

Machine Learning and Statistical Combination Assisted Searches for Dark Higgs and Dark Photon with ATLAS experiment at LHC

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上海交通大学博士学位论文

在大型强子对撞机ATLAS实验中基于机器学习
与联合统计分析技术寻找暗希格斯粒子和
暗光子

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**MACHINE LEARNING AND STATISTICAL
COMBINATION ASSISTED SEARCHES FOR DARK
HIGGS AND DARK PHOTON WITH ATLAS
EXPERIMENT AT LHC**

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摘要

暗物质 (Dark Matter), 作为一种未知的物质存在形式, 被众多宇宙学观测证据所支持。标准模型 (Standard Model) 作为目前诠释物质基本组成最为完备的理论, 无法对暗物质给出预测和解析。研究暗物质的本质是当前粒子物理领域的关键课题之一。大型强子对撞机LHC为寻找暗物质并揭示其性质和相互作用提供了独特的机会。

本论文主要关注两个在大型强子对撞机 ATLAS 实验中进行的物理分析。第一个课题是搜寻暗希格斯玻色子并尝试回答暗物质是否可以通过希格斯机制获得质量。这一搜寻在低质量区间进行并利用了 ATLAS 实验的第二期数据采集结果。一种新的基于机器学习技术的大半径喷注 (Jet) 味鉴别算法的开发和应用, 显著提升了分析的灵敏度。该分析首次将暗物质残存密度(Relic Density)的宇宙学观测结果直接纳入到对模型参数空间的扫描中, 提高了对模型多维参数空间扫描的效率。该研究对于标准参数组合的暗希格斯模型, 在95%置信区间下将质量在30至150GeV范围内的暗希格斯玻色子全部排除, 对于重媒介粒子 Z' 的质量排除至最高3.5TeV。对于符合暗物质残存密度观测的参数组合也获得了目前最严格的统计排除结果, 对于70GeV质量的暗希格斯粒子和700GeV以下的马约拉纳暗费米子, 重媒介粒子 Z' 的质量可以排除到微扰理论计算的上限。

本论文的另一个中心课题是寻找暗光子, 它为暗物质与标准模型粒子之间的非常弱的耦合提供了一个潜在解释, 认为其之间的相互作用仅通过暗光子与标准模型光子的动力学混合产生。这一分析对目前ATLAS实验中搜寻具有希格斯耦合的无质量暗光子的结果进行了统计联合分析, 建立了目前最严格的对撞机实验限制。在95%置信区间下, 标准模型希格斯玻色子衰变到光子和无质量暗光子的分支比不超过1.3%; 对于具有超标准模型重希格斯粒子耦合的无质量暗光子模型, 希格斯粒子质量在1.5TeV以下的假设均被排除。

本论文还探讨了一种创新的模型无关暗物质搜寻技术。通过基于自监督机器学习异常检测技术 (Anomaly Detection), 暗物质信号可以被识别为不同于标准模型的异常事件。对模拟数据集的研究表明, 这种方法可以利用事件里的喷注特征提高对未知模型暗物质信号的搜寻灵敏度, 对于未来在对撞机实验中进行暗物质搜寻具有重要的意义。

关键词：大型强子对撞机，暗物质，暗希格斯，暗光子，喷注鉴别

Abstract

The existence of dark matter is strongly supported by numerous cosmological observations. The Standard Model (SM), as the most complete understanding of elementary particles to date, cannot predict or explain the nature of dark matter. Unveiling the properties and interactions of dark matter remains a central question in modern particle physics. Searching for dark matter at the Large Hadron Collider (LHC), the highest-energy particle collider on Earth, offers a unique opportunity to address this fundamental mystery.

This thesis focuses on two analyses performed using data from the ATLAS experiment at the LHC. The first study searches for the dark Higgs boson, exploring whether dark matter acquires its mass through a Higgs-like mechanism. This search targets low-mass dark Higgs bosons and utilizes the full Run-2 dataset from the ATLAS experiment. A novel machine learning-based boosted jet tagging algorithm was developed and applied, significantly enhancing the sensitivity. Relic density observations were incorporated for the first time to directly constrain the model's parameter space, improving the efficiency of multidimensional parameter scans. The results exclude dark Higgs bosons with masses between 30 and 150 GeV and heavy mediator particles Z' up to 3.5 TeV at 95% confidence level. For parameters consistent with relic density observations, stringent exclusions are set, including Z' masses up to the perturbative limit for a 70 GeV dark Higgs boson and Majorana dark fermions below 700 GeV.

The second focus of this thesis is the search for dark photon, which provide a potential explanation for the extremely weak coupling between dark matter and SM particles. This coupling is hypothesized to occur exclusively via kinetic mixing between dark photon and SM photon. The analysis combines ATLAS searches for massless dark photon with Higgs coupling, establishing the most stringent collider limits. At 95% confidence level, the branching ratio of SM Higgs bosons decaying into photons and massless dark photons is less than 1.3%, while massless dark photon with couplings to heavy BSM Higgs bosons and Higgs masses below 1.5 TeV is excluded.

Additionally, this thesis explores a novel technique for model-independent dark matter searches. Using self-supervised machine learning-based anomaly detection, dark matter

signals can be identified as anomalous events deviating from SM expectations. Studies on simulated datasets demonstrate that this method leverages jet features to enhance sensitivity to unknown dark matter model. This approach holds significant promise for future dark matter searches in collider experiments.

Key words: Large Hadron Collider, Dark Matter, Dark Higgs, Dark Photon, Jet Tagging

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Chapter 1 Introduction

The existence of an unknown form of matter, known as dark matter, is strongly supported by numerous cosmological observations. Dark matter constitutes approximately 26.8% of the current universe, yet it remains one of the greatest mysteries in modern physics. Despite the successes of the Standard Model (SM) of particle physics, which represents our best understanding of the material world, it provides no explanation for dark matter. Searching for dark matter at the highest energy scales achievable on Earth offers a unique opportunity to uncover its properties and interactions. These searches not only probe conditions akin to those of the early universe but also aim to recreate the processes that might have led to the generation of dark matter.

This thesis focuses on two analyses performed using the data collected by the ATLAS experiment at the Large Hadron Collider (LHC), the world's largest particle collider, which achieves proton-proton collisions at a center-of-mass energy of up to 13 TeV.

A key focus of this work is the search for the so-called dark Higgs boson, which addresses the fundamental question of why dark matter possesses mass, given its gravitational interactions. This search, conducted in the low-mass regime, utilizes the full Run-2 dataset from the ATLAS experiment. A novel machine learning technique, boosted Xbb tagging, was developed during this study to enhance the analysis sensitivity. Additionally, for the first time, cosmological constraints from relic density were incorporated into the search, directly linking collider physics with cosmology. This innovative approach provided non-trivial constraints on model parameters and improved the efficiency of scanning multidimensional parameter spaces.

Another central topic of this thesis is the search for the dark photon, which offers a potential explanation for the weak coupling of dark matter to SM particles. The dark photon hypothesis posits that dark matter interacts with the SM exclusively through kinetic mixing between a dark photon and the SM photon via higher-order interactions. This analysis involves a statistical combination of previous ATLAS results and establishes the most stringent collider constraints to date on models involving a dark photon with Higgs coupling.

Beyond these model-specific searches, this thesis also explores a model-independent approach to dark matter detection. A novel anomaly detection technique based on self-supervised machine learning is introduced. Preliminary results on simulated datasets demonstrate the effectiveness of this method in learning features of jets and improving sensitivity to unknown physics models. This work represents an important step toward implementing model-independent dark matter searches at collider experiments in the near future.

The thesis is organized as follows. The theoretical background and unresolved mysteries surrounding dark matter are discussed in Chapter 2, followed by an introduction to the experimental techniques used in the ATLAS experiment at the LHC in Chapter 3. Utilizing the novel boosted double b -jet tagging method introduced in Chapter 4, the search for the dark Higgs boson decaying into two b -quarks is detailed in Chapter 5. The combination of dark photon searches with Higgs coupling at ATLAS is described in Chapter 6, while Chapter 7 presents the study of a self-supervised anomaly detection method for model-independent dark matter searches. The thesis concludes with a summary and outlook in Chapter 8.

Chapter 2 The Theory and Mystery

2.1 Introduction to Standard Model (SM) Theory

2.1.1 The History

The Standard Model (SM)^[1] is the most comprehensive and profound framework for understanding the current physical world, developed through the efforts of theorists and experimentalists over more than half a century. It describes the elementary particles that constitute matter—leptons and quarks. Three of the four fundamental interactions underlying all observable phenomena—electromagnetic, weak, and strong interactions—are unified within the SM 's gauge theory framework. These interactions are mediated by gauge bosons, while the Higgs boson interacts with all particles to generate their masses.

With the discovery of the electron by Thomson, the understanding of atomic structure by Rutherford and Bohr, the realization of particle spin by Stern and Gerlach, and the implications of antiparticles proposed by Dirac and confirmed by Anderson, as well as the precise measurements of atomic fine structure by Lamb and Retherford, significant experimental and theoretical advancements occurred during the early to mid-1900s. These efforts culminated in the formal development of Quantum Electrodynamics (QED)^[2], the quantum and relativistically consistent description of electromagnetic interactions. As a cornerstone of the SM , it describes the interaction between electrically charged particles and photons in a Lorentz-invariant framework, with foundational contributions by Tomonaga, Feynman, and Schwinger.

In parallel, efforts to understand the binding of positively charged protons within atomic nuclei led to Yukawa's 1935 proposal of the strong interaction^[3]. He predicted the existence of mesons and estimated their mass based on the size of strong interaction-bound states (nuclei). This prediction was experimentally confirmed with the discovery of the pion in cosmic rays by Powell in 1947, followed by observations of various other mesons. The terminology introduced during this period persists today: leptons (light particles such as electrons and muons, the latter discovered alongside pions in cosmic rays), baryons (heavy particles like protons), and mesons (intermediate-mass particles).

In another line of study focused on weaker interactions, the discovery of the neutron by

Chadwick in 1932 and the brilliant proposal of the neutrino by Pauli, followed by Fermi's theoretical formulation to account for the missing energy in neutron beta decay, laid the foundation for understanding weak interactions. Subsequent experimental efforts, including the detection of neutrinos by Cowan and Reines in 1956, identified neutrino interactions and their types. The astonishing discovery of parity violation in weak interactions, proposed by Yang and Lee and experimentally confirmed by Wu, further advanced this field. The theory of beta decay, grounded in weak interactions, was ultimately unified with electromagnetic interactions by Glashow, Salam, and Weinberg, leading to the Electroweak (*EWK*)^[4] sector of the Standard Model. This unification also predicted the existence of massive intermediate vector bosons that mediate weak interactions.

The discovery of "strange" particles put the two interactions together, identified the particle which could produced by strong interaction while decay with weak interaction and inspired the theory by first Pais then Gell-mann and Nishijima the to assign particle the property such as strangeness, which converse only in strong interaction impliciting special symmetry structure of strong interaction and the modern version of "periodic table" of hadrons (mesons and baryons). This finally become clear with the discovery of a lot of hadrons and put them firstly in the eightfold way and then the quark model in 1964 by Gell-mann and Zweig and shortly the color by Greenberg which is proposed to resolve symmetry issues in the quark model, ensuring consistency with the Pauli exclusion principle in hadrons composed of identical quarks. The theory finlly formulated as Quantum Chromodynamics (*QCD*)^[5] part of the *SM*.

On the theoretical side, the modern formulation of the *SM* theory is founded on Yang-Mills theory^[6], which generalizes gauge theory from an Abelian group as in *QED*, to a non-Abelian group as in *QCD*. With the Higgs mechanism^[7], the correct mass terms are generated within the *EWK* gauge theory, providing an explanation for the origin of mass for all elementary particles. This incorporation results in the modern formulation of the *SM*, unifying all components into a cohesive theoretical framework.

Subsequently, a series of remarkable advancements in both theory and experiment have further developed and confirmed the success of the *SM*. These include the prediction of the fourth quark (charm) through the GIM mechanism^[8], in addition to the up and down quarks that form protons and neutrons, and the strange quark responsible for strange particles. The

charm quark was indirectly confirmed during the "November Revolution" of 1974 with the discovery of the J/ψ particle by Ting and Richter. Other milestones include the discovery of the third lepton, the tau, by Perl et al. in 1975, the subsequent discoveries of the bottom (b) and top (t) quarks, the identification of the W and Z vector bosons, and finally the discovery of the Higgs boson in 2012^{[9][10]}. Today, all the predicted components of the *SM* have been observed, and all the cards are on the table.

2.1.2 Elementary Particle

The *SM* consists of three generations of fermions, four gauge bosons, and the Higgs boson, which together form the elementary particles. The spin and charge carried by these particles dictate their behavior under specific symmetries. The elementary fermions in the *SM* have spin- $\frac{1}{2}$ and obey Fermi-Dirac statistics, which enforce the Pauli exclusion principle, stating that no two identical fermions can occupy the same quantum state. Fermions, which constitute the matter in the universe, are divided into two categories: quarks and leptons.

In contrast, bosons carry integer spins and are divided into two types in the *SM*: gauge bosons, which have spin-1 (vector bosons), and the Higgs boson, which has spin-0 (scalar boson). These bosons mediate fundamental forces and provide mass to particles through the Higgs mechanism. The complete set of *SM* particles is illustrated in Fig. 2.1¹.

2.1.3 The Formalism

The quantum field theory (QFT)^[11-12] provides the theoretical framework within which the Standard Model (SM) is formulated.^[13] In this framework, the dynamics and interactions of particles are encoded in the Lagrangian, and all particles are described as fields that depend on space-time coordinates. Starting from the Lagrangian in relativistic field theory, free fields are categorized based on their spin and are described by specific formulations, such as the Klein-Gordon Lagrangian Eq. 2.1, Dirac Lagrangian Eq. 2.2, and Proca Lagrangian Eq. 2.3:

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)(\partial^\mu \phi) - \frac{1}{2} \left(\frac{mc}{\hbar} \right)^2 \phi^2 \quad (2.1)$$

$$\mathcal{L} = i(\hbar c)\bar{\psi}\gamma^\mu \partial_\mu \psi - (mc^2)\bar{\psi}\psi \quad (2.2)$$

¹ Figure credits to the author Cush

Standard Model of Elementary Particles

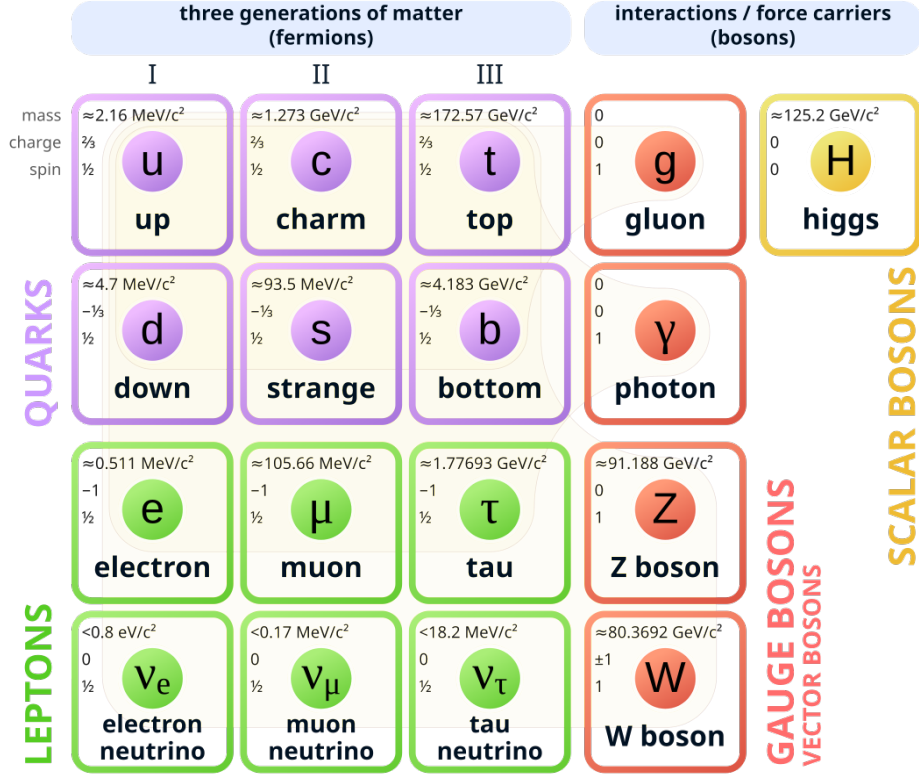


Figure 2.1 Elementary Particles of the Standard Model. ¹

$$\mathcal{L} = -\frac{1}{16\pi}(\partial^\mu A^\nu - \partial^\nu A^\mu)(\partial_\mu A_\nu - \partial_\nu A_\mu) + \frac{1}{8\pi}\left(\frac{mc}{\hbar}\right)^2 A^\nu A_\nu \quad (2.3)$$

By applying the Euler-Lagrange equations, which are derived from the principle of least action, one can obtain equations describing particles with specific masses and spins. These include the Klein-Gordon equation Eq. 2.4 for a particle with mass m and spin-0, the Dirac equation Eq. 2.5 for spin- $\frac{1}{2}$ particles, and the Proca equation Eq. 2.6 for spin-1 particles, where $F^{\mu\nu}$ is defined as $\partial^\mu A^\nu - \partial^\nu A^\mu$. In the case of a massless spin-1 particle, the Proca equation reduces to Maxwell's equations.

$$\partial_\mu \partial^\mu \phi + \left(\frac{mc}{\hbar}\right)^2 \phi = 0 \quad (2.4)$$

$$i\partial_\mu \bar{\psi} \gamma^\mu + \left(\frac{mc}{\hbar}\right) \bar{\psi} = 0 \quad (2.5)$$

$$\partial_\mu F^{\mu\nu} + \left(\frac{mc}{\hbar}\right)^2 A^\nu = 0 \quad (2.6)$$

The modern formulation of the Standard Model (SM) interactions is based on gauge theory. The requirement that the system and its Lagrangian exhibit global invariance, and that this invariance must hold locally, when applied to the free-field Lagrangian, generates all interaction dynamics and specifies the current produced by sources.

In more detail, "gauge" refers to the regulation of redundant degrees of freedom in the theory. If a system remains invariant under gauge transformations belonging to a certain symmetry group, it is said to exhibit gauge invariance. A global gauge transformation implies that the transformation parameters are identical at every point in space-time, whereas a local gauge transformation allows these parameters to vary as functions of space-time coordinates.

The requirement of local gauge invariance under the symmetry group $SU(3) \times SU(2) \times U(1)$ forms the theoretical foundation of the Standard Model.

To derive the formalism of QCD, start from the free Dirac Lagrangian describing 3 color of quarks in Eq. 2.7, assuming the mass is same in different color and 3 color fields are defined as $\psi = (\psi_r \ \psi_b \ \psi_g)^T$

$$\mathcal{L} = i\hbar c \bar{\psi} \gamma^\mu \partial_\mu \psi - mc^2 \bar{\psi} \psi \quad (2.7)$$

Requiring local gauge invariance under the $SU(3)$ group introduces the covariant derivative $D_\mu = \partial_\mu + ig_s G_\mu^a T^a$, which translates global symmetry into local symmetry. Adding the free Lagrangian of the gauge field G , known as the gluon, the QCD Lagrangian can be expressed as Eq. 2.8:

$$\mathcal{L}_{\text{QCD}} = \bar{\psi} i \gamma^\mu D_\mu \psi - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} \quad (2.8)$$

where ψ is the quark field, G_μ^a is the gluon field, $D_\mu = \partial_\mu + ig_s G_\mu^a T^a$ is the covariant derivative, $G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a + g_s f^{abc} G_\mu^b G_\nu^c$ is the gluon field strength tensor, g_s is the strong coupling constant and the structure constants f^{abc} the Dirac matrices, and T^a the $SU(3)$ generators.

