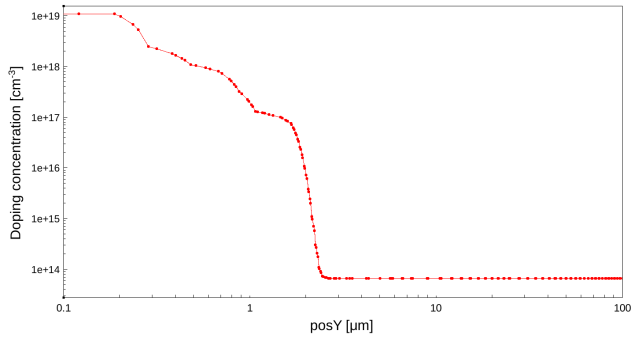


Figure 8.52 – Overall view of the simulated pixel structure. NetActive in the legend represents the doping concentration.



(a)



(b)

Figure 8.53 – a) Detail of a bias electrode. The shallow doping profile is shown. b) Doping profile along the dashed line in sub-figure (a)

8.6 Physics model

The electrical properties of silicon detectors are defined by the poisson equation and the continuity equations for electrons and holes:

$$\begin{cases} \frac{dp}{dt} - \nabla \cdot \vec{J}_p = G_h - R_h \\ \frac{dn}{dt} - \nabla \cdot \vec{J}_n = G_e - R_e \\ -\Delta V = \frac{\rho}{\epsilon} \end{cases} \quad (8.7)$$

with

$$\vec{J}_n = -\mu_n n \nabla V + D_n \nabla n \quad ; \quad \vec{J}_p = -\mu_p p \nabla V + D_p \nabla p \quad (8.8)$$

where n (p) is the electron (hole) density, $\mu_{n(p)}$ is the electron (hole) mobility, $D_{n(p)}$ is the diffusivity constant for electrons (holes), $\vec{J}_{n(p)}$ is the current density, $G_{e(p)}$ is the electron (hole) generation rate and $R_{e(p)}$ the recombination rate, as described by the Shockley-Read-Hall model [138].

Boundary conditions are also required to define the electric field lines at the interfaces. Three types of boundary conditions were implemented in our model: in the semiconductor/insulator boundary the current is not allowed to flow through the surface of the insulator, this is mathematically implemented using the Von-Neumann boundary condition⁶. At the metal-semiconductor surfaces, instead, the boundaries between the silicon bulk and metallic electrodes form an ohmic contact thus current is allowed to flow through them. The voltage V is constant and equals the bias voltage applied to the sensor by an external power supply. For these reason, the Dirichlet boundary condition was applied. The last condition concerns guard rings. A guard ring is a metal semiconductor interfaces where the metallic electrode is self-biased. To represent this case, null current flow on this contact was imposed. The bias voltages at the floating contacts are then found by the solver of the TCAD software.

In order to characterize the parameters in the equations 8.7, a set of models are used to describe the mobility, generation and recombination rates. TCAD softwares offer a large variety of different options. In most of the cases these models are phenomenological parametrization of experimental data for different conditions of the device in analysis (e.g. doping concentration, temperature of operation, dimension of the device). The most appropriate choices for the model in this analysis are summarized in the following:

⁶This condition specifies the values of the derivative of the solution. In case of electrical simulation this means that the electric field is kept constant and perpendicular to the surface not allowing any current to flow in the direction of the insulator.

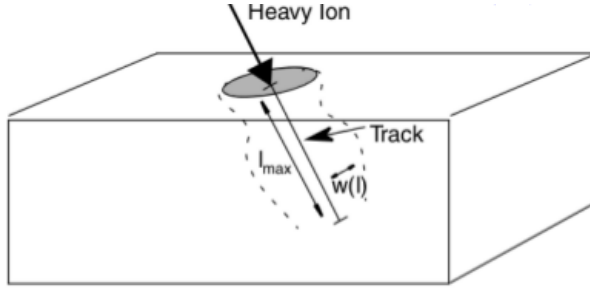


Figure 8.54 – A particle penetrating a semiconductor; its track is defined by a length and the transverse spatial influence is assumed to be symmetric about the track axis [137].

- **Mobility** Masetti model [139]: degradation of the mobility due to scattering through impurities.
- **Mobility** Canali model [140]: velocity saturation due to high electric field.
- **Recombination** SRH model [138]: generation/recombination occurs through shallow traps in the band due to the impurities. The carriers lifetime has been increased to $\tau = 10^{-6} \mu s$ because of the high purity of the silicon of the H35Demo.
- **Recombination** Scharfetter relation [141] : recombination lifetime degradation due to impurities.
- **Band gap narrowing** SlotBoom model[142]: decrease the gap for highly doped substrate.

In addition to the static simulation used to study the voltage, the ramo potential and the depletion depth, an $e-h$ pair distributions emulating the passage of a real charged particle can be implemented to study the induced charge at the electrode. The energy released from the incoming particle is modeled using a Linear Energy Transfer (LET) function as shown in figure 8.54. The LET function is expressed by the following relation:

$$G(l, w) = G_{LET}(l)R(w, l) \quad (8.9)$$

where l is the longitudinal direction with respect to the incoming particle, w is the transverse direction, $G_{LET}(l)$ is the linear energy transfer generation density and $R(w, l) = \exp(-\frac{w}{\sigma_w})$ is the spatial distribution in the transverse direction. Table 8.5 shows the values used in simulation.

Parameter	Units	Value
$G_{LET}(l)$	e^-/h pairs per μm	80
σ_w	μm	0.05

Table 8.5 – LET parameters [137].

One of the critical parameter of the simulation is the strategy adopted to define the meshing elements. The value of $G_{LET}(l)$ might change significantly in each of the elements leading to a difference of the generation density with respect to the initial value given in simulation. To cope with this fact, different meshing strategies were used and the corresponding results were compared to verify the stability of the overall interpretation given by simulation. However, this compromises the quantitative estimation of the results. A detailed comparison between data and simulation was out of the scope of this study, which aims to describe qualitatively the collection properties of HV-CMOS sensors.

Results

The electric field distribution within a single pixel for a biasing voltage of $HV = 120\text{ V}$ is shown in Figure 8.55 for the four nominal resistivities of the H35 Demo (20, 80, 200, 1000 Ωcm). The depletion depth, outlined with a white line in the Figure, extends into the bulk of the detector for a region of $\sim 10\text{ }\mu\text{m}$ for the lowest resistivity of 20 Ωcm and increases, following approximately $d \approx \sqrt{\rho V}$, up to 70 μm for the highest resistivity of 1000 Ωcm . It is also interesting to compare the electric field strength for the different resistivities. For the simulation using 20 and 80 Ωcm the electric field is homogenous within the depleted region but, as soon as the resistivity increases, the electric field grows laterally until most of its strength is dissipated between the biasing n -well and the collection electrode. In particular, for $\rho = 200\text{ }\Omega\text{cm}$ and 1000 Ωcm , the absolute value of the electric field is large enough to produce a deep depletion depth, but most of its strength is dissipated among the p -implant and the deep n -well resulting in a low field at the boundary of the depleted region in the deep bulk of the silicon. Such an effect can be understood by looking at the electric field lines (shown in black in the Figure).

The potential difference between the biasing and collecting electrode is defined as the integral of the electric field over a given field line: $\int_l E(x, y) dl = \Delta V_{bias}$. Since the HV is applied at the top of the sensor, it is clear that in the region between the two electrodes, where the field lines have the shortest path, the electric field must be large. On the contrary, in the case of the deep-bulk region, the field lines must come back to the collecting electrode such that $l_{field} \propto 2d_{depletion}$ resulting in a low-field region in the deep bulk and below the n -well. To further investigate this effect, a simulation featuring a biasing strategy from the back of the sensor was implemented. A p -doped layer and a metallic electrode at the back of the sensor were also implemented to ensure a resistive contact between the biasing electrode and the bulk of the silicon, while the deep n -well was left floating. The results of the simulation are shown in Figure 8.56. As expected,

the field lines mostly form straight vertical lines in between the collecting and biasing electrodes and thus the electric field distribution resemble the one of a standard planar detector.