After the realization of the possibility of unifying the electromagnetic and weak interactions, the underlying symmetry group of *EWK* was identified as $SU(2)_L \times U(1)_Y$, with

conservation of weak isospin (T_3) and weak hypercharge (Y_W). Their relationship with electric charge is expressed as:

$$Q = T_3 + \frac{1}{2}Y_W \quad (2.9)$$

The formalism of *EWK* theory is then established as Eq. 2.10:

$$\begin{aligned} \mathcal{L}_{\text{EWK}} = & \bar{Q}_{Lj} i\gamma^\mu D_\mu Q_{Lj} + \bar{\ell}_{Lj} i\gamma^\mu D_\mu \ell_{Lj} \\ & + \bar{u}_{Rj} i\gamma^\mu D_\mu u_{Rj} + \bar{d}_{Rj} i\gamma^\mu D_\mu d_{Rj} + \bar{e}_{Rj} i\gamma^\mu D_\mu e_{Rj} \\ & - \frac{1}{4} W_a^{\mu\nu} W_{\mu\nu}^a - \frac{1}{4} B^{\mu\nu} B_{\mu\nu} \end{aligned} \quad (2.10)$$

And D_μ is the covariant derivative, defined as Eq. 2.11:

$$D_\mu = \partial_\mu - ig W_\mu^a T^a - ig' \frac{Y}{2} B_\mu, \quad (2.11)$$

where W_μ^a are the $SU(2)_L$ gauge fields, B_μ is the $U(1)_Y$ gauge field, T^a are the generators of $SU(2)_L$, and Y is the weak hypercharge, and the fields defined as,

- Q_{Lj} are the left-handed quark doublets of the three generations, while ℓ_{Lj} are the left-handed lepton/neutrino doublets. These fields interact with both the weak and electromagnetic interactions, having non-zero weak hypercharge Y_W and weak isospin T .
- u_{Rj} , d_{Rj} , and e_{Rj} are the right-handed singlets for up quarks, down quarks, and charged leptons, respectively, in each generation. These fields interact only with the electromagnetic interaction and have non-zero weak hypercharge Y_W .

These chiral fermion states are combinations of flavor states, taking into account quark mixing through the Cabibbo-Kobayashi-Maskawa (CKM) mechanism. Chirality projection unifies the vectorial and axial natures of the electroweak interaction. Explicitly in Eq. 2.12 and 2.13:

$$Q_L \equiv \begin{pmatrix} u_L \\ d_L \end{pmatrix}, \quad \ell_L \equiv \begin{pmatrix} \nu_L \\ e_L \end{pmatrix} \quad (2.12)$$

$$U_R \equiv u_R, \quad D_R \equiv d_R, \quad e_R \equiv e_R \quad (2.13)$$

The Lagrangian terms consist of the first five kinetic terms, describing fermion dynamics and their interactions with gauge bosons via the covariant derivative, and the last two terms, representing gauge boson self-interactions.

The Lagrangian satisfying local gauge invariance only allows the existence of massless gauge fields, as the $A_\mu A^\mu$ term in Eq. 2.3 is not invariant. This fits well with QCD, where gluons are massless, but fails in the case of *EWK* interactions. The gauge bosons associated with $SU(2)_L \times U(1)_Y$ must be massive to account for the short-range weak interactions, which is experimentally verified. The Higgs mechanism is introduced to resolve this difficulty.

The Higgs potential is designed to have non-zero ground states (vacuum), where the perturbative calculations are performed. The chosen ground state does not share the same symmetry as the original Lagrangian, causing spontaneous symmetry breaking (SSB). This process leads to a rewritten Lagrangian expanded around the non-vanishing vacuum expectation value. The spontaneous breaking of global symmetry typically results in the appearance of unphysical massless scalar bosons, as demonstrated by the Goldstone theorem^[14]. However, when local gauge invariance is combined with spontaneous symmetry breaking and the gauge is fixed properly, the Lagrangian correctly exhibits terms for massive gauge bosons and one massive scalar particle, the Higgs boson^[7].

In the Standard Model electroweak theory, the Higgs field is described as an $SU(2)_L$ doublet complex field: $\varphi = (\varphi^+, \varphi^0)^T$ and the Lagrangian is written as Eq. 2.14:

$$\mathcal{L}_H = (D_\mu \varphi)^\dagger (D^\mu \varphi) - V(\varphi), \quad (2.14)$$

where D_μ stands for the covariant derivative (defined in Eq. 2.11), and the potential is given in Eq. 2.15:

$$V(\varphi) = -\mu^2 \varphi^\dagger \varphi + \lambda (\varphi^\dagger \varphi)^2. \quad (2.15)$$

where $\lambda > 0$ ensures the potential is bounded from below.

The illustration of the shape of the potential for a simplified case where one field with two degree of freedom and defined in one space is shown in Fig. 2.2¹ where the symmetry is the $SO(2)$ rotation between the two degree of freedom, or equally the $U(1)$ with one complex field representation.

¹ Figure credits to the author Janosh Riebesell

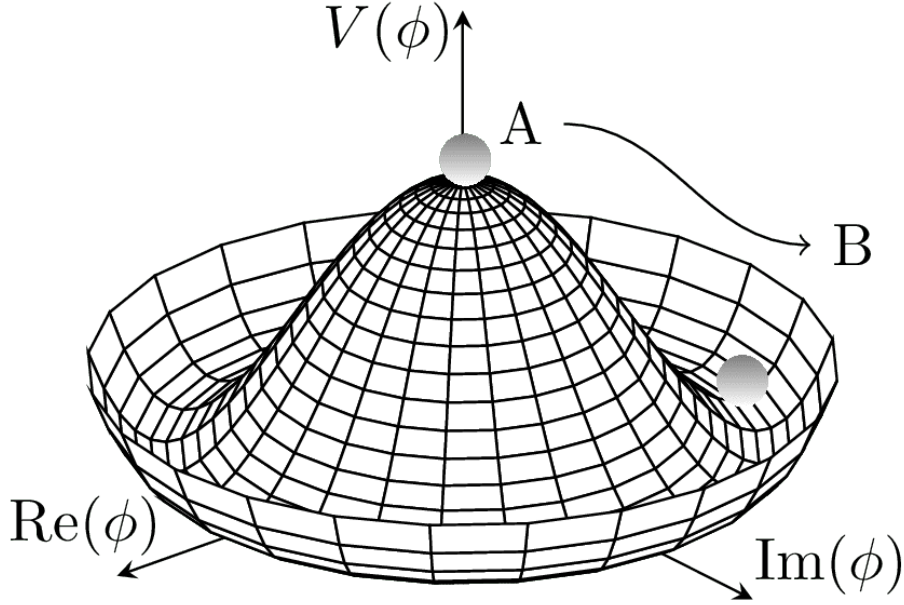


Figure 2.2 The Higgs Potential U(1) Toy Model. ¹

The minimum of Higgs potential is not at zero field but $\phi^\dagger \phi = \frac{\mu^2}{2\lambda} \equiv \frac{v^2}{2}$, where v is called the vacuum expectation value (vev). We choose the vacuum state $\varphi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}$, breaking the symmetry, and rewrite the field in Eq. 2.16, just as Eq. 21.38 in^[12]:

$$\varphi = \frac{1}{\sqrt{2}} \begin{pmatrix} -i(\phi_1 - i\phi_2) \\ v + h(x) + i\phi_3 \end{pmatrix}, \quad (2.16)$$

where ϕ_1 , ϕ_2 , and ϕ_3 are the Goldstone bosons. Applying the unitarity gauge^[15], all three Goldstone bosons are rotated to zero, leaving the physical field as Eq. 2.17:

$$\varphi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h(x) \end{pmatrix}, \quad (2.17)$$

With this spontaneous symmetry breaking, the electroweak symmetry $SU(2)_L \times U(1)_Y$ is broken down to the electromagnetic symmetry $U(1)_{\text{em}}$. The electroweak Lagrangian, after symmetry breaking, is formulated as Eq. 2.18:

$$\begin{aligned}
\mathcal{L}_{\text{EWK}} = & \sum_f \bar{f} (i \not{\partial} - m_f - \frac{gm_f}{2m_W} H) f \\
& - \frac{1}{4} A_{\mu\nu} A^{\mu\nu} - \frac{1}{2} W_{\mu\nu}^+ W^{-\mu\nu} - \frac{1}{4} Z_{\mu\nu} Z^{\mu\nu} + \frac{1}{2} (\partial^\mu H) (\partial_\mu H) \\
& + m_W^2 W_\mu^+ W^{-\mu} + \frac{1}{2} m_Z^2 Z_\mu Z^\mu - \frac{1}{2} m_H^2 H^2 \\
& + e J_\mu^{\text{em}} A^\mu + \frac{g}{\cos \theta_W} (J_\mu^3 - \sin^2 \theta_W J_\mu^{\text{em}}) Z^\mu \\
& - \frac{g}{\sqrt{2}} \left[\bar{u}_i \gamma^\mu \frac{1 - \gamma^5}{2} M_{ij}^{\text{CKM}} d_j + \bar{\nu}_i \gamma^\mu \frac{1 - \gamma^5}{2} e_i \right] W_\mu^+ + \text{h.c.} \\
& - \frac{gm_H^2}{4m_W} H^3 - \frac{g^2 m_H^2}{32m_W^2} H^4 \\
& + \left(gm_{\text{HV}} + \frac{g^2}{4} H^2 \right) \left(W_\mu^+ W^{-\mu} + \frac{1}{2 \cos^2 \theta_W} Z_\mu Z^\mu \right) \\
& - ig \left[\left(W_{\mu\nu}^+ W^{-\mu} - W^{+\mu} W_{\mu\nu}^- \right) (A^\nu \sin \theta_W - Z^\nu \cos \theta_W) \right. \\
& \quad \left. + W_\nu^- W_\mu^+ (A^{\mu\nu} \sin \theta_W - Z^{\mu\nu} \cos \theta_W) \right] \\
& - \frac{g^2}{4} \left\{ \left[2W_\mu^+ W^{-\mu} + (A_\mu \sin \theta_W - Z_\mu \cos \theta_W)^2 \right]^2 \right. \\
& \quad \left. - \left[W_\mu^+ W_\nu^- + W_\nu^+ W_\mu^- + (A_\mu \sin \theta_W - Z_\mu \cos \theta_W) (A_\nu \sin \theta_W - Z_\nu \cos \theta_W) \right]^2 \right\}
\end{aligned} \tag{2.18}$$

where the $W^\pm$, A_μ , and Z_μ are the physical boson fields, mixed from the massless gauge bosons W and B before spontaneous symmetry breaking (SSB) as described in Eq. 2.10. The mixing is described by the Weinberg angle θ_W .

The physical interpretation of each term in the Lagrangian, line by line, is as follows:

- The dynamics of fermions, including their propagation, mass terms, and Yukawa coupling to the Higgs field H which generates fermion masses.
- Kinetic terms of the photon A , charged $W^\pm$ bosons, Z^0 boson and Higgs boson which describes their propagations.
- Mass terms for the $W^\pm$, Z^0 bosons arising from their interaction with the Higgs field and Higgs boson mass term due to the potential.
- Neutral current which describes the electromagnetic interaction and the Z^0 boson interaction with fermions, modified by the Weinberg angle θ_W . $J_\mu^{\text{em}} = \sum_f Q_f \bar{f} \gamma_\mu f$, $J_\mu^3 = \sum_f T_f^3 \bar{f} \gamma_\mu f$, where Q_f the electric charge and T_f^3 the weak isospin of corre-

sponding fermion state.

- Charged current interactions mediated by $W^\pm$ bosons, including quark mixing via the CKM matrix M_{ij}^{CKM} .
- Higgs boson self-interaction terms, describing cubic and quartic Higgs boson couplings.
- Higgs boson interaction with $W^\pm$ and Z^0 gauge bosons. $m_{HV} = v$.
- The rest is other gauge bosons self interactions in the form of 3-point WWV and 4-point $WWVV$.

All the parameters in the Lagrangian are determined by experimental measurements.

■

Completing with the discovery of the last missing piece of the SM , the Higgs Boson, in 2012 at the Large Hadron Collider (LHC)^[9-10], all the predicted particles have been confirmed by experiments. Furthermore, all observations and measurements of their basic properties, such as mass, spin, charge, and cross-sections, align with the SM predictions with remarkable accuracy.

However, despite its great success, the SM faces significant challenges. It fails to account for all the matter in the universe, particularly the mysterious dark matter, which constitutes a substantial portion of the universe's mass-energy density. Understanding the nature of dark matter remains one of the most compelling questions in modern physics and is the central topic of this thesis.

2.2 Dark Matter

2.2.1 Dark Matter From Cosmology

One of the open questions of the SM is its inability to predict all the matter constituents of the universe, as revealed by studies in cosmology. Observations in cosmology indicate that a large proportion of the universe's matter is of unknown origin. This unknown matter is proposed to satisfy a variety of astrophysical and cosmological observations, including the motion of galaxies^[16], the anisotropies in the cosmic microwave background (CMB) from the early universe^[17], X-ray emissions from merging galaxy clusters^[18], gravitational lensing effects^[19], and the formation of large-scale structures in the universe^[20].

This unknown matter is referred to as "dark matter" due to its electromagnetically neutral

or nearly neutral nature and its classification as non-baryonic. In the most widely accepted cosmological model, known as the Λ CDM model, dark matter constitutes approximately 84.4% of the total matter density of the universe. However, the only particle in the SM that satisfies the non-baryonic, electromagnetically neutral properties of dark matter—neutrinos—has been found to account for only about 1.6% of the non-baryonic matter in the universe^[21].

This significant discrepancy strongly indicates the existence of physics beyond the Standard Model (BSM). The search for new physics to account for dark matter is one of the most active and compelling areas of research in particle physics and cosmology.

The major evidences supporting the existence of dark matter are:

- **The motion of galaxies and clusters:** Numerous observations of galaxy rotation curves^[16] and velocity dispersions^[22] predict a mass distribution significantly different from that of visible matter. To reconcile these observations, an additional invisible matter component must be included. For example, the spiral galaxy Messier-33 exhibits a rotation curve that cannot be explained solely by luminous matter, as shown in Fig. 2.3^[23].
- **The structure formation of the universe^[24]:** The density perturbations following the Big Bang are crucial for forming cosmic structures, such as stars and galaxies. Ordinary matter interacts strongly with radiation, dominating perturbations only during the early universe. With only baryonic matter, the predicted fluctuation at present is $\delta\rho_b/\rho_b|_{\text{today}} \approx 10^{-2}$, far below the observed value $\delta\rho_b/\rho_b|_{\text{obs}} \gg 1$. Dark matter, which does not interact electromagnetically, is necessary to sustain perturbations over long periods, enabling the structures we observe today to form.
- **The merging galaxy clusters, such as the Bullet Cluster^[25]:** Observations of phenomena such as gravitational lensing, galaxy motions, and X-ray emissions provide compelling evidence for the existence of additional mass from invisible matter. These observations show a spatial separation between visible matter and the mass inferred from gravitational lensing, strongly supporting the dark matter hypothesis.
- **Other supporting evidence:**
 - The failure of dark matter-free modified gravity theories to predict the identical speeds of gravitational waves and light during the gravitational wave event GW170817^[26].

- The anisotropies in the cosmic microwave background (CMB), where perturbations from ordinary and dark matter leave distinct imprints^[27].
- Type Ia supernova distance measurements, which indicate a flat universe and provide evidence for the total energy density required, including dark matter^[17].
- Precise cosmological parameter measurements combining CMB observations with baryon acoustic oscillations (BAO) from galaxy redshift surveys^[28].

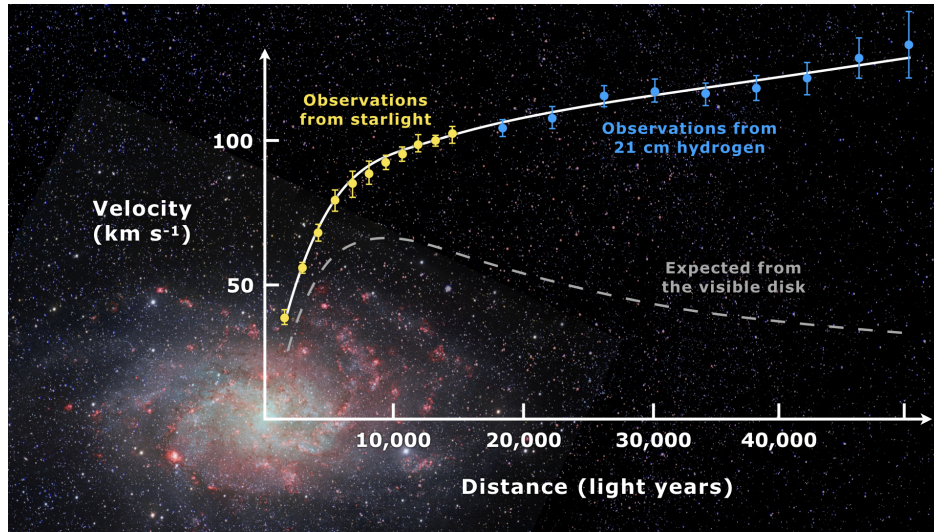


Figure 2.3 Rotation curve of the Messier 33. The observation of rotation from starlight and 21 cm hydrogen match very well and both are notable different from the prediction from visible matter^[23].

2.2.2 Lambda-CDM Cosmology Model

The most accepted cosmological model predicting the existence and behavior of dark matter is the Λ CDM framework^[29]. In this model, dark matter is considered to be "cold," meaning it has very small velocity dispersion, and it constitutes the universe along with ordinary (baryonic) matter and dark energy governed by the cosmological constant Λ . The Λ CDM model provides an excellent fit to a wide range of observations, including the cosmic microwave background, large-scale structure formation, and galaxy clustering.

The properties of dark matter are predicted within the Λ CDM framework based on cosmological observations. Some important ones are summarized below^[21]:

- **Abundance:** Dark matter constitutes 26.4% of the critical density of the universe and 84.4% of the total matter density.
- **Relic density:** This is a crucial parameter in the Λ CDM model that reflects the

evolution of dark matter in the early universe. Dark matter initially tracks thermal equilibrium until its production and annihilation slow down and eventually stop as the universe expands and cools. At this point, the abundance "freezes out", becoming constant until today. An example of this process for a weakly interacting massive particle (WIMP) dark matter candidate is shown in Fig. 2.4^[30]. The latest measured relic density is^[17]:

$$\Omega_c h^2 = 0.1200 \pm 0.0012 \quad (\text{from CMB observations}),$$

$$\Omega_c h^2 = 0.1193 \pm 0.0009 \quad (\text{combined with BAO measurements}).$$

- **Density:** Estimates for local dark matter density range from 0.2 to 0.6 GeV/cm³ based on global extrapolations of rotation curve measurements, assuming a Galactic halo shape, and 0.3 to 1.5 GeV/cm³ from Gaia satellite measurements.^[31]
- **Velocity:** The velocity dispersion of dark matter particles in the Galactic halo is estimated to be between 218 km/s and 246 km/s based on multiple measurements of velocities and radial forces^[32].
- **Self-interaction cross-section:** Limits on the self-interaction of dark matter are constrained to^[33]:

$$\sigma_{DM-DM}/m_{DM} < 0.84 \text{ barn/GeV}.$$

- **Mass:** To account for the observed gravitational effect, the DM mass has lower limit for different kind. For fermionic dark matter candidates, the mass is constrained to be $m > 70 \text{ eV}$ ^[34-35], obtained from the upper bound of phase-space density due to Pauli's principle with the parameters of Fornax dwarf. For bosonic dark matter candidates, the lower limit is $m > 10^{-22} \text{ eV}$ which is required to form the correct small-scale structure and to be consistent with a set of measurements including CMB and luminosity function^[21]. The upper limit on dark matter mass is approximately $5 M_\odot$ to make the structure of cosmology system immersed in DM halos safe, such as binary stars and clusters, from tidal disruption^[21].