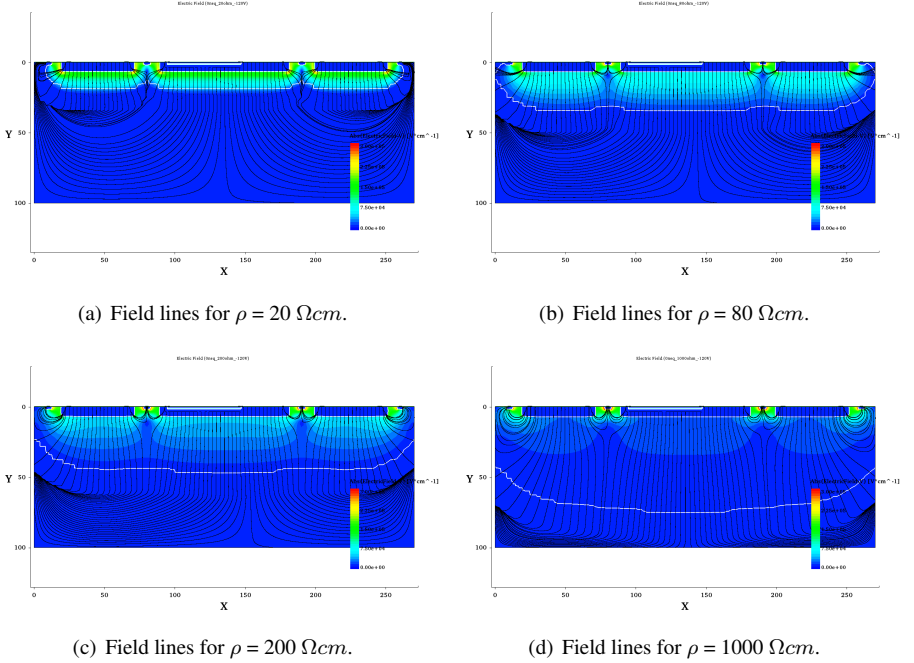


Figure 8.55 – Electric field distributions for different resistivities and a $HV = 120 \text{ V}$. The white line represents the boundary of the depleted region.

In order to study the induced signal at the collecting electrode, a *mip* passing through the center of the pixel has been simulated. Figure 8.57 shows the simulated electron distribution for different time intervals. At the initial time of the interaction ⁷ the charge is still homogenous in the detector showing the simulated profile of the LET function. After 5 ns, the charge in the depleted region is collected by drift while, in the deep bulk, the generated charges slowly move by means of diffusion. At 50 ns the charge in the depleted region is mostly collected while the slowing diffusion component is still visible in the deep bulk. The charge randomly diffusing from the deep bulk into the depleted region is then further accelerated even after 50 ns.

⁷The time that a *mip* needs to pass through the simulated structure is of the order of fs. Since we are interested in effect which in takes place in $\sim \text{ns}$, the interaction is considered instantaneous.

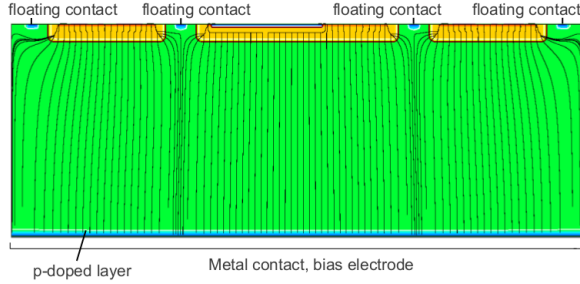


Figure 8.56 – Field line distribution for the simulation when biasing voltage is applied at the back of to the sensor.