Different models explicitly propose candidates for dark matter, and these candidates are widely searched for using a variety of experimental approaches, beyond cosmological observations. These approaches include direct detection, indirect detection, and collider searches. The candidates and their associated detection methods are categorized and illustrated in Figure 2.5.

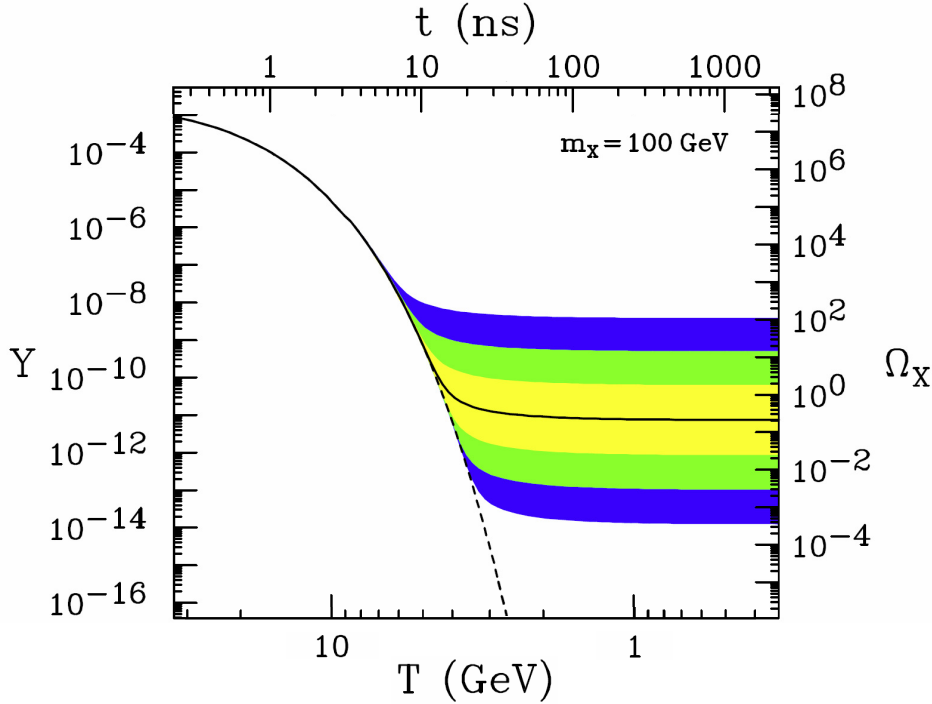


Figure 2.4 Demonstration of the relic density of dark matter. The comoving number density (left), defined as the ratio of WIMP number density to entropy density and resulting thermal relic density (right) evolve as a function of temperature T (bottom) and time t (top), assuming 100 GeV, P-wave annihilating WIMP DM candidate. The line of the freeze-out is for an annihilation cross section yields the correct relic density and the shaded are for a cross-section varied by 100,100,1000 respectively. The dashed line marks the thermal equilibrium.^[30]

Among these methods, collider experiments offer a unique opportunity to potentially generate dark matter on Earth and study it in detail using advanced particle detectors. The high energies achieved in particle collisions recreate the conditions of the early universe, enabling the production of massive dark matter particles directly, which can then be analyzed through their interactions or missing energy signatures. This is the primary method explored in this thesis to search for dark matter.

2.2.3 Dark Higgs

How does dark matter obtain its mass? The dark Higgs model provide one fascinating explanation by porting the Higgs mechanism and Yukawa interaction into the dark sector to account the mass origin. It extends the SM by introducing a hidden sector with its own spontaneously broken $U(1)$ gauge symmetry, leads to a configuration with dark matter fermion χ , massive gauge boson Z' , the dark Higgs field S and the physical dark Higgs s formulated

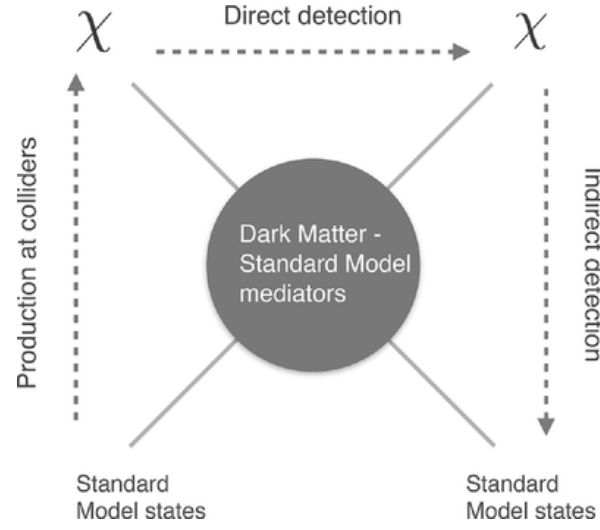


Figure 2.5 General Idea of Experimental Dark Matter Searches. Direct detection experiments probe dark matter through interactions with SM particles, typically employing large volumes of detector material to observe rare signals, as demonstrated by experiments like PANDAX and XenonNT. Indirect detection focuses on anomalies in kinematic distributions and abundances of observed SM particles, often relying on satellite-based experiments such as AMS and DAMPE. Collider experiments, on the other hand, aim to produce dark matter directly and detect its presence via interactions with SM particles at the highest achievable energies.

in $S = \frac{1}{\sqrt{2}}(w + s)$ where the w is the vacuum expectation value of the field^[36]. The Lagrangian interaction terms after SSB is described as fermion interaction

$$\mathcal{L}_\chi = -\frac{1}{2}g_\chi Z'^\mu \bar{\chi} \gamma^5 \gamma_\mu \chi - g_\chi \frac{m_\chi}{m_{z'}} s \bar{\chi} \chi + 2g_\chi Z'^\mu Z'_\mu (g_\chi s^2 + m_{Z'} s) \quad (2.19)$$

where the main parameters are shown in Tab. 2.1.

Table 2.1 Main Parameters of the Dark Higgs Model

Parameter	Explain
m_s	mass of Dark Higgs
m_χ	mass of DM
$m_{Z'}$	mass of heavy mediator
g_χ	coupling in dark sector, between s , χ , Z'
g_q	coupling with SM: $q \leftrightarrow Z'$, fixed 0.25 as benchmark
θ	mixing angle of SM Higgs $\leftrightarrow$ dark Higgs, fixed at 0.01

The experimental constraints and considerations for parameter settings are described in detail in Section 5.2.

In the most common parameter setting of the dark Higgs model, the dark Higgs is chosen

to be the lightest particle in the dark sector. This configuration allows the annihilation channel $\chi\chi \rightarrow ss \rightarrow SM$, which reduces the dark matter abundance without requiring significant fine-tuning of the coupling constants. This parameter choice relaxes the cosmological constraint on the relic density, which is a common issue in standard WIMP models, as they often predict an overabundance of dark matter. This is discussed further in Section 2.2.2.

In terms of production mechanisms, SM quarks are also charged under the dark Higgs field, enabling interactions where the Z' boson couples to SM quarks. This makes production channels into the dark sector accessible in collider experiments, as illustrated in the Feynman diagram in Fig. 2.6 and described by the Lagrangian in Eq. 2.20.

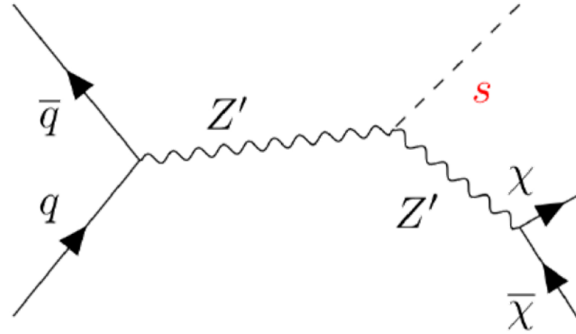


Figure 2.6 Feynman Diagrams of Dark Higgs Model. One of the production channels is shown. The Z' mediates the interaction between SM and the dark sector.

$$\mathcal{L}_{q-Z'} = -g_q Z'^\mu \bar{q} \gamma_\mu q. \quad (2.20)$$

The dark Higgs mixes with the SM Higgs boson, allowing it to decay into SM particles. This mixing provides efficient and detectable signatures for the dark Higgs model. The decay channels of the dark Higgs boson depend on its mass assumptions, leading to a rich phenomenology. For instance, at high masses, the dominant decay channel is $s \rightarrow VV$ (where V represents SM gauge bosons such as W or Z), while at low masses, the decay channel is predominantly $s \rightarrow b\bar{b}$. These decay modes are demonstrated in Fig. 2.7.

2.2.4 Dark Photon

The Dark Photon is another extension of the SM that introduces an additional abelian $U(1)$ gauge symmetry, focusing on kinetic mixing between the SM and the dark sector. This mechanism is described in the Lagrangian in Eq. 2.21, which includes the kinetic mixing of

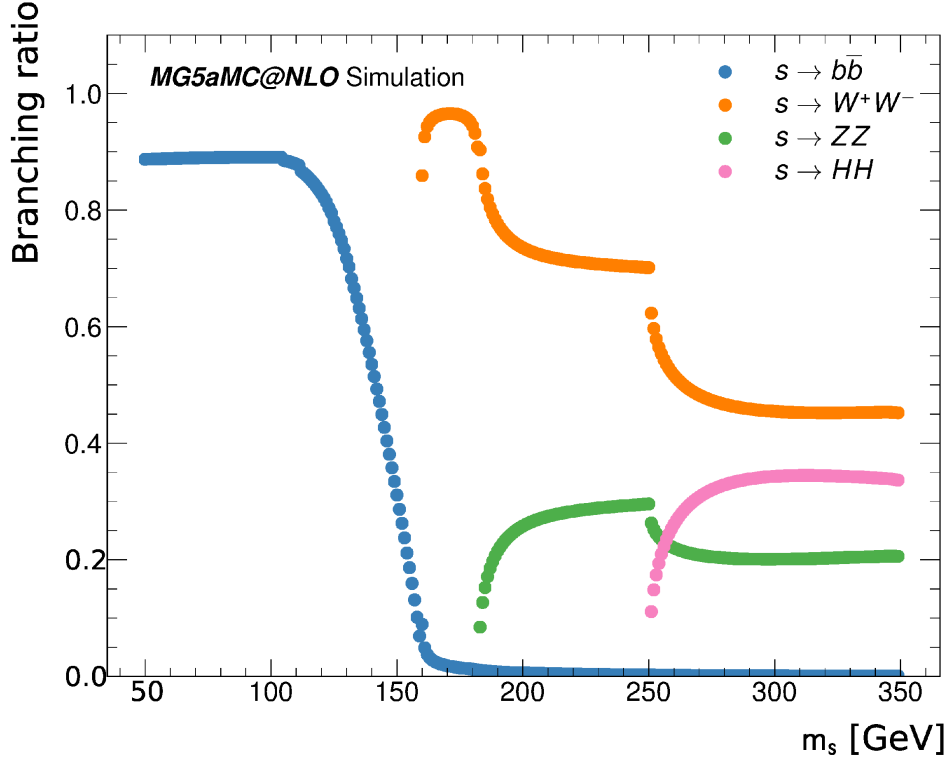


Figure 2.7 Decay Modes of Dark Higgs. Decay branching ratio of dark Higgs to different SM particles depending on the mass. At low mass the dark Higgs boson dominately decay into b quark pair, while at high mass the decay into vector boson pair and even Di-Higgs is leading.^[37]

the two $U(1)$ gauge fields.^[38]

$$\mathcal{L}_0 = -\frac{1}{4}F_{a\mu\nu}F_a^{\mu\nu} - \frac{1}{4}F_{b\mu\nu}F_b^{\mu\nu} - \frac{\epsilon}{2}F_{a\mu\nu}F_b^{\mu\nu} \quad (2.21)$$

The dark photon, as the gauge boson of the dark $U(1)$ gauge field, can be either massless or massive, depending on the mechanism of mass generation. These mechanisms include the SM Higgs mechanism, beyond Standard Model (BSM) Higgs fields (such as the dark Higgs discussed in the previous section), or the Stueckelberg mechanism^[39]. The coupling between the dark photon and the SM photon leads to a rich phenomenology, which has been extensively studied in both collider experiments and direct detection experiments^[38]. The production and decay channels of the dark photon are illustrated in Fig. 2.8.

The two gauge fields can be orthogonally rotated to form the SM photon field and the dark photon field, which diagonalize the kinetic terms, as Eq. 2.22. This rotation also clarifies the interactions between the currents (generated by particles carrying charge under one of the gauge fields) and their corresponding gauge fields.

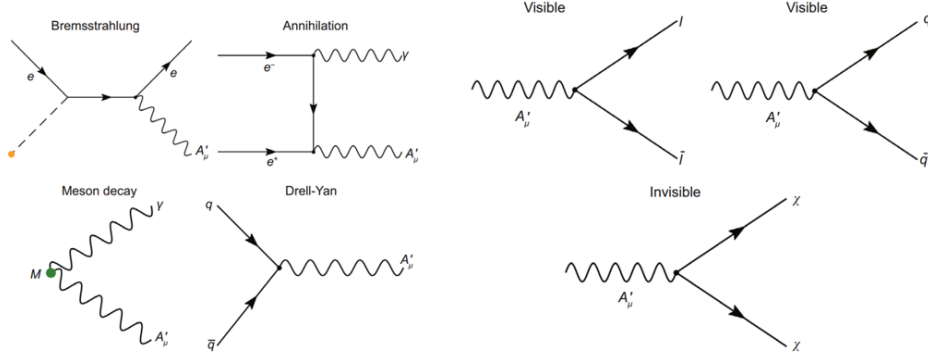


Figure 2.8 Typical Production and Decay Modes of Dark Photo

$$\begin{pmatrix} A_a^\mu \\ A_b^\mu \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{1-\epsilon^2}} & 0 \\ \frac{-\epsilon}{\sqrt{1-\epsilon^2}} & 1 \end{pmatrix} \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} A'^\mu \\ A^\mu \end{pmatrix} \quad (2.22)$$

The rotation angle determines the interaction between the SM and dark currents with the SM and dark photon fields. Two extreme cases can be considered. In the first case, the interaction between the SM photon field and the dark current is rotated to zero. As a result, the SM photon interacts exclusively with SM particles, while the dark photon interacts with both dark and SM particles, as described in Eq. 2.23.

$$\mathcal{L}_1 = \left[\frac{e'}{\sqrt{1-\epsilon^2}} J'_\mu - \frac{e\epsilon}{\sqrt{1-\epsilon^2}} J_\mu \right] A'^\mu + e J_\mu A^\mu \quad (2.23)$$

Another case occurs when the dark photon interacts exclusively with dark particles, while the SM photon interacts with dark particles through a milli-charge^[40], where the normal electric charge is modified by a small coupling constant, as described in Eq. 2.24.

$$\mathcal{L}_2 = e' J'_\mu A'^\mu + \left[\frac{-e'\epsilon}{\sqrt{1-\epsilon^2}} J'_\mu + \frac{e}{\sqrt{1-\epsilon^2}} J_\mu \right] A^\mu \quad (2.24)$$

For the massless dark photon, the rotation angle is arbitrary. In this scenario, the dark photon can mediate long-distance interactions and couples to the SM sector only through high-dimensional effective operators. Consequently, the direct generation of a massless dark photon at colliders via quarks or gluons is generally suppressed.

While for the massive dark photon, the rotation angle is fixed as Eq. 2.25,

$$\theta = \arctan \left[\frac{\delta \sqrt{1-\epsilon^2}}{1-\delta\epsilon} \right] \quad (2.25)$$

where $\delta = M_b/M_a$. The Lagrangian becomes the one shown in Ref^[38] as Eq. 2.26,

$$\mathcal{L}_m = \frac{1}{\sqrt{1-2\delta\epsilon+\delta^2}} \left[e'(1-\delta\epsilon) \frac{J'_\mu}{\sqrt{1-\epsilon^2}} + e(\delta-\epsilon) \frac{J_\mu}{\sqrt{1-\epsilon^2}} \right] A'^\mu + \frac{1}{\sqrt{1-2\delta\epsilon+\delta^2}} [eJ_\mu - \delta e'J'_\mu] A^\mu. \quad (2.26)$$

At collider experiments where the Higgs boson can be generated, the interaction between the Higgs and the dark photon provides a unique probe of the dark photon model^[41-42]. This production channel for the dark photon is not sensitive to the very high ultraviolet (UV) energy scales of effective operators but instead operates at the *EWK* scale, owing to the non-decoupling nature of the Higgs boson^[42].

To connect the Higgs with the dark sector, a set of messenger-scale fields is introduced in the model. The Yukawa coupling in this scenario is assumed to be effective and radiatively induced by the dark sector^[43], rather than being a fundamental coupling. The interaction is described in Eq. 2.27.

$$Y_i = Y_0 \left(\frac{M_i}{\bar{m}} \right) \exp \left(-\frac{2\pi}{3\bar{\alpha}q_i^2} \right) \quad (2.27)$$

where $\bar{\alpha}$ and q_i are the fine structure constant of and dark fermion charge of i flavor under the $U(1)_F$ gauge group. $Y_0(M_i/\bar{m})$ is the loop function of the ratio of dark fermion mass M_i and the universal average mass of messenger fields $\bar{m}$.

And after electroweak symmetry breaking, this interaction leads to the Higgs boson decaying into a photon and a dark photon, as illustrated in the diagrams in Fig. 2.9^[42]. Combined with the extensive production channels of Higgs bosons, this enables an efficient search for dark photons in hadron collider experiments.

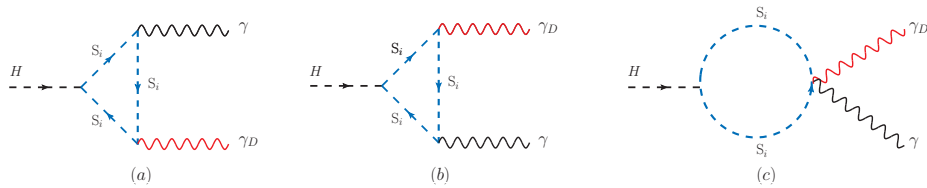


Figure 2.9 Feynman diagrams of dark photon with Higgs coupling. Higgs boson coupled with photon γ and dark photon γ_D via mass eigenstates S_i of portal messenger scalar fields.^[42]

Chapter 3 The Large Hadron Collider (LHC) and ATLAS Experiment

3.1 Overview of LHC

The collider is one of the most important instrumentation to study the elementary particle at high energy frontier. With head-on colliding, the kinetic energy T of accelerated particle with mass m is well utilized in the interaction, leads to roughly $2T/m$ times amplification of relative kinetic energy in the rest frame^[13] and enable the access to physics at higher energy compared with fixed-target experiment. The Large Hadron Collider (LHC) is the biggest particle collider facility in the world with the highest energy proton-proton beam at 7TeV ($7 \times 10^{12}\text{eV}$) of each. Crossing the border between Switzerland and France and being underground at a depth of more than 100 meter, the main ring of the LHC has a circumference of 26.7km where two energetic beams of particle circle and collide. And the collisions being recorded provide valuable data to probe the most fundamental and deepest nature of the world.

The LHC complex consists of several parts, as illustrated in Fig. 3.1¹ where the most notable components are the accelerators and detectors. The linear accelerator, Linac4, located in the north side of the LHC accelerates first the H^- ion which is basically the proton surrounded by electrons and obtained from the hydrogen with inductive surface plasma ignited by radio frequency (RF) electromagnetic wave. Then the circular accelerator Proton Synchrotron Booster further accelerates the particle to 2GeV and removes the electron, resulting in the proton beam. With further acceleration by two synchrotrons, the Proton Synchrotron (PS) and Super Proton Synchrotron (SPS), the beam reaches 450GeV energy and is injected into the main ring bunch by bunch. In the main ring two proton beams are finally accelerates up to 7TeV, circle the ring 11245 times per second and collide in the bunches at a frequency at 40MHz. Characterized in the term of luminosity L , which is defined in Formula 3.1 which stands for the number of events detected from the collision dN in a certain period of time dt and of unit cross-section σ , The LHC is designed to deliver very intensive beam at $10^{34}\text{cm}^{-2}\text{s}^{-1}$ which is actually doubled in the operation of 2017.

¹ Figure Credits to CERN

$$L = \frac{1}{\sigma} \frac{dN}{dt}. \quad (3.1)$$

The collision generates billions of particles and in the end they are recorded by detectors which are designed to measure the momentum of energy of different type particles.

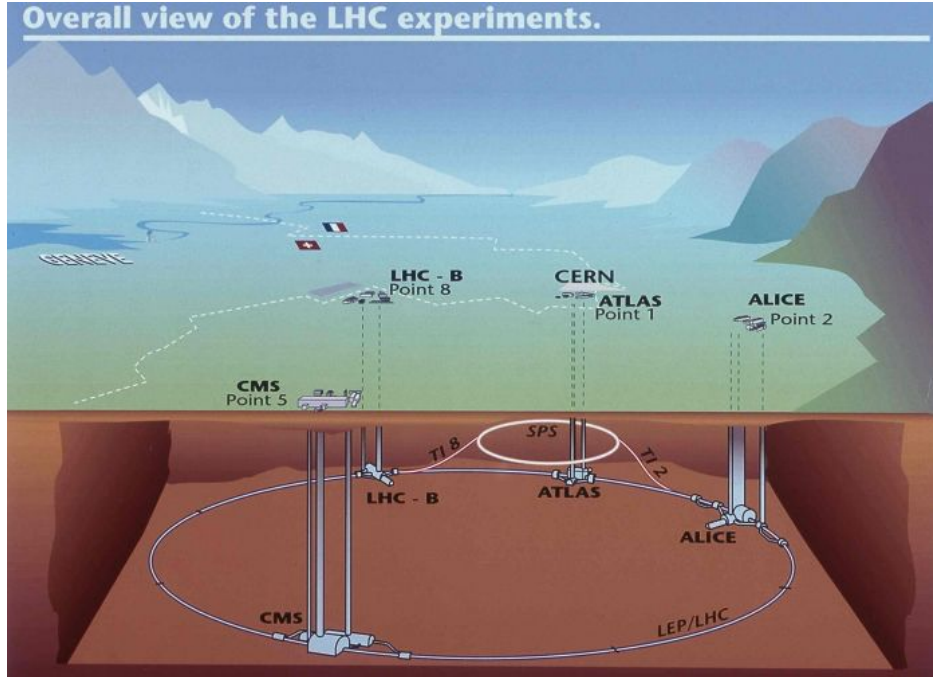


Figure 3.1 Sketch of the Large Hadron Collider ¹

Four crossing points where the collision happens are positioned on the LHC ring and multiple detectors and experiments are located to study different phenomena. ATLAS (A Toroidal LHC Apparatus) and CMS (Compact Muon Solenoid) are the two general purpose particle detector experiments lying on the opposite sites on the ring and host variety of physics programme, including the precise measurements of Standard Model and searches for the Beyond Standard Model phenomenology. Another experiments includes ALICE (A Large Ion Collider Experiment) which is designed for the study of quark-gluon plasma, LHCb (LHC-beauty) experiment focuses on b-physics and more experiments which take full advantage of the unprecedented energy at LHC facility and probes the fundamental physics in different aspect.

This thesis is mainly based on the data taken from ATLAS experiment while the prospective study in the last part covers the phenomenology in the context of general collider experiment.

3.2 The ATLAS Detector

With the largest general-purpose detector at the LHC, the ATLAS experiment^[44] is designed to maximize the potential for the discovery of new physics while maintaining the capability for high-accuracy measurements of the Standard Model. It has a size of 46 meters in length by 25 meters in diameter and weighs more than 7000 tons. It features the following subsystems and aims to provide as many signatures and as accurate and precise measurements as possible in the high-luminosity environment.

- Inner Detector (ID) system^[45-46], surrounded by solenoid magnets^[47], operational at high luminosity for the measurement of lepton momentum at high p_T , identification of electrons/photons, τ -lepton identification, b-quark tagging, and full event reconstruction at lower luminosity.
- Electromagnetic calorimeter (ECAL) system^[48] for electron/photon identification and measurement. A complementary hadronic calorimeter (HCAL)^[48] with full coverage designed for measurements of jet and missing transverse energy (E_T^{miss}) accurately.
- Stand-alone muon system^[49] for accurate measurement of muon momentum at the highest luminosities, utilizing toroid magnets^[47].
- Trigger and Data Acquisition (TDAQ) system^[50-51], integrated with each sub-detector, providing full azimuthal angle ϕ coverage and large acceptance range of pseudo-rapidity η , to measure particles with low- p_T thresholds and high efficiency for most processes.

The quantitative expected performance of detector is list in Tab. 3.1^[52].

Table 3.1 General performance goals of the ATLAS detector^[52]. σ denotes the overall absolute resolution in GeV. $\oplus$ marks the constant term of uncertainty.

	Resolution	Coverage in η	
		for Measurement	for Trigger
Tracker	$\sigma_{p_T}/p_T = 0.05\% p_T (GeV) \oplus 1\%$	± 2.5	
ECAL	$\sigma_E/E = 10\% \sqrt{E (GeV)} \oplus 0.7\%$	± 3.2	± 2.5
HCAL			
Barrel&Cap	$\sigma_E/E = 50\% \sqrt{E (GeV)} \oplus 3\%$	± 3.2	± 3.2
Forward	$\sigma_E/E = 100\% \sqrt{E (GeV)} \oplus 10\%$	$3.1 < \eta < 4.9$	$3.1 < \eta < 4.9$
Muon Spectrometer	$\sigma_{p_T}/p_T = 10\%$ at $p_T = 1\text{TeV}$	± 2.7	± 2.4

The overall layout of ATLAS detector is visualized in Fig. 3.2^[52] and detailed in the following sections.

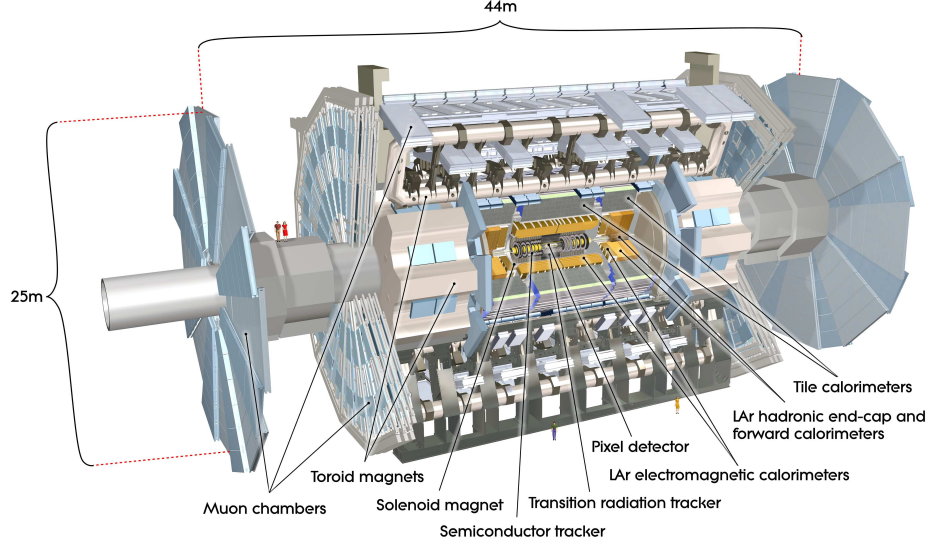


Figure 3.2 Overview layout of ATLAS detector^[52]

3.2.1 Inner Detector (ID)

The Inner Detector (ID) system^[53-54], located closest to the interaction point, plays a crucial role in achieving precise measurements of the vertex and momentum of charged particles. It combines silicon-based detectors—the Pixel and Silicon Microstrip Tracker (SCT)—with the gas-based Transition Radiation Tracker (TRT). These sub-detectors offer high granularity, enabling accurate measurements in an environment with extremely dense track multiplicity, where approximately 1000 particles traverse the detector every 25ns. The entire ID system is immersed in a 2T axial magnetic field, as illustrated in the inner region of Fig. 3.3¹. This magnetic field bends the trajectories of charged particles, facilitating precise momentum measurements. The overview layout of the ID is illustrated in Fig. 3.4. The barrel and end-cap structure of detectors provide η coverage from -2.5 to +2.5, with the detailed coverage shown in Fig. 3.5. The main parameters are detailed in Ref.^[52].

At the innermost region, the silicon-based detector is placed to ensure precise tracking measurements. The pixel detector^[53-54], located at the core, comprises three layers of pixel sensors in the barrel and three disks in each end-cap. The pixel dimensions are $50 \times 400 \mu\text{m}^2$

¹ Credit to Rodriguez Vera, Ana Maria; Antunes Pequeno, Joao

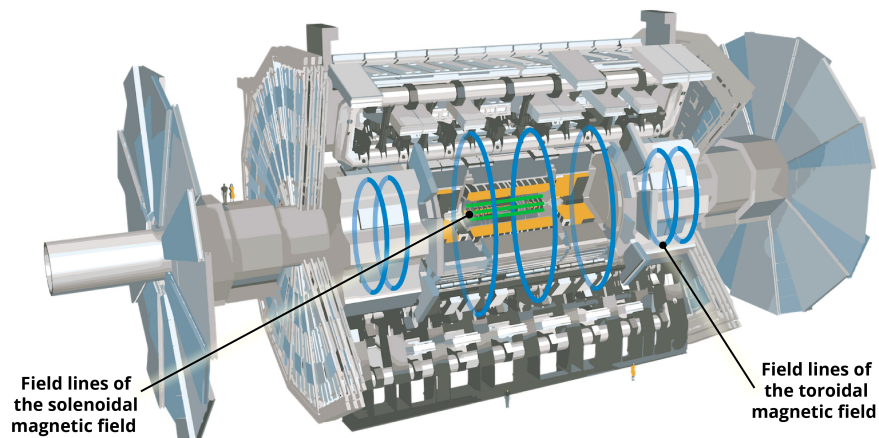


Figure 3.3 Overview layout of Magnet System in ATLAS detector^[1]

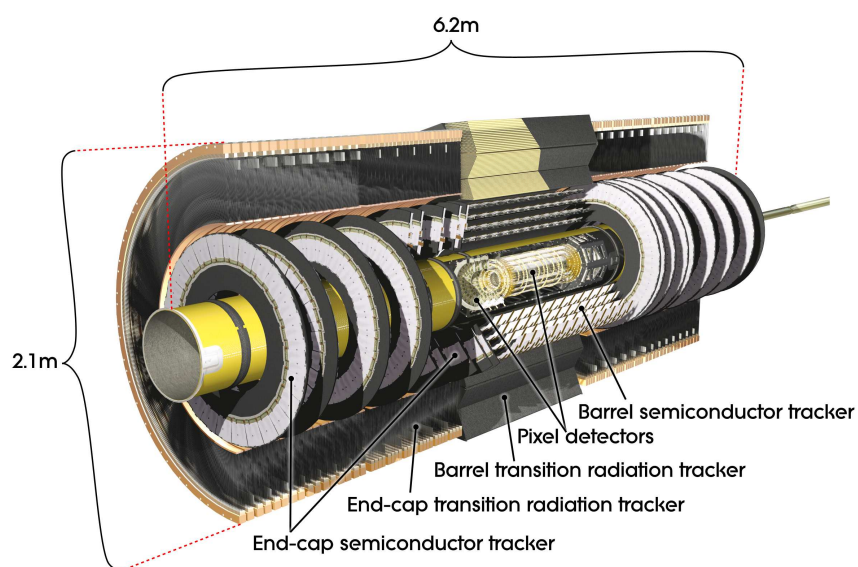


Figure 3.4 Overview layout of ATLAS Inner Detector^[52]

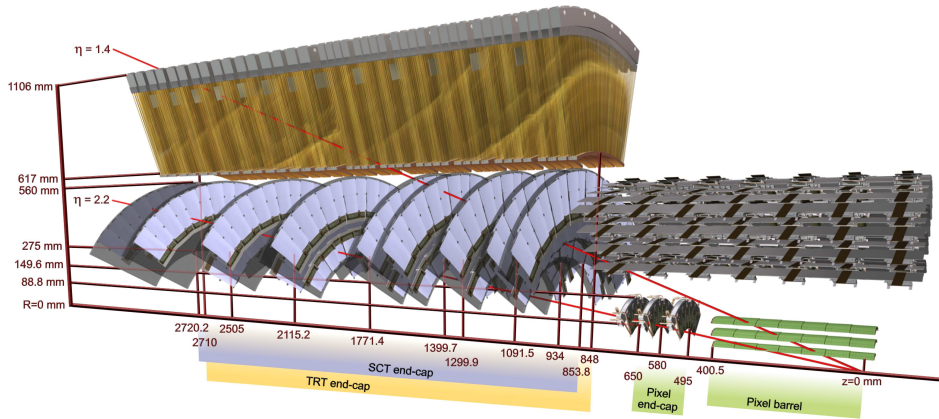


Figure 3.5 Coverage of ATLAS Inner Detector^[52]

in the barrel and $50 \times 600 \mu\text{m}^2$ in the end-cap, with a thickness of $250 \mu\text{m}$. Novel oxygenated n-type wafers are fabricated for use in the sensors, with the readout pixels located on the n^+ -implanted side. The Semiconductor Tracker (SCT)^[55] surrounds the pixel detector and features four layers of silicon microstrip sensors in the barrel and nine disks in each end-cap. The strip widths are $80 \mu\text{m}$ in the barrel and $122 \mu\text{m}$ in the end-cap, employing reliable, cost-effective single-sided p-in-n technology with AC-coupled readout. Together, the pixel detector and SCT enable highly accurate track and vertex measurements, with resolutions of $10 \mu\text{m}$ and $17 \mu\text{m}$, respectively. Prior to the 2015 data-taking year, the Insertable B-Layer (IBL)^[56] was installed as the innermost layer of the pixel detector, positioned closer to the beam pipe. The IBL incorporates advanced technologies, including planar n-in-n sensors with slim edges, 3D sensors, and a new 130nm CMOS front-end readout ASIC. This upgrade significantly enhances tracking precision, particularly for vertexing and b-tagging, while also facilitating maintenance of the beam pipe, electronics, and innermost sensors following exposure to high radiation doses.

At the outermost region, the gas-based Transition Radiation Tracker (TRT)^[45-46] ensures continuous tracking and facilitates electron identification while remaining cost-effective. The TRT consists of polyimide straw tubes with 4mm diameter $\times$ 144cm length, constructed from $35 \mu\text{m}$ thick multi-layer films. The central anode is made of the gold-plated tungsten wire. The tubes are filled with a gas mixture (70% Xe, 27% CO_2 , 3% O_2). This xenon-based gas mixture allows for efficient separation of low-energy transition radiation photons from minimum-ionizing charged particles, as the former are absorbed, generating a stronger signal. The TRT achieves a tracking resolution of $130 \mu\text{m}$ per straw tube and complements other

sub-detectors by enhancing electron identification through transition radiation detection.

3.2.2 Calorimeter

The calorimeter system^[48] is designed for the measurement of the energy and position of particles, primarily electrons, photons, and hadronic particles forming jets. It consists of two main components: the electromagnetic calorimeter (ECAL) and the hadronic calorimeter (HCAL), as illustrated in Fig. 3.6. The ECAL, based on liquid-argon technology, is optimized for precise energy measurements of electrons and photons, offering high granularity and excellent resolution while covering the pseudorapidity range $|\eta| < 3.2$. In contrast, the HCAL utilizes scintillator-tile technology for $|\eta| < 1.7$ and liquid-argon technology for $|\eta| > 1.5$, and is designed to measure precisely the energy of hadronic particles, such as jets, and to estimate missing transverse energy (E_T^{miss}). The forward liquid-argon calorimeter extends the coverage to $|\eta| < 4.9$ and functions as both an electromagnetic and hadronic calorimeter. Both the ECAL and HCAL are sampling calorimeters, specifically designed to handle the high energy and radiation environment of the LHC. The ECAL has a total thickness exceeding 22 radiation lengths (X_0) in the barrel region and more than $24 X_0$ in the end-caps, ensuring effective absorption of electromagnetic particles. For the hadronic component, the thickness is 9.7 interaction lengths (λ) in the barrel and 10λ in the end-caps, which is sufficient to achieve high-resolution measurements for high-energy jets. The total thickness, including the support materials, reaches 11λ at $\eta = 0$, significantly reducing the punch-through of muons into the outer sub-detectors. This design ensures the calorimeter system's capability to accurately reconstruct jet energies while minimizing background from penetrating particles.

The ECAL is a lead-liquid argon (LAr) sampling calorimeter with an accordion geometry as shown in Fig. 3.7, optimized for measuring the energy and position of electrons and photons with high precision. Its unique design ensures complete azimuthal coverage without cracks, enhancing the detector's ability to accurately reconstruct electromagnetic showers. The ECAL is divided into three sections along its depth with $|\eta| < 2.5$. In the case of the end-cap inner wheel (EMEC), it features two depth segments and a comparatively coarser lateral granularity than the other regions within its coverage. The presampler was added in the $|\eta| < 1.8$ with 1.1cm thickness LAr in barrel and 0.5cm at end-cap. It is designed to measure the energy loss of particles before entering the calorimeter. The

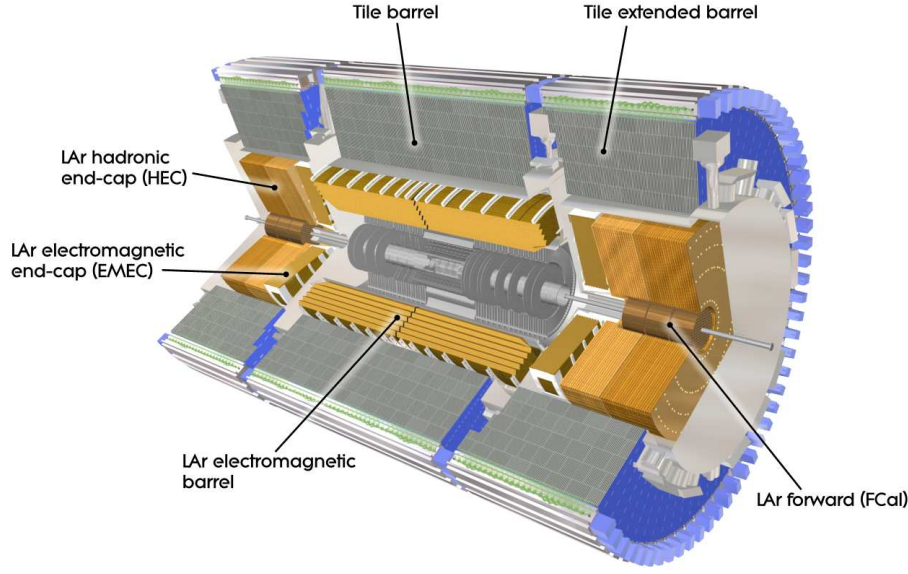


Figure 3.6 Overview layout of ATLAS Calorimeter System^[52]

beam test of barrel module with the material setup before the ECAL module close to the real detector^[57] gives the energy resolution of barrel ECAL is measured to be $\sigma_E/E = (10.1 \pm 0.4)\%/\sqrt{E(GeV)} \oplus (0.2 \pm 0.1)\%$ and 0.5% linearity with energy range 20-250 GeV.