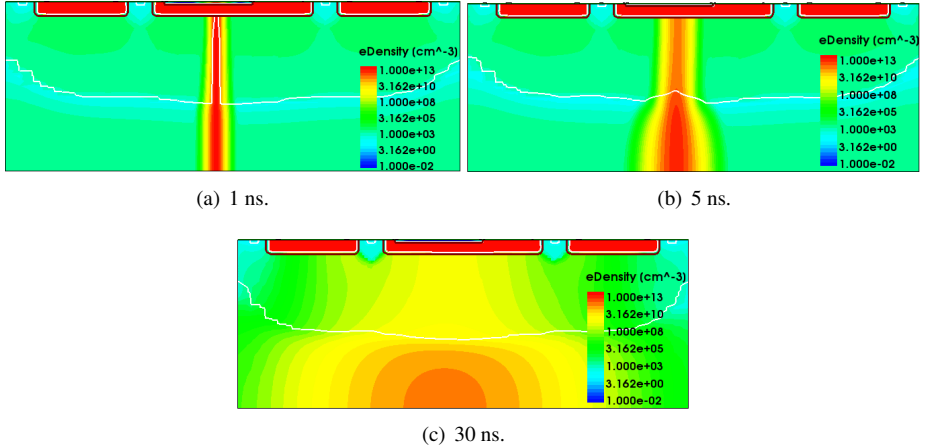


Figure 8.57 – Snapshot of the distribution of electron for different time intervals for $\rho = 200 \, \Omega\text{cm}$ and $HV = 50 \, \text{V}$.

The induced current at the electrode is shown in Figure 8.58. At the initial time of the interaction, the collected charge is larger for $20 \, \Omega\text{cm}$ and $80 \, \Omega\text{cm}$ compared to the higher resistivity values of $200 \, \Omega\text{cm}$ and $1000 \, \Omega\text{cm}$. For the latter resistivities, the low electric field in the deep-bulk region leads to a slow collection time. These results give a picture of the collection mechanism in HV-CMOS pixel sensor. A more complete simulation infrastructure, which include also the simulation of the electronics on-sensor and subsequent processing of the signal by the FEI4 is out of the scope of this thesis.

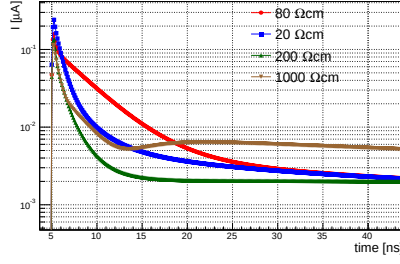


Figure 8.58 – Induced current for a top-biased simulated H35DEMO pixel sensor as a function of time at HV = 50 V.

In summary, the characterization of HV-CMOS pixel sensor at different irradiation levels was performed. The studies presented in this chapter represent one of the first evidence of the feasibility of this new pixel technology at extreme radiation conditions.

CHAPTER 9

Conclusions

From 2015 to the end of 2018 the LHC provided p - p collisions at an unprecedented center-of-mass energy of 13 TeV. During this period, the ATLAS experiment collected almost 140 fb^{-1} of LHC data. The high energy reached by the LHC and the high luminosity collected by the LHC detectors enable the experiments to investigate physics processes that cannot be explored by other high-energy physics laboratories. An important fraction of these processes involve b -quarks in the final state. The identification of jets originating by heavy-quarks is thus a fundamental task for the LHC experiments. In this thesis, four main topics were discussed: the characterization of the b -tagging performance at high transverse momentum; the application of this tool to a physics analysis looking for high-mass resonances decaying to one or two b -quarks; a search for boosted Higgs bosons and other resonances decaying into $b\bar{b}$ pairs and finally a study to characterize the performance of a novel pixel detector technology based on the CMOS manufacturing process.