The HCAL contains several sections: Tile Calorimeter (TileCal) is built with the steel (absorber) and scintillating tiles (active material). The barrel covers $|\eta| < 1.0$ and two extended barrels the range $0.8 < |\eta| < 1.7$. Azimuthally the TileCal has 64 modules and radially range from 2.28m to 4.25m. In depth it is segmented in three layers and in total 9.7λ at $\eta = 0$. The scintillating tiles are read out from two sides and the scintillation light is guided by wavelength shifting fibres into two photomultiplier tubes (PMT). The combined beam test of barrel ECAL and TileCal yields the energy resolution of $\sigma_E/E = (52.0 \pm 1.0)\%/\sqrt{E(GeV)} \oplus (3.0 \pm 0.1)\%$ with $1.6\text{GeV} \pm 0.1\%$ electronic noise for the hadron response.

The end-cap HCAL (HEC) consists of two wheels per side, constructed with interleaved 8.5mm liquid-argon (LAr) gaps and 25mm/50mm copper plates for the front and rear wheels, respectively, covering the range $1.5 < |\eta| < 3.2$.

The forward calorimeter (FCal) comprises three modules, also utilizing LAr technology. The first module, similar to the ECAL, uses copper, while the second and third modules,

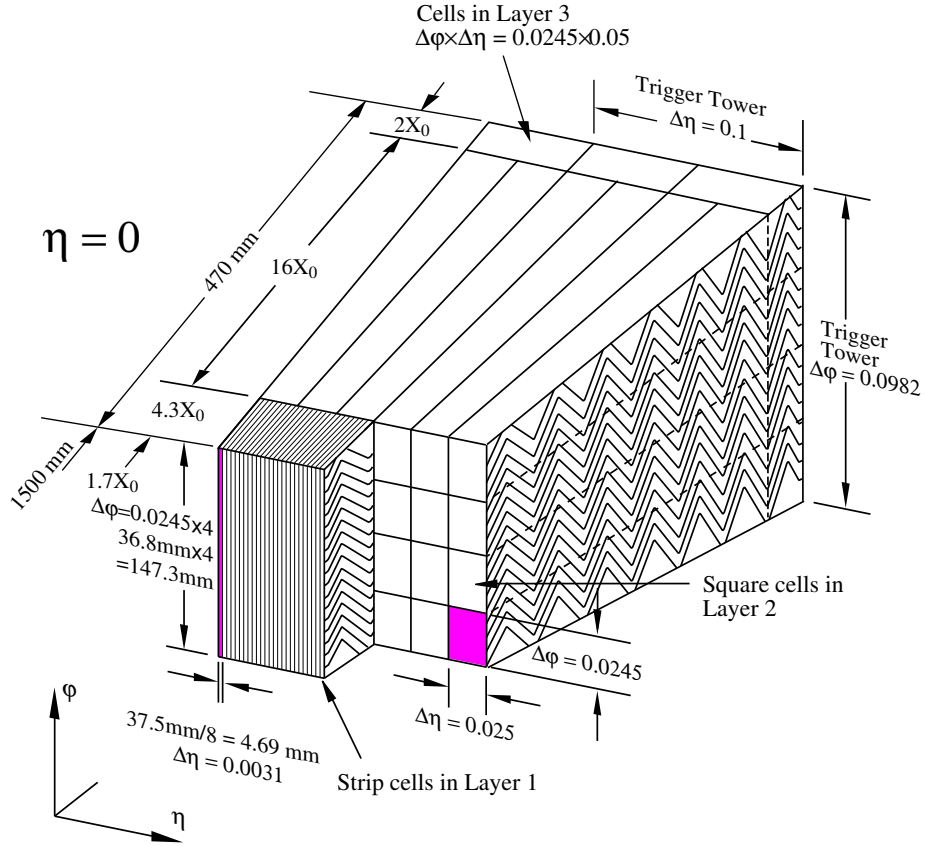


Figure 3.7 Layout of ATLAS ECAL Unit^[52]

functioning as the HCAL, use tungsten. The FCal covers the range $3.1 < |\eta| < 4.9$ and provides a total depth of approximately 10 interaction lengths. To handle the extremely high particle flux in the forward region, the LAr gap is reduced to as small as 0.25mm.

3.2.3 Muon System

The muon spectrometer^[49] is designed for the measurement of the muon momentum in conjunction with the magnet system, which provides a toroidal magnetic field of 0.5T in the central region and 1.0T in the end-cap region. The system consists of four main components: Monitored Drift Tubes (MDT), Cathode Strip Chambers (CSC), Resistive Plate Chambers (RPC), and Thin Gap Chambers (TGC). The MDTs are used for precise muon tracking, while the CSCs complement coverage in the large pseudorapidity range of $2 < |\eta| < 2.7$. The RPCs and TGCs are primarily employed for triggering at a resolution of 1.5-4ns, covering $|\eta| < 2.4$, with the former used in the barrel region and the latter in the end-cap region. The RPCs and TGCs also measure the muon coordinates in the orthogonal direction, provide

bunch-crossing identification, and determine p_T thresholds.

The muon system occupies a large volume, making the alignment of each module, as well as the measurement of the magnetic field over the entire area, critical to achieving the required measurement resolution. The MDT and CSC chambers are monitored using laser sensors precisely installed inside the modules, which are sensitive to deformations of the module as well as the variations in the relative positions. On a larger scale, the initial alignment of the system is achieved through precise installation, with tolerances of 5mm and 2mrad. The alignment is then refined using track-based method with high-momentum muon during data-taking and the targeted $30\ \mu\text{m}$ precision is achieved. The magnetic field is continuously monitored using Hall probes distributed throughout the system.

The layout of the muon system is illustrated in Fig. 3.8 and the design parameters detailed in Ref.^[52].

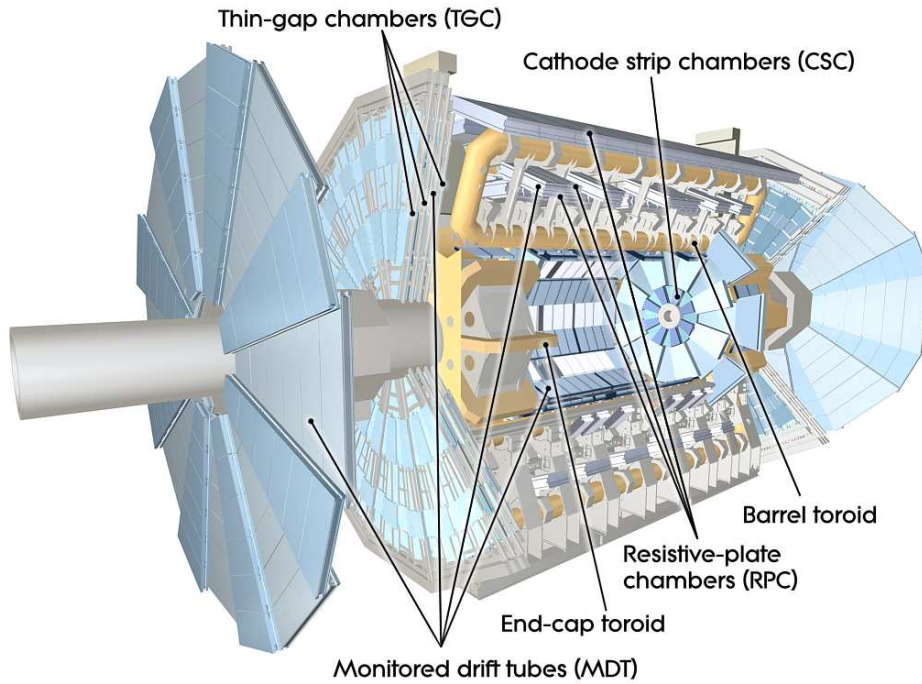


Figure 3.8 Overview layout of ATLAS Muon Spectrometer^[52]

The four detector in the muon system are all gaseous detectors optimized for different functions. The Monitored Drift Tubes (MDTs), the primary tracking detectors, consist of tubes approximately 3 cm in diameter filled with the gas mixture (93% Ar, 7% CO_2). MDTs provide a spatial resolution of $80\ \mu\text{m}$ in the bending direction but are limited to a maximum

counting rate of $150\text{Hz}/\text{cm}^2$.

The Cathode Strip Chambers (CSCs) are one type of the multiwire proportional chambers with cathode strip readout and anode wires. They are designed for higher-rate environments, handling up to $1000\text{Hz}/\text{cm}^2$, making them suitable for the end-cap regions. CSCs also offer superior resolution of $60\mu\text{m}$ in the bending direction.

The Resistive Plate Chambers (RPCs) are parallel-plate detectors with resistive plates separated by a 2mm gas gap. And the Thin Gap Chambers (TGCs) are multiwire proportional chambers featuring a 1.4mm wire pitch. TGCs utilize a high-field, low-gain gas mixture and thin gaps to achieve excellent timing resolution.

3.3 Data Acquisition and Simulation

3.3.1 Trigger System

The proton-proton bunch crossings at the LHC occur at a design rate of 40 MHz, far exceeding the data storage and processing capabilities of even today's technology. The trigger system is designed to reduce the event rate by selecting events of physics interest for further processing. There are two levels of trigger system: the Level-1 (L1) trigger and the High-Level Trigger (HLT).

The L1 trigger is hardware-based and reduces the event rate down to 100 kHz, while the HLT is software-based and it further reduces the rate to 1 kHz. The L1 trigger uses the information from calorimeters and muon systems to make quick decisions, whereas the HLT utilizes full event information to apply more complex selection criteria. The trigger system is designed to be both flexible and configurable, leveraging programmable hardware (L1) and software-based logic (HLT). This flexibility enables the selection of diverse physics signatures and event topologies, such as electrons and photons^[58], $E_{\text{T}}^{\text{miss}}$ ^[59], muons^[60], b -jets^[61], and objects with specific patterns, combinations, or topologies^[62-63].

The architecture of the ATLAS trigger system is illustrated in Fig. 3.9.

The Level-1 (L1) trigger system is based on custom electronics and FPGAs, designed to make fast decisions within $2.5\mu\text{s}$ and reduce the event rate to fit within the data transfer bandwidth. The L1 trigger system consists of calorimeter trigger, muon trigger and central trigger processor.

The calorimeter trigger (L1Calo) utilizes information from the calorimeter system to iden-

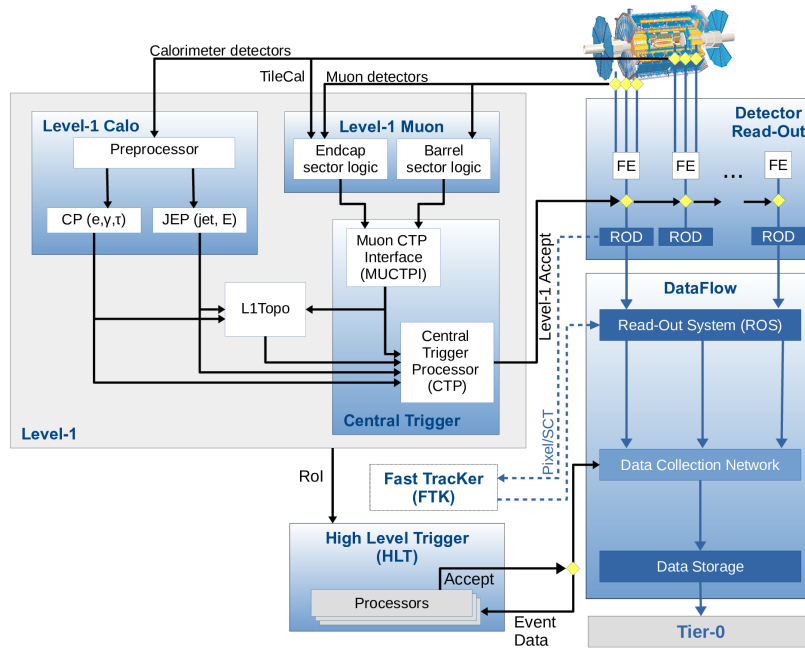


Figure 3.9 Diagram of the Trigger system designed in Run 2. The FTK system was proposed but was not commissioned during Run 2.^[64]

tify high-energy objects, such as electrons, photons, and jets. The muon trigger (L1Muon) leverages data from the muon system to identify high-momentum muons. The L1Topo trigger takes kinematic information from input triggers and makes decision based on simple event topologies and global event quantities, such as mass and E_T^{miss} . The central trigger processor combines the information from both the calorimeters and muon triggers to make a final decision. Due to limited processing time and bandwidth, objects at the L1 trigger level are not fully reconstructed with full precision and granularity. Instead, the system provides regions of interest (RoIs) for further processing at the High-Level Trigger (HLT).

The HLT is a software-based trigger system that operates on a farm of CPUs. It utilizes full event information to perform more complex selections than the L1 trigger, aiming to replicate full reconstruction at the analysis level but with a limited processing time. This includes identifying specific objects or event topologies. The HLT is designed to reduce the event rate to around 1 kHz, shared among triggers with different physics interests defined in the *trigger menu*. This is limited as the maximum event rate that can be stored to disk. The stored data are subsequently processed offline for further analysis.

3.3.2 Event Simulation

One important task for collider experiments is to separate the unknown from the known. To incorporate the best known knowledge of particle physics, collision events are simulated and widely used in analyses. Simulated events are essential for detector optimization, background process estimation, and new physics signal searches.

The known knowledge used in the simulation includes SM theory/phenomenology describing particle interactions and outcomes derived from perturbative/non-perturbative approaches, the physics of detectors modelling particle-material interaction and electronics for decoding and recording detector signals. The process involves two major steps to simulate realistic data:

Event Generation: Various Monte Carlo (MC) generators are employed to simulate events starting from matrix element (ME) calculations, parton showering (PS), hadronization, and immediate decays. Extra effects such as initial- and final-state radiation (ISR/FSR), multiple parton-parton interactions (MPI), and underlying events (UE) are also included. The SM theory and empirical knowledge are used to compute cross-sections and kinematic distributions of particle outcomes. New physics events can also be simulated according to specific models, such as dark matter production from SM quark interactions. This step generates the kinematics of free particles, such as leptons and hadrons, which are then passed to the next step. This information, often referred to as *truth* information, represents the pure physics outcomes before detector, allowing direct decoding of the hard-scattering physics.

Detector Simulation and Digitization^[65]: The particles from event generation are then passed through a GEANT4-based^[66] detector simulation to replicate realistic detector responses. Particle-material interactions are simulated using models for different energy scales, such as the QGSP (quark-gluon string model with the Pre-compound model)^[67] for energies up to the TeV scale and parameterized models for lower-energy excitations down to the keV range. Secondary particles are sampled using MC methods and traced recursively. The simulation incorporates detailed geometry, material effects, magnetic fields, and operational conditions (e.g., inactive detector regions due to defects).

The detector simulation produces *hits*, which represent the response on detector material before electronic processing. These hits are then passed to the digitization step, where they are converted into detector signals. Electronics simulations are applied to mimic the

real detector readout. The output of the digitization process is in a similar format as real taken data, which serves as input for reconstruction. Additional effects, such as electronic noise and pile-up, are incorporated at this stage. Pileup arises from additional proton-proton interactions occurring in the same (*in-time pileup*) or adjacent bunch crossings (*out-of-time pileup*) as the primary interaction and other reasons such as cavern background, beam halo events and beam gas events^[68]. The pileup effect is added to the simulation following the procedure illustrated in Fig. 3.10.

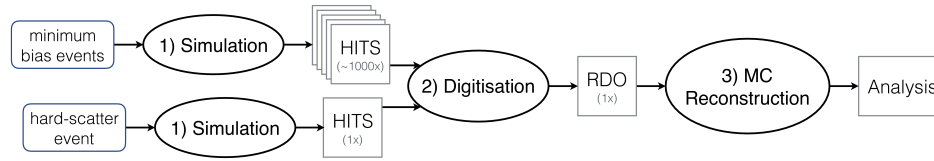


Figure 3.10 Simulation of Pileup Events^[69]

3.4 Object Reconstruction

3.4.1 Low-level objects

The tracks of charged particles in the tracker and clusters of energy deposition in the calorimeter serve as low-level objects used in the reconstruction of physics objects. Their reconstruction relies on a detailed understanding of the detector, its operational conditions, and sophisticated algorithms designed to address realistic effects such as pileup, noise, quenching, saturation, dynamic range limitations, defects, and the intrinsic physical properties of the detector. A brief introduction to the reconstruction process is provided below.

3.4.1.1 Tracks^[70]

- **Clusterization:** Energy deposits in the pixel and SCT detectors are grouped into clusters using connected component analysis (CCA)^[71] and are then used to create three-dimensional space-points representing the particle's path. Closely spaced particles can produce merged clusters and necessitates precise identification techniques to maintain reconstruction efficiency.
- **Iterative Combinatorial Track Finding:** The combinatorial Kalman filter^[72] is used. Track reconstruction begins with seed formation from three space-points in the inner detector layers. These seeds are extended outward by adding compatible clusters layer by layer, forming track candidates. The process iterates, refining the selection by

removing clusters associated with successful tracks and reprocessing the remaining data to identify additional tracks.

- **Track Candidates and Ambiguity Solving^[70]**: Multiple track candidates can share clusters, leading to ambiguities. An ambiguity solver evaluates these candidates based on criteria such as the number of shared clusters, track fit quality, and consistency with the detector model. It assigns scores to each candidate, resolving conflicts by selecting the most probable tracks while minimizing shared clusters, thus enhancing reconstruction accuracy.
- **Neural-Network Pixel Clustering^[73]**: To address merged clusters from closely spaced particles, neural networks are employed to predict the number of particles contributing to a cluster and estimate their positions. This method improves the precision of cluster position and error estimates, particularly in high-density regions, by effectively distinguishing overlapping signals.
- **Track Fit^[70]**: High-resolution fit is applied to the selected track candidates using all associated clusters. This fitting process refines the track parameters, ensuring accurate momentum and trajectory determination, which are crucial for subsequent physics analyses.

3.4.1.2 Topo-Cluster

The energy deposition in the calorimeter is clustered to form candidates used in lepton and jet reconstruction. The topo-cluster method^[74-75] is employed due to its favorable properties for reconstructing electromagnetic (EM) and hadronic energy.

For EM energy, the topo-cluster method effectively recovers energy losses caused by bremsstrahlung photons or photon conversions, utilizing the dynamic supercluster technique^[76]. With proper calibration^[77], it also achieves excellent linearity and stability, even in high pile-up environments, comparable to the performance of previous fixed-size clustering methods^[78]. For hadronic energy, the method efficiently suppresses noise, providing significant improvements to jet and E_T^{miss} reconstruction.

The topo-clustering process is recursive, beginning with proto-clusters, where the cell energy exceeds four times the noise level (determined by electronic noise and pile-up noise estimated from the expected instantaneous luminosity). The cluster grows to include neighboring cells if their energy exceeds two times the noise level. This condition applies to the

absolute value of energy, allowing negative energy to be included if it meets the threshold. Finally, clusters are merged if adjacent cells are selected, and they are split if multiple local minima are identified. A local minimum is defined as a cell with energy exceeding 500 MeV and surrounded by at least four neighboring cells with lower energy.

3.4.2 Electron and Photon

The electron and photon reconstruction procedures are summarized in Fig. 3.11 and illustrated schematically for electrons in Fig. 3.12.

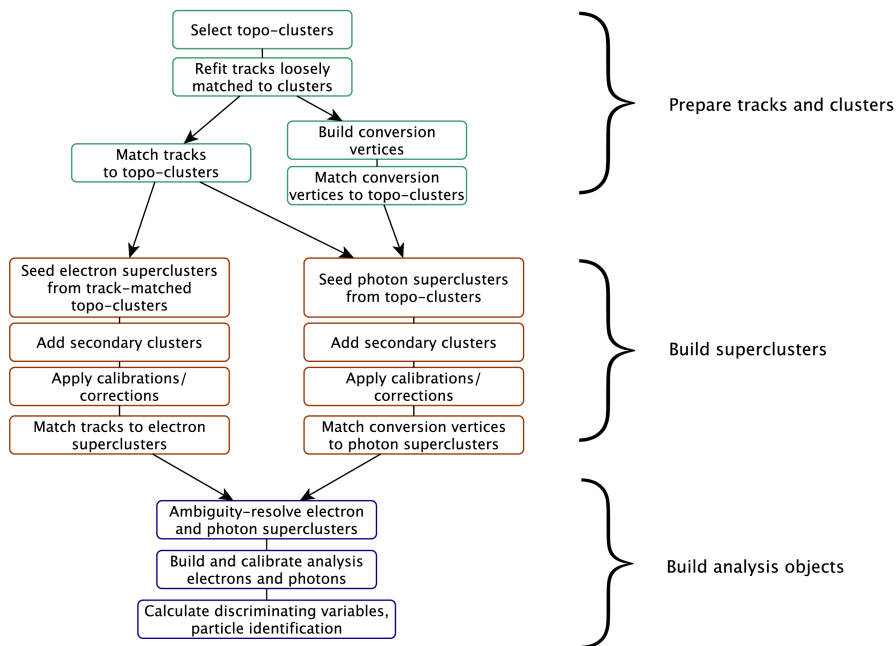
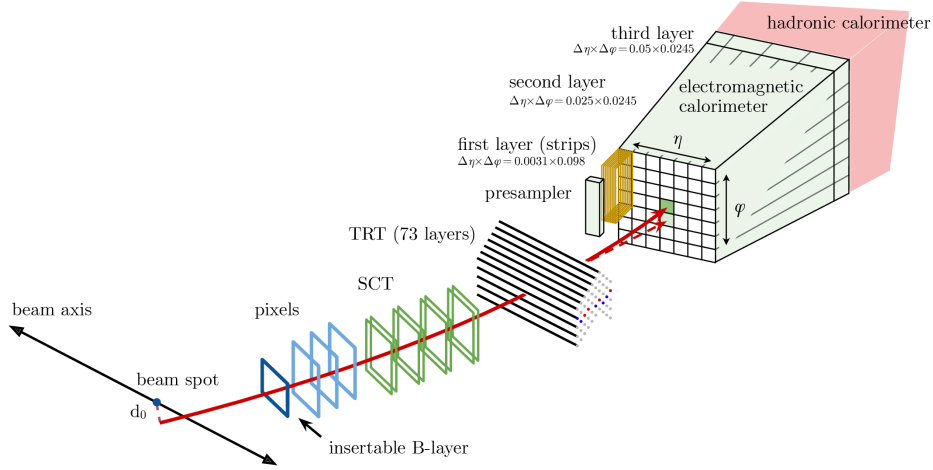


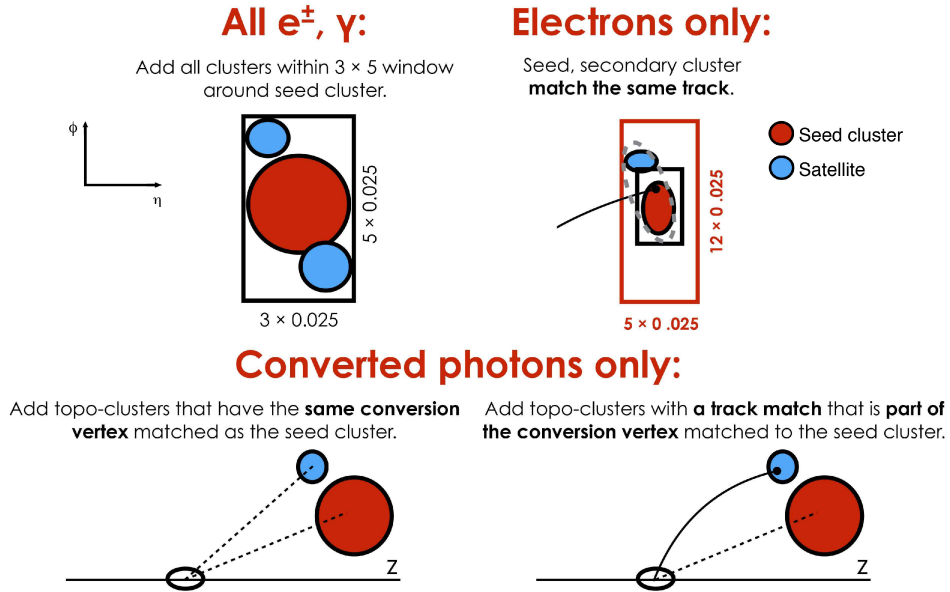
Figure 3.11 Reconstruction of Electron and Photon in ATLAS Run2.^[76]

Starting from the track and topo-clustering information discussed earlier, superclusters are created using the method illustrated in Fig. 3.13. Initial corrections and calibrations are then applied, as detailed in Ref.^[77], and electron tracks or photon conversion vertices are matched to the corresponding supercluster.

To reconstruct unique electron or photon candidates, ambiguities are resolved using the algorithm illustrated in Fig. 3.14. A set of identification and isolation^[79] criteria, named "identification working points" and "isolation working points", are calculated based on variables derived from the supercluster and track information. These criteria enable different analyses to select purer and more isolated objects tailored for specific physics goals. Finally,

Figure 3.12 Electron hits in Detector used in Reconstruction^[79]

calibrations^[76-77] are performed, and systematic uncertainties are assigned to the resulting objects.

Figure 3.13 Super-cluster for Electron and Photon Reconstruction in Run2.^[76]

3.4.3 Muon

Muons are first independently reconstructed using the inner detector (ID) tracks, as described in Section 3.4.1.1, and the muon spectrometer (MS). The combined muons are then used for physics analysis. The reconstruction of muons from the MS and takes full advantage of the components of the MS, as introduced in Section 3.2.3. Initially, segments

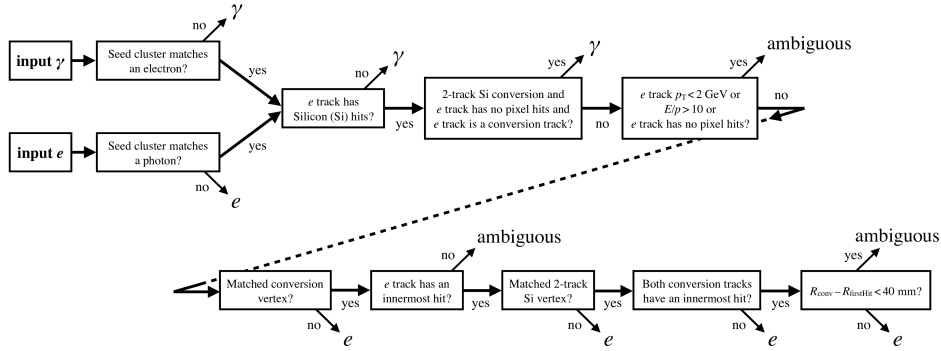


Figure 3.14 Algorithm for Resolving Ambiguities Between Electron and Photon Reconstruction^[76]

are formed from MDT, RPC, and TGC, as well as the CSC for the high- η region.

The combined muon is formed using information from the ID and MS, employing various algorithms^[80] and with assistance from the calorimeter data. Four kinds of muons are reconstructed as detailed in Ref.^[81].

- **Combined (CB) muon:** from global refit of the hits from both Inner Detector and Muon Spectrometer
- **Segment-tagged (ST) muon:** track in Inner Detector and extrapolated to at least 1 local track segment in the MDT or CSC subdetector at Muon Spectrometer
- **Calorimeter-tagged (CT) muons:** track in Inner Detector and matched to minimum-ionizing particle (mip) in calorimeter
- **Extrapolated (ME) muons:** reconstructed with the Muon Spectrometer track only

Several muon identification and isolation criteria^[81], similar to those for electrons and photons, are defined. The identification is mainly designed to suppress the muons from the in-flight kaon and pion decay and is defined using the fit quality and the agreement of independent measurements with the ID and MS. This defines Medium, Loose, Tight, and High- p_T muons to be used in different analyses, as the requirements for efficiency and purity vary. The isolation is based on track-based and calorimeter-based variables. These criteria essentially measure the activity, such as track p_T or calorimeter energy, within a cone around the muon. The goal is to distinguish muons from particle decays, such as those from W , Z , or Higgs bosons, from muons embedded within jets.

Calibrations are applied to the muon objects to correct their energy and momentum scales as well as resolutions, and systematic uncertainties are assigned accordingly.^[81]

3.4.4 Tau

Tau leptons decay either leptonically (into one lepton and two neutrinos) or hadronically (into several hadrons and one neutrino), typically before reaching the detector. Tau reconstruction can be performed as a composite object identified from several signatures, particularly in the leptonic decay channel. Specific algorithms have been developed to identify and calibrate hadronic taus, as their response in different detector components is more interconnected and can overlap with jets originating from quarks or other particles^[82].

In the physics topics discussed in this thesis, taus are often treated as a background for standard jets. Consequently, tau veto requirements are typically applied, involving both object- and event-level selections. Taus also represent a non-negligible source of background in zero-lepton regions due to the low identification efficiency. To estimate this contribution, dedicated control regions are defined. Leveraging lepton universality, tau contributions are constrained using control regions defined for other leptons, such as muons and electrons. This process is discussed in detail, for example, in Section 5.

3.4.5 Jet and Missing Momentum

3.4.5.1 Jet definition

As we know, confinement prevents quarks and gluons from existing freely in space, and the only detectable signatures in the detector come from the showered and hadronized particles. These particles leave footprints in the tracker, calorimeter, and sometimes the muon spectrometer. A jet is defined as a collection of particles clustered together in the detector, resulting from such as the hadronization of quarks and gluons.

ATLAS mainly uses two types of jets with different radii. The small- R jet aims to capture particles originating from a single quark or gluon, while the large- R jet clusters the hadronic decay products of massive particles, such as W , Z , Higgs bosons, and top quarks. The separation between the decay products, roughly the radius of the jet, is approximately $\Delta R \approx 2m/p_T$, where m is the mass of the particle.

Jet reconstruction^[83] starts with inputs from the calorimeter and tracker. The topoclusters^[74] from the calorimeter, as described in Section 3.4.1.2, are the primary inputs for jet reconstruction in ATLAS. These clusters define the EM jet or the local cell weighting (LCW) jet based on different calibration scales. At the EM scale, the cell energies of the

topo-cluster are summed to form the cluster energy, and EM jets are mainly used for small- R jets. The LCW scale accounts for the differences between electromagnetic and hadronic interactions, correcting the topo-cluster to the hadronic energy scale on average. This makes the LCW scale more suitable for large- R jets, where more hadronic interactions are clustered.

A new jet reconstruction method developed in ATLAS combines track information, as described in Section 3.4.1.1, with calorimeter data to form the PFlow jet^[84], improving the resolution of jet reconstruction. The steps involved in forming the PFlow jet are summarized in Fig. 3.15.

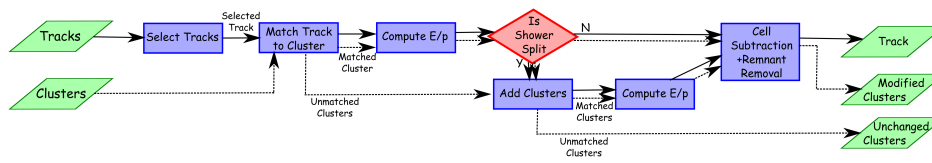


Figure 3.15 Reconstruction of Particle Flow Jet^[84]

Pile-up activity is the primary source of noise affecting the inputs for jet clustering. There are two types of pile-up: in-time pile-up, which occurs when many interactions happen simultaneously in the same bunch crossing as the hard-scattering collision we study, and out-of-time pile-up, which arises from interactions in previous or subsequent bunch crossings due to the detector's processing time.

Topo-cluster-based jets have intrinsic pile-up suppression, as noise cells are excluded from clustering if their energy is below a specific threshold determined based on the average pile-up level and electronic noise. The impact of pile-up is further mitigated using various techniques^[85], along with jet calibration and grooming methods.

The jet grooming procedure for large- R jets is designed to mitigate the pile-up effects that are clustered into the jet. A series of algorithms have been developed^[86-89], with trimming^[87] being the technique typically used in ATLAS. Trimming is performed with parameters $f_{cut} = 5\%$ and $R_{sub} = 0.2$. In this procedure, the k_t algorithm^[90] is applied to the constituents of the original jet with a sub-jet radius R_{sub} . Constituents are removed if they are clustered into a k_t sub-jet with p_T less than f_{cut} of the large- R jet.

Once the clusters are prepared, a standard jet clustering algorithm is applied to form the jets. The anti- k_t algorithm^[91] is the most widely used algorithm in ATLAS. It is a sequential recombination algorithm with the distance metric defined as:

$$d_{ij} = \min \left(\frac{1}{k_{ti}^2}, \frac{1}{k_{tj}^2} \right) \frac{\Delta R_{ij}^2}{R^2}, \quad (3.2)$$

where k_{ti} is the transverse momentum of particle i , ΔR_{ij} is the distance between two particles in the η - ϕ plane, and R is the jet radius parameter. The anti- k_t algorithm effectively forms jets dominated by high- k_t particles due to the inverse- k_t^2 weighting in the distance metric, associating lower- k_t particles with these jets as the clustering proceeds. The anti- k_t algorithm typically produces more cone-like jet shapes and is robust to the addition of soft radiation due to the suppression by k_t^{-2} , as illustrated in Fig. 3.16.

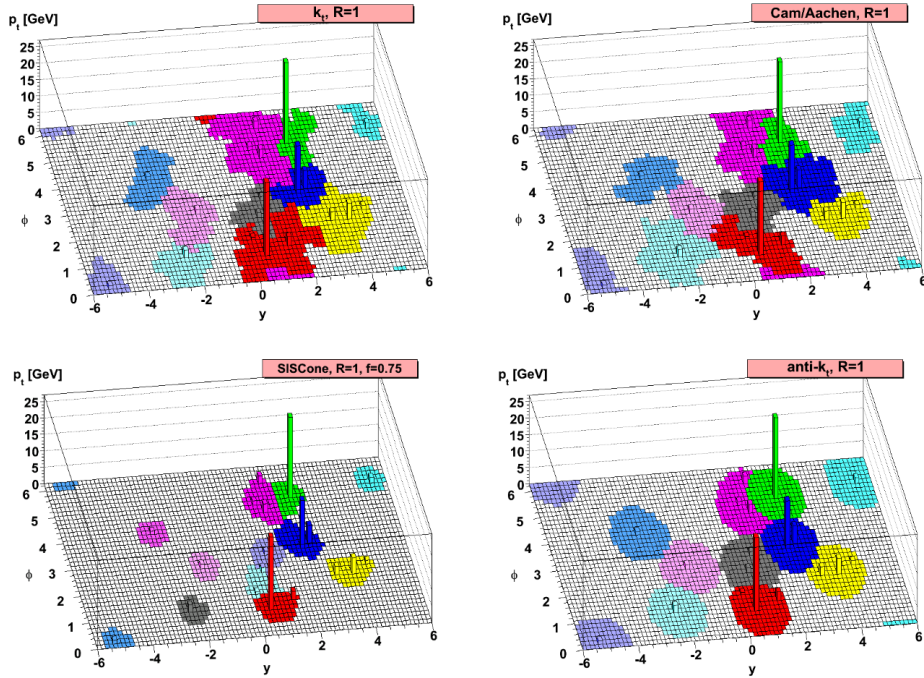


Figure 3.16 Demonstration of the jet shape from Anti- k_t and other Algorithms^[91]

The typical parameter R used in ATLAS is 0.4 for small- R jets and 1.0 for large- R jets.

There are also other types of jets defined in ATLAS, such as track jets, which are formed solely from the tracks in the tracker and are particularly useful for b-tagging and studying the substructure of jets. Another type is the reclustering jet, which is typically used to reconstruct jets outside the phase space supported by standard jet definitions and calibrations, such as low-mass large- R jets. These jet types differ only in their inputs, as the standard jet clustering algorithm is still applied. Various radii are also used for specific purposes, such as $R = 0.2$ or variable radii determined by the jet p_T .

3.4.5.2 Jet calibration

The jet must be calibrated to correct for various effects from the detector and the reconstruction process. The calibration process is divided into several steps, which are summarized in Fig. 3.17.

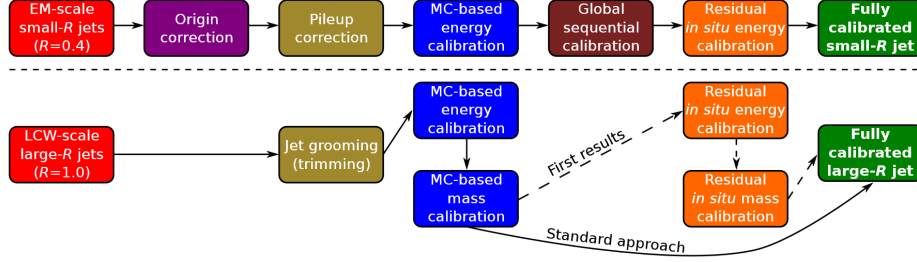


Figure 3.17 Calibration workflow of the Jet object designed for ATLAS Run2^[83]

The workflow starts from the pile-up suppression. For large- R jets, jet grooming techniques, as discussed earlier, are employed to remove clustered pile-up particles (topoclusters). For small- R jets, pile-up suppression relies primarily on energy subtraction and corrections applied on average. The jet origin is first corrected to the primary vertex. Then, the pile-up energy density ρ within $|\eta| < 2.0$, the number of primary vertices per event N_{PV} , and the average number of interactions per bunch crossing μ are obtained to apply the correction. The corrected transverse momentum is calculated using the formula:

$$p_T^{\text{corr}} = p_T - \rho \mathcal{A}_{\text{jet}} - \alpha(N_{PV} - 1) - \beta\mu,$$

where $\mathcal{A}_{\text{jet}}$ is the jet area obtained for each jet, and the residual factors α and β are derived from a specific dataset. Jets originating directly from pile-up can be removed in later analyses using the (Forward) Jet Vertex Tagger (fJVT/JVT)^[92-93].

The MC-based calibration^[94] uses well-defined MC samples to correct the jet energy scale (JES), accounting for the large fraction of invisible energy in hadronic activity. The small- R jet is further refined with Global Sequential Calibration^[95], which considers additional properties of jet response, such as flavor differences, and narrows the jet energy resolution (JER). For large- R jets, the mass (JMS/JMR) is also calibrated using MC samples.

The MC-based calibrations are further corrected to data using in-situ methods^[94,96-97], where well-understood objects are used to calibrate other jets in the same event. For example, the forward jet can be calibrated with the central jet in p_T -balanced dijet events. Track-based

objects are also used for large- R jet mass in-situ calibration when statistics are limited for other methods.

These methods yield well-calibrated performance for both small- R jets^[94], achieving JES uncertainty at or below the 1% level for central jets over a wide p_T range of 100 GeV to 1 TeV, and for large- R jets^[96], with JES uncertainty at 1-2% for a p_T range of 200 GeV to 2 TeV, as shown in Fig. 3.18 and JMS uncertainty at 2-10% as shown Fig. 3.19.