Identifying heavy-quark initiated jets at high transverse momentum is experimentally challenging. The algorithms used for b - or c -tagging exploit the weak decay modes of the heavy hadrons by reconstructing secondary and tertiary vertices, as well as using the impact parameters of the tracks within a jet. The collimation between the decay products of the heavy-quarks scales as $\frac{1}{\gamma}$, where γ is the boost factor of the decaying hadron. At high energy, the high boost factor leads to very collimated particles. In addition, the number of particles originating during the fragmentation processes increases at high energy and in turn also the probability to generate fake vertices or misreconstructed tracks, thus degrading the b -tagging performance. In the context of this

thesis, the performance of the b -tagging algorithms in such harsh environments was improved by a factor of ~ 3 for a jet- p_T of around 700 GeV. These improvements originate from a novel training strategy for the b -tagging algorithms at high transverse momentum and from the addition of a new multivariate algorithm, a recurrent neural network which is able to exploit the correlations of the track parameters in the jet. These improvements, which became part of the standard reconstruction flow of the ATLAS experiment, were evaluated in the context of an analysis searching for heavy resonances decaying into b -quarks. The analysis was performed using the full data-set collected at 13 TeV by the ATLAS experiment, corresponding to 139 fb^{-1} . No new physics signals were found and 95 % exclusion limits were set for a variety of benchmark models with masses above $\sim 1 \text{ TeV}$, including a dark matter mediator model. The upgraded b -tagging configuration led to improvements in the exclusion limits of around a factor of ~ 2.5 compared to the previous b -tagging configuration. In addition, a new approach to b -tagging very energetic jets was also investigated using the ATLAS detector. At very high energy, the b -hadron life-time increases and the heavy-hadron can eventually decay within the fiducial volume of the inner detector. Profiting from the high spatial resolution of the tracking detector, a small cone around the jet-axis can be used to count the number of silicon *hits* in between detector layers. It was shown that this algorithm is able to exploit complementary information with respect to the other track-based b -tagging algorithms. Therefore, further improvements of the performance at very high transverse momentum can be achieved.

The second analysis presented in this thesis is a search for inclusive boosted Higgs bosons and Dark Matter mediators decaying into bottom-quarks. The analysis was performed using 80.5 fb^{-1} of data. This analysis was previously considered to be impossible due to the overwhelming QCD background. However, profiting from the experimental developments in the reconstruction of boosted objects, it is now possible to search for Higgs bosons inclusively at high transverse momentum. The analysis, performed for the first time by the ATLAS experiment, largely relies on the b -tagging performance in boosted environment and on the reconstruction of large- R jets with radius parameter of 1.0 that capture the collimated decay products of the Higgs bosons. A measurement of the $Z/W + \text{jets}$ process was performed with an observed significance of 5σ in the $b\bar{b}$ final state. This represents the first evidence by the ATLAS experiment of vector bosons in final states enriched with heavy-quarks in the boosted regime. An excess, compatible with the Higgs boson at a significance of 1.6σ , was also observed. In addition to the SM interpretation, the analysis set limits on dark matter mediator models in the mass range between $[100, 200] \text{ GeV}$, thus complementing the mass reach of the other analysis presented in this thesis.

The search for boosted Higgs bosons is statistically limited. At the HL-LHC, where the integrated luminosity will be increased to 3000 fb^{-1} , the determination of the differential cross-section of the Higgs boson transverse momentum constitutes one of the most important measurements of the HL-LHC physics programme. However, due to this high luminosity, the detectors will have to function in unprecedented radiation conditions. In

this thesis, a novel pixel sensor based on the HV-CMOS technology was characterized. The analysis of test-beam data showed the high detection efficiency of this technology up to an irradiation level of $1 \cdot 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$, a value compatible with the expected fluence of the outer pixel layers of the ATLAS tracking detector at the HL-LHC.

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