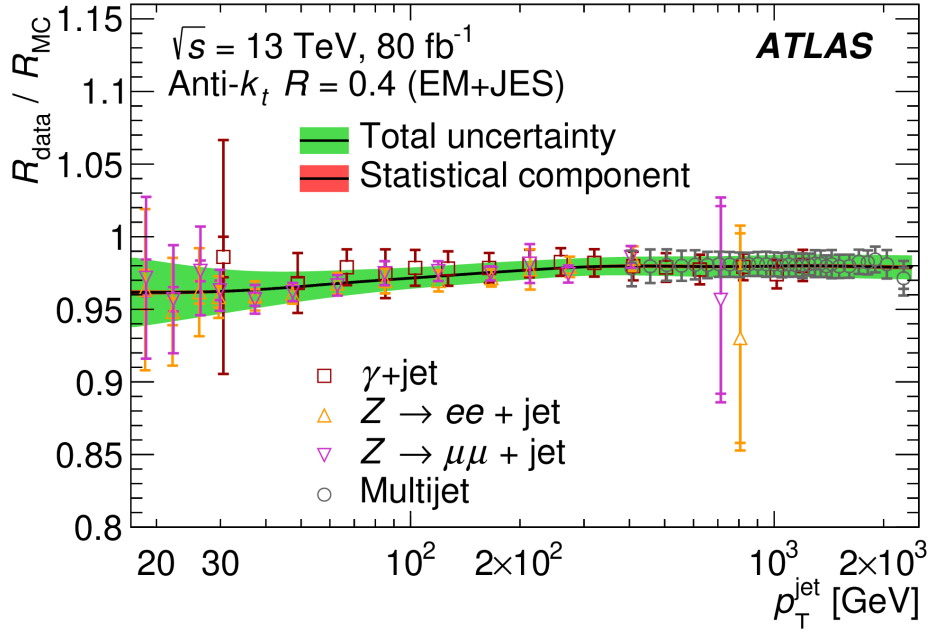


Figure 3.18 EM+JES calibration: Jet response ratio in data to that in the nominal MC event generator as a function of jet p_T for Z +jet, γ +jet, and multijet in situ calibrations. Statistical unc. is shown with inner horizontal ticks and total unc. (stat. unc. and syst. unc. summed in square) in outer. The final correction and its statistical and total unc. bands are also shown.^[94]

3.4.5.3 E_T^{miss} reconstruction^[98]

Missing transverse energy (E_T^{miss}) reconstruction involves subtracting the transverse energy contributions from all reconstructed objects to recover the missing component. Complicated handling is required to address overlaps or duplications in the original detector signals that are used by different object reconstruction algorithms. The general composition of E_T^{miss} is described in 3.3.

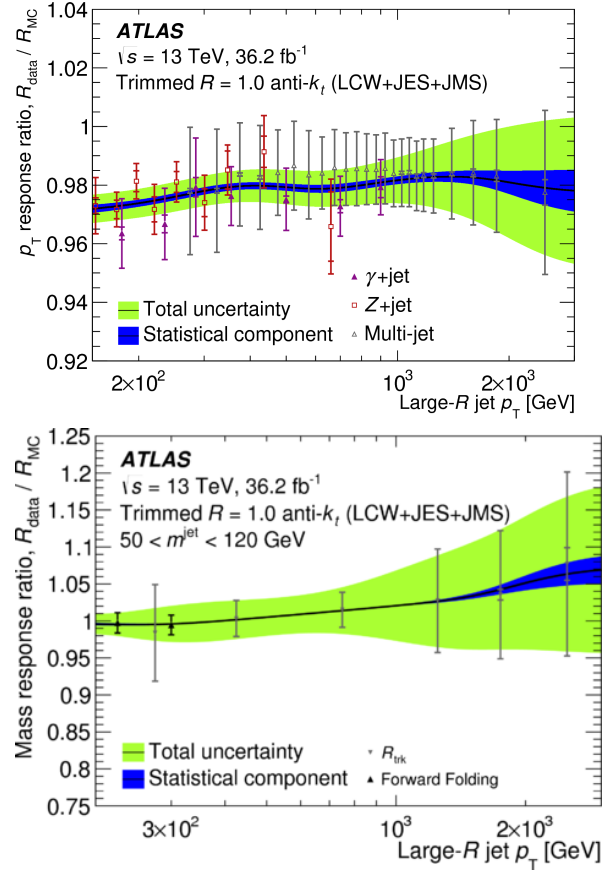


Figure 3.19 LCW+JES+JMS calibration of Anti-kt $R=1.0$ jets.

Up: Data/MC ratio of average jet p_T response. The X-axis shows the large- R jet p_T . In situ techniques are used including the balance method of Z+jets, γ +jet and multijet, shown in open squares, closed triangles and open triangles respectively.

Down: Data/MC ratio of average jet mass response. The X-axis shows the large- R jet p_T . In situ techniques are combined to provide the correction including R_{trk} and forward-folding approaches. The W mass window (50-120 GeV) is used for the large- R jet mass fitting.

For both plots, the statistical error is shown in the inner error bars and total uncertainty in the outer, summed up the stat. and syst. unc. in square. Smoothing is applied with a sliding Gaussian kernel.^[96]

$$p_T^{\text{miss}} = - \left(\underbrace{\sum_{\text{selected } e/e^-} p_T^e + \sum_{\text{accepted } \gamma} p_T^\gamma + \sum_{\text{accepted } \tau\text{-leptons}} p_T^\tau + \sum_{\text{selected } \mu} p_T^\mu + \sum_{\text{accepted jets}} p_T^{\text{jet}}}_{\text{hard term}} + \underbrace{\sum_{\text{unused tracks}} p_T^{\text{track}}}_{\text{soft term}} \right). \quad (3.3)$$

The hard term in the E_T^{miss} calculation generally consists of well-calibrated objects and can be selected based on the specific analysis requirements. For instance, in the analysis this thesis describes, a "lepton-invisible" E_T^{miss} is defined, where the lepton is treated as invisible, aiming to estimate the contribution from missing reconstructed lepton.

The soft terms represent low-level signals that are not associated with reconstructed objects. These can be calculated either from the calorimeter or from tracks. The track-based approach, while excluding neutral soft particles, often performs better in high-pileup environments due to its reliance on ID-tracks associated with the hard-scatter vertex.

From the E_T^{miss} vector, the magnitude of E_T^{miss} and its azimuthal angle can be obtained as:

$$p_T^{\text{miss}} = |\vec{p}_T^{\text{miss}}| = \sqrt{(p_x^{\text{miss}})^2 + (p_y^{\text{miss}})^2}, \quad (3.4)$$

$$\phi^{\text{miss}} = \tan^{-1} \left(\frac{p_y^{\text{miss}}}{p_x^{\text{miss}}} \right). \quad (3.5)$$

The scalar sum of all E_T^{miss} components is another important observable. While distinct from the E_T^{miss} magnitude, it reflects the overall "hardness" of the process.

A signal ambiguity resolution procedure is employed to address cases where the same detector signals are used by different object reconstruction algorithms, which can distort the E_T^{miss} calculation. This procedure involves associating reconstructed objects with low-level tracks, topo-clusters, or PFlow objects to determine their relationships. Ambiguities are resolved through a sequential process, as described in^[98], which considers overlaps between different objects. Ultimately, this leads to the construction of object-based E_T^{miss} using mutually exclusive detector signals.

The absolute scale of E_T^{miss} can be evaluated using the p_T^Z distribution in $Z \rightarrow \ell\ell$ events, where the true E_T^{miss} is expected to be zero. The systematic uncertainty of E_T^{miss} reconstruction arises from both the hard-term and soft-term contributions. Hard-term uncertainties are

propagated from the uncertainties of individual objects selected in the analysis, while soft-term uncertainties are derived from calibration procedures using leptonic Z decay events.

In addition, the E_T^{miss} significance (S)^[98] is defined to quantify the likelihood that the reconstructed E_T^{miss} originates from genuine sources, such as neutrinos or invisible BSM particles. This is especially critical for analyses relying on E_T^{miss} , such as dark matter searches and supersymmetry (SUSY) particle searches, where the primary signature is missing detector response. Both event-based and object-based E_T^{miss} significance measures are used, with the latter offering superior performance as it adheres to the same object selection criteria as the object-based E_T^{miss} calculation.

The evaluation of E_T^{miss} significance relies on the resolution of reconstructed hadronic activity or other objects, as well as their correlations. Detailed procedures and methodologies for calculating E_T^{miss} significance are well documented in^[98].

3.4.5.4 Jet flavor^[99]

Jet flavor tagging is a crucial technique for distinguishing heavy-flavor jets, originating from b -quarks, from light-flavor jets. This is particularly important for analyses in hadronic channels, such as those involving $b\bar{b}$ final states originating from Higgs boson decays or beyond-the-Standard-Model (BSM) heavy particles.

Jet flavor identification relies on tracks from charged particles, primary vertices (PVs), and the jets themselves. A key characteristic of heavy-flavor jets is the presence of displaced tracks and the secondary vertices (SV), as illustrated in Fig. 3.20. Several algorithms developed within ATLAS aim to tag jet flavor using these low-level features. Examples include impact-parameter-based (IP-based) algorithms, for example, IP2D and IP3D^[100], the track-based recurrent neural network tagger RNNIP^[101], secondary-vertex-tagging algorithms SV1^[102] and SVKine^[99], and the topological multi-vertex finding algorithm JetFitter^[103].

High-level algorithms, such as DL1r^[99], combine information from these lower-level features using deep neural networks. More recently, graph network-based taggers (GN1/GN2) and transformer-based taggers have been developed, targeting enhanced performance in future data-taking periods.

The detailed information utilized by flavor tagging algorithms is summarized in Tab. 3.2, taken from Ref.^[99]. The significance improvements achieved through these advancements, driven by over a decade of technological development, are highlighted in Fig. 3.21. This

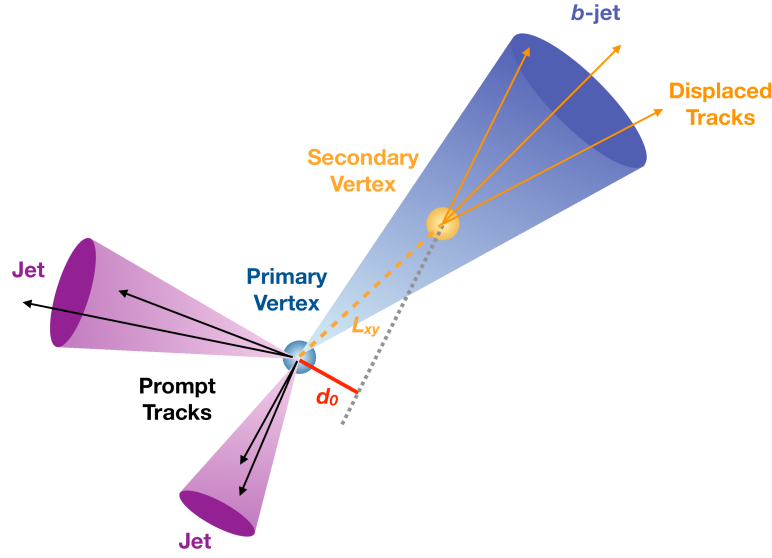
Figure 3.20 Principle of Jet Flavor Tagging^[61]

figure demonstrates the remarkable progress and success of the continuous evolution in experimental techniques.

Building upon small- R jet tagging, the tagging of composite large- R jets becomes feasible by associating sub-jets with well-defined flavor information. However, for the boosted jet with high- p_T , where sub-jets are highly merged, the reconstruction and single jet flavor tagging of sub-jet become extremely challenging. This difficulty has led to the development of a new concept: boosted flavor tagging, or double- b tagging, which overlaps with techniques originally developed for $W/Z/\text{Top}$ tagging as part of the large- R jet reconstruction algorithm^[108].

The development and performance of boosted double- b tagging are critical to the primary physics topic of this thesis: the search for dark matter associated with $b\bar{b}$ final states. The study and improvement of this algorithm have been a central focus throughout my PhD. These efforts are documented in detail in Chapter 4, as part of my PhD research contributions.

Table 3.2 Input variables used by the SVKine, JFKine, DL1 and DL1r algorithms.^[99]

Input	Variable	Description	SVKine	JFKine	DL1	DL1r
Kinematics	p_T	Jet p_T	✓	✓	✓	✓
	η	Jet $ \eta $	✓	✓	✓	✓
IP2D, IP3D	$\log(P_b/P_{\text{light}})$	Likelihood ratio (LR) of hypotheses: the b -jet to light-flavour jet			✓	✓
	$\log(P_b/P_c)$	LR of hypotheses: the b -jet to c -jet			✓	✓
	$\log(P_c/P_{\text{light}})$	LR of hypotheses: the c -jet to light-flavour jet			✓	✓
RNNIP	P_b	b -jet probability				✓
	P_c	c -jet probability				✓
	P_{light}	light-flavour jet probability				✓
SV1	m	Invariant mass of tracks at the secondary vertex (SV) (assuming pion mass)	✓		✓	✓
	f_E	Jet energy fraction of the tracks which associated with the SV	✓		✓	✓
	N_{TrkAtVtx}	No. of the tracks used in the SV	✓		✓	✓
	$N_{2\text{TrkVtx}}$	No. of the two-track vertex candidates	✓		✓	✓
	L_{xy}	Transverse distance between the primary vertex (PV) and SV	✓		✓	✓
	L_{xyz}	Distance between the PV and SV	✓		✓	✓
	S_{xyz}	Distance between the PV and SV divided by its uncertainty	✓		✓	✓
	$\Delta R(\vec{p}_{\text{jet}}, \vec{p}_{\text{vtx}})$	ΔR between the jet axis and the direction of the SV relative to the PV.	✓		✓	✓
	m	Invariant mass of the tracks from displaced vertices		✓	✓	✓
JetFitter	f_E	Jet energy fraction of the tracks associated with displaced vertices		✓	✓	✓
	$\Delta R(\vec{p}_{\text{jet}}, \vec{p}_{\text{vtx}})$	ΔR between the jet axis and the vectorial sum of momenta of all tracks attached to displaced vertices		✓	✓	✓
	S_{xyz}	Significance of the average distance between PV and displaced vertices		✓	✓	✓
	N_{TrkAtVtx}	No. of tracks from multi-prong displaced vertices		✓	✓	✓
	$N_{2\text{TrkVtx}}$	No. of two-track vertex candidates (prior to decay chain fit)		✓	✓	✓
	$N_{1\text{-trk vertices}}$	No. of single-prong displaced vertices		✓	✓	✓
	$N_{\geq 2\text{-trk vertices}}$	No. of multi-prong displaced vertices		✓	✓	✓
	$L_{xyz}(2^{\text{nd}})$	Distance of 2 nd vertex (SV) from PV		✓	✓	✓
	$L_{xy}(2^{\text{nd}})$	Transverse displacement of the SV		✓	✓	✓
	$m_{\text{Trk}}(2^{\text{nd}})$	Invariant mass of the tracks associated with the SV		✓	✓	✓
	$E(2^{\text{nd}})$	Energy of the tracks associated with the SV		✓	✓	✓
	$f_E(2^{\text{nd}})$	Jet energy fraction of the tracks associated with the SV		✓	✓	✓
	$N_{\text{TrkAtVtx}}(2^{\text{nd}})$	No. of tracks associated with the SV		✓	✓	✓
	$\eta_{\text{tk}}^{\text{min,max,avg}}(2^{\text{nd}})$	Min., max. and avg. pseudorapidity of tracks at the SV		✓	✓	✓

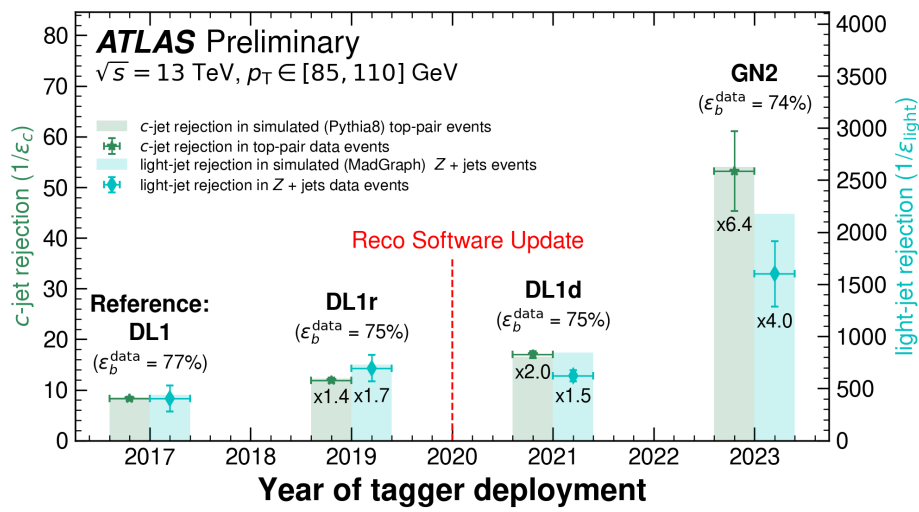


Figure 3.21 Evolution of the improvement of flavour tagging algorithms. The filled bar represents the expected performance, the background rejections (defined as the inverse of the mistagging rates of c- and light-jets), computed on the ttbar MC sample corresponding to a 70% jet expected efficiency. Data points show the performance measured by the calibration analyses with their uncertainties, using events for b-jets^[104], c-jets^[105] and light-jets^[106]. The number on the bar denotes the relative improvement in the measured rejections of light- and c- jet with respect to ones from the DL1 tagger.^[107]

Chapter 4 Study of Novel Boosted Jet Tagging Algorithm

The identification of particles such as the Higgs boson decaying into pairs of b-quarks is crucial in many physics analyses.

In analyses such as searching for large missing momentum or high-mass BSM particles decaying into Higgs bosons, the resulting high-momentum particles create a highly boosted topology. In such cases, the jet constituents are highly collimated and merged, posing a challenge for jet flavor identification using conventional algorithms, as described in Section 3.4.5.4. Boosted jet tagging is therefore of great importance.

In the specific scenarios such as SM measurements of boosted Higgs boson^[109-110] and BSM searches for heavy particles decaying into Higgs bosons with high p_T ^[111-115], the decay products are produced highly collimated and this results in the large-radius (large- R) jet reconstructed. New techniques are needed to analyze the large- R jet. A neural network (NN)-based $X \rightarrow b\bar{b}$ tagging algorithm named $DXbb$ ^[116] has been developed in ATLAS and it extends the jet flavor identification to the large- R jet level. With the help of machine learning, this algorithm efficiently combines the information from the kinematics of the large- R jet and the tagging variables of subjets (variable-radius track-jets) and achieves notable improvement in performance.

In this chapter, the development and calibration of the novel $X \rightarrow b\bar{b}$ tagging algorithm are presented, with a focus on mistagging efficiency calibration, which is the main area of my study.

4.1 Introduction to Algorithm

The $DXbb$ algorithm combines the inputs of kinematic variables of the large- R jet, including p_T , η , and the flavor information of up to three subjets. The neural network is trained to discriminate jets using MC-simulated $H \rightarrow b\bar{b}$, top quark, and QCD multijet samples, and outputs three probability values for the jet. The architecture of the tagger is illustrated in Figure 4.1.

The three probability values are combined to define a single discriminant, as described in Eq. 4.1, in the form of a log-likelihood ratio. This method is proven to be optimal for

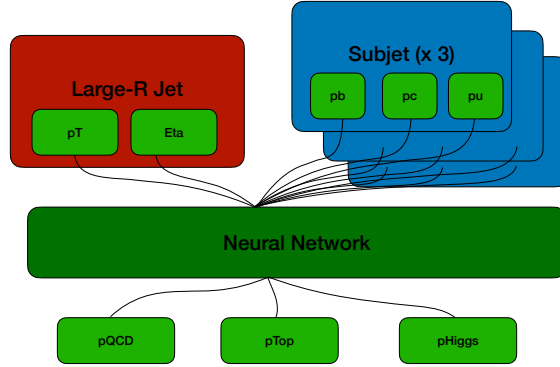


Figure 4.1 Architecture of the *DXbb* algorithm for boosted jet tagging. The inputs are shown at the top, and the output at the bottom. This algorithm takes at most three sub-jets and the large-*R* jet kinematic information as inputs and trains the neural network maximizing the discrimination between three categories.

constructing the discriminant, assuming a proper top fraction f_{top} is set close to that of the testing sample, according to the Neyman-Pearson lemma^[117].

$$D_{Xbb} = \ln \frac{P_{Higgs}}{f_{top} \cdot p_{top} + (1 - f_{top}) \cdot p_{multijet}}, \quad (4.1)$$

An important principle of the tagger is to ensure that the output is decorrelated from sensitive single variables such as mass and p_T . This is crucial to avoid the so-called sculpting effect, where the tagger preferentially selects events with specific mass or p_T values regardless of other information, thereby biasing the results and distorting the mass shape. Such distortions could hinder further analyses relying on the jet mass.

The mass-agnostic property is achieved through the design of the tagger and its training strategy. Several methods were tested, including adversarial training^[118], DisCo loss^[119], and feature engineering. The final solution involves selecting a small set of inputs with minimal mass dependence and reweighting the p_T distribution to be flat across all samples during training. This approach results in the final design described above and exhibits excellent mass decorrelation performance, as shown in Figure 4.2. The mass spectrum of multijet events shows minimal distortion after tagging, comparable to the performance of the single b-jet tagger (DL1r).

The performance of *DXbb* is shown in Figure 4.3, compared with other single b-tagging methods. The X-axis represents the signal efficiency, while the Y-axis corresponds to the

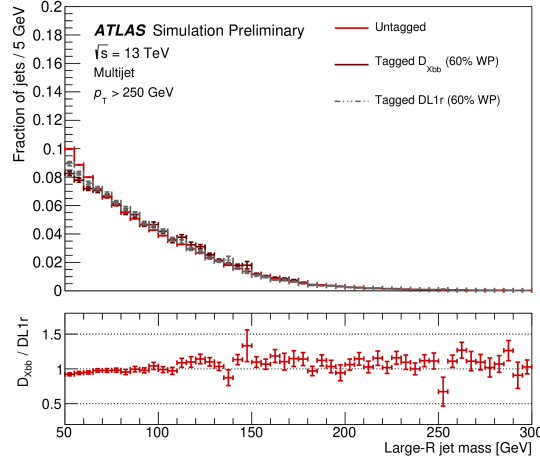


Figure 4.2 Mass decorrelation feature of D_{xbb} tagger. The mass spectrum of multijet events shows little change before and after tagging, comparable to the one with single b-jet tagger (DL1r) which is believed to be mass-decorrelated.^[116]

background rejection, defined as the inverse of the background efficiency and higher values indicate better performance. Four tagging algorithms are compared: two variants of the MV2 algorithm, which represent the first generation of multivariate tagging method developed in ATLAS, as well as DL1r as mentioned before and the D_{Xbb} algorithm demonstrates a clear improvement.

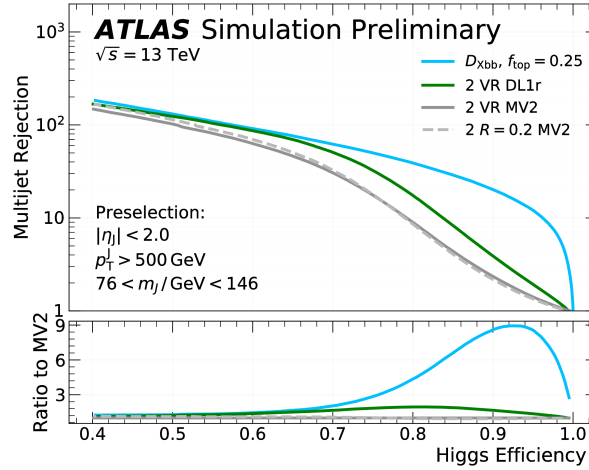


Figure 4.3 D_{Xbb} tagger performance measured in simulated samples. At the same signal efficiency, the D_{Xbb} shows significant improvement of the QCD multijet rejection compared with single b-tagging.^[116]

4.2 Signal Tagging Efficiency Calibration

The tagging efficiency on signal events such as Higgs boson decaying to $b\bar{b}$ is calibrated using the $Z \rightarrow b\bar{b}$ events where the topology and tagger performance is believed to be similar due to the mass-agnostic property of the DXbb tagger^[116]. Two type of events are used in the calibration: the $Z(\rightarrow b\bar{b}) + \gamma$ events and the $Z(\rightarrow b\bar{b}) + jets$ events in different p_T range. For the event with jet p_T in 200-450GeV, $Z(\rightarrow b\bar{b}) + \gamma$ events are used where the photon trigger is efficient. For events with a jet p_T greater than 450GeV, $Z(\rightarrow b\bar{b}) + jets$ events are used due to the high statistics and the clear signature, where the Z-jet and recoiled jet are back-to-back, forming two high- p_T boosted jets.

The Zbb calibration is based on the formula shown in Equation 4.2 where the number of events passing or failing the tagger are linked using the tagging efficiency. The scale factor defined as the correction between MC efficiency and the data efficiency, can be derived from the two data/MC ratio before and after passing the tagger. This enables the calibration performed in two steps, measuring the data/MC ratio without tagging from the pure modelling difference, and measuring of number of events difference passing tagger in data and MC. The former is named $\mu_{\text{pre-tag}}$ measurement and due to the overwhelming background, the proxy $Z \rightarrow ll$ are measured instead of $Z \rightarrow b\bar{b}$ while measured in a same phase space. The later is named $\mu_{\text{post-tag}}$ measurement and the $Z \rightarrow b\bar{b}$ events are used. The diagrams of the events are illustrated in Figure 4.4

$$\text{SF} = \frac{\epsilon^{\text{data}}}{\epsilon^{\text{MC}}} = \frac{\frac{N^{\text{data}}_{\text{passed}}}{N^{\text{data}}_{\text{total}}}}{\frac{N^{\text{MC}}_{\text{passed}}}{N^{\text{MC}}_{\text{total}}}} = \frac{\frac{N^{\text{data}}_{\text{passed}}}{N^{\text{MC}}_{\text{passed}}}}{\frac{N^{\text{data}}_{\text{total}}}{N^{\text{MC}}_{\text{total}}}} = \frac{\mu_{\text{post-tag}}}{\mu_{\text{pre-tag}}}. \quad (4.2)$$

The selection of the calibration using $Z + \gamma$ and $Z + jet$ are described in Table 4.1 and 4.2.

In the $\mu_{\text{pre-tag}}$ measurement, only the event yield is measured and both signal and background are well modelled with MC, while in the $\mu_{\text{post-tag}}$ measurement, the Zbb mass shape is necessary to extract the correction and the dominant background $\gamma + jets$ (or multijets in high p_T calibration) do not have good modelling. Data-driven methods are used to estimate the contribution and mutiple techniques and intensive validations are performed^[116].

The final results are shown in Figure 4.5 as well as the Table 4.3 with the systematic uncertainty listed.

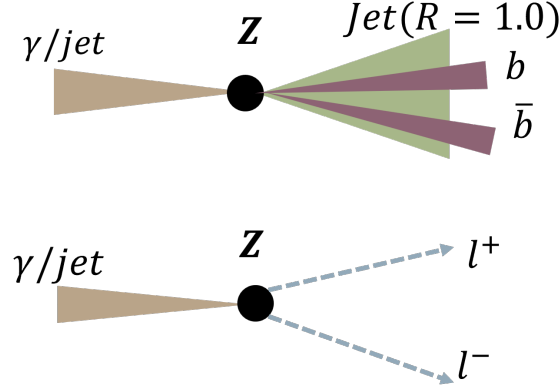


Figure 4.4 Diagrams of the $Z + \gamma/jet$ events used in the calibration. The upper plot shows the $Z(\rightarrow b\bar{b}) + \gamma/jet$ events which are used to measure the $\mu_{post-tag}$ while the lower plot shows the $Z(\rightarrow ll) + \gamma/jet$ events used in $\mu_{pre-tag}$ study.

Table 4.1 Selections for $Z + \gamma$ Calibration

	$\mu_{post-tag}$	$\mu_{pre-tag}$
Photon	Single photon trigger, $p_T > 200$ GeV	
	$200 \text{ GeV} < p_T < 450 \text{ GeV}$	
	≥ 2 track jets with $p_T > 7$ GeV	2 same flavor leptons with $p_T > 20$ GeV
Z-candidate	$50 \text{ GeV} < m_J < 150 \text{ GeV}$	$70 \text{ GeV} < m_{ll} < 110 \text{ GeV}$
	$\Delta R_{J,\gamma} > 1.0$	opposite sign (muon channel)
	$2m_J/p_T < 1.0$	lepton p_T balance
Topology	$\Delta\phi_{Z,\gamma} > \pi/2$	

Table 4.2 Selections for $Z + jet$ Calibration

	$\mu_{post-tag}$	$\mu_{pre-tag}$
Trigger	single large-R jet	single lepton
	$450 \text{ GeV} < p_T < 100 \text{ GeV}$	
Z-candidate	≥ 2 track jets with $p_T > 7$ GeV	2 $ee/\mu\mu$ with $p_T > 25(27)$ GeV
	$50 \text{ GeV} < m_J < 150 \text{ GeV}$	$66 \text{ GeV} < m_J < 116 \text{ GeV}$
Balance	$\Delta p_T^{J,J} < 0.15 \sum p_T^J$	$\Delta p_T^{ll,J} < 0.15 \sum p_T^{ll(J)}$
	$\Delta y_{J,J} < 1.2$	$\Delta y_{ll,J} < 1.2$
	-	$66 \text{ GeV} < \Delta p_T^{l,l} < 0.8 \sum p_T^l$
Extra	-	$p_T^{ll} > p_T^J$

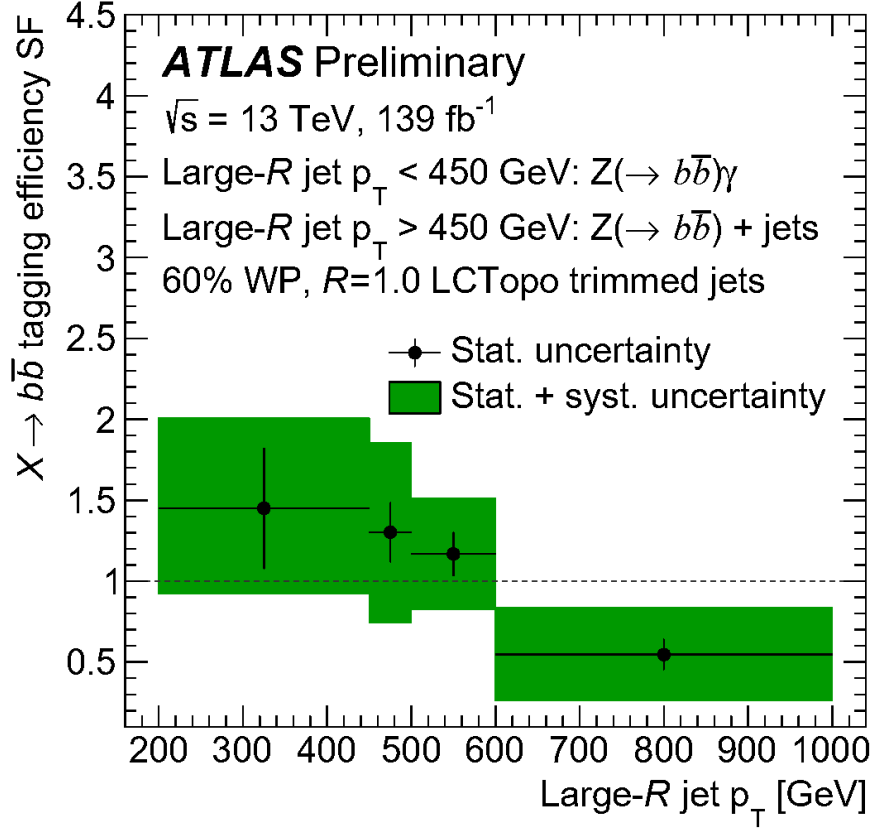


Figure 4.5 Calibration scale factor of the $DXbb$ signal efficiency. The X-axis shows the large- R jet p_T . The color band denotes the total uncertainty and the vertical line indicates the statistical uncertainty.^[116]

Table 4.3 Scale factors and the uncertainties of the Zbb calibration. The parameters of interest, $\mu_{\text{pre-tag}}$ and $\mu_{\text{post-tag}}$ are shown for each p_T bin at 60% efficiency working point.^[116]

Calibration p_T [GeV]	$Z(\rightarrow b\bar{b})\gamma$ 200 – 450	450 – 500	$Z(\rightarrow b\bar{b}) + \text{jets}$	
			500 – 600	600 – 1000
$\mu_{\text{post-tag}}$	1.33	1.32	1.10	0.51
$\mu_{\text{pre-tag}}$	0.92	1.01	0.94	0.93
SF	1.45	1.30	1.17	0.55
Uncertainties ($\pm\sigma$)				
Statistical	± 0.37	± 0.18	± 0.13	± 0.09
Z-boson modelling	$+0.24$ -0.19	–	–	–
Z + jets modelling	–	$+0.21$ -0.28	± 0.15	± 0.18
Fit model	0.14	0.39	0.22	0.16
Spurious signal	± 0.26	± 0.11	± 0.07	± 0.07
Other background modelling	± 0.05	± 0.03	± 0.02	± 0.01
Lepton & Photon related	± 0.02	$+0.06$ -0.07	$+0.06$ -0.07	± 0.03
Jet mass scale	± 0.05	$+0.02$ -0.01	± 0.01	$+0.02$ -0.01
Jet mass resolution	$+0.03$ -0.02	$+0.22$ -0.15	$+0.11$ -0.09	$+0.09$ -0.07
Jet energy scale	$+0.06$ -0.07	± 0.09	± 0.09	± 0.05
Others	$+0.14$ -0.16	± 0.01	$< \pm 0.01$	$< \pm 0.01$
Total uncertainty	$+0.33$ -0.56	$+0.55$ -0.56	$+0.35$ -0.34	$+0.29$ -0.28

4.3 Background Mis-tagging Efficiency Calibration

This section introduces the calibration of mis-tagging rate using $t\bar{t}$ events and the text is modified from the section from ATLAS public note^[116] where I contributed as the author of the calibration.

4.3.0.1 Methodology

The top-jet mis-tag efficiency, which measures the probability of misidentifying a top-quark jet as an $X \rightarrow b\bar{b}$ signal jet, is determined using semileptonic $t\bar{t}$ events. In these events, one of the W bosons decays into a charged lepton and a neutrino, while the other W boson undergoes a hadronic decay. The leptonically decaying W boson, together with the b -quark originating from the same top quark, creates a distinct signature that is easily separable from other SM processes.

The event is triggered using charged lepton and tagged with the lepton associated b -jet and E_T^{miss} . The hadronically decaying W boson, along with the neighboring b -quark, forms a characteristic top jet.

The scale factor of calibration is defined as the tagging efficiency on MC to the one on data is the target deliverable of the calibration. It is linked to the event number both passing or failing the tagger. The number of semileptonic $t\bar{t}$ events in MC, which contains a top jet passing a given $X \rightarrow b\bar{b}$ tagger requirement ($N_{\text{pass}}^{\text{t}\bar{\text{t}},\text{MC}}$), can be written as:

$$N_{\text{passed}}^{\text{t}\bar{\text{t}},\text{data}} = \text{SF} \cdot \frac{N_{\text{total}}^{\text{t}\bar{\text{t}},\text{data}}}{N_{\text{total}}^{\text{t}\bar{\text{t}},\text{MC}}} \cdot N_{\text{passed}}^{\text{t}\bar{\text{t}},\text{MC}} = \text{SF} \cdot f^{\text{t}\bar{\text{t}}} \cdot N_{\text{passed}}^{\text{t}\bar{\text{t}},\text{MC}}, \quad (4.3)$$

where $N_{\text{total}}^{\text{t}\bar{\text{t}},\text{data}}$ ($N_{\text{total}}^{\text{t}\bar{\text{t}},\text{MC}}$) is the number of semileptonic $t\bar{t}$ events in data (MC) before tagging and $N_{\text{pass}}^{\text{t}\bar{\text{t}},\text{data}}$ is the number of semileptonic $t\bar{t}$ events in data after tagging. The $t\bar{t}$ correction factor, $f^{\text{t}\bar{\text{t}}} = \frac{N_{\text{total}}^{\text{t}\bar{\text{t}},\text{data}}}{N_{\text{total}}^{\text{t}\bar{\text{t}},\text{MC}}}$, is introduced to account for differences in the total $t\bar{t}$ normalisation and modelling of the jet p_T distributions in data and MC simulation.

The yield $N_{\text{passed}}^{\text{t}\bar{\text{t}},\text{data}}$ is obtained by subtracting the contribution from the non- $t\bar{t}$ processes, estimated from the simulation ($N_{\text{passed}}^{\text{non-t}\bar{\text{t}},\text{MC}}$), from the data yield ($N_{\text{passed}}^{\text{data}}$):

$$N_{\text{passed}}^{\text{t}\bar{\text{t}},\text{data}} = N_{\text{passed}}^{\text{data}} - N_{\text{passed}}^{\text{non-t}\bar{\text{t}},\text{MC}}. \quad (4.4)$$

In order to constrain $f^{\text{t}\bar{\text{t}}}$, the events containing the leading top jet failing the $X \rightarrow b\bar{b}$ tagger requirement are studied:

$$N_{\text{failed}}^{\bar{t}\bar{t},\text{data}} = N_{\text{failed}}^{\text{data}} - N_{\text{failed}}^{\text{non-}\bar{t}\bar{t},\text{MC}}, \quad (4.5)$$

where $N_{\text{failed}}^{\text{data}}$ ($N_{\text{failed}}^{\bar{t}\bar{t},\text{data}}$) is referred to the total number of data ($\bar{t}\bar{t}$ in data) events. And $N_{\text{failed}}^{\text{non-}\bar{t}\bar{t},\text{MC}}$ represents the contribution from the non- $\bar{t}\bar{t}$ processes, estimated from the MC simulation. Given

$$N_{\text{failed}}^{\bar{t}\bar{t},\text{data}} = N_{\text{total}}^{\bar{t}\bar{t},\text{data}} - N_{\text{passed}}^{\bar{t}\bar{t},\text{data}} = f^{\bar{t}\bar{t}} \cdot N_{\text{total}}^{\bar{t}\bar{t},\text{MC}} - f^{\bar{t}\bar{t}} \cdot \text{SF} \cdot N_{\text{passed}}^{\bar{t}\bar{t},\text{MC}} = f^{\bar{t}\bar{t}} \cdot N_{\text{total}}^{\bar{t}\bar{t},\text{MC}} \cdot (1 - \epsilon^{\text{MC}} \cdot \text{SF}), \quad (4.6)$$

$$N_{\text{total}}^{\bar{t}\bar{t},\text{MC}} = N_{\text{failed}}^{\bar{t}\bar{t},\text{MC}} \cdot \frac{1}{1 - \epsilon^{\text{MC}}}, \quad N_{\text{passed}}^{\bar{t}\bar{t},\text{MC}} = N_{\text{failed}}^{\bar{t}\bar{t},\text{MC}} \cdot \frac{\epsilon^{\text{MC}}}{1 - \epsilon^{\text{MC}}}, \quad (4.7)$$

the number of fail-tag events of the data and the simulation is linked as :

$$N_{\text{failed}}^{\text{data}} = f^{\bar{t}\bar{t}} \cdot \frac{1 - \epsilon^{\text{MC}} \cdot \text{SF}}{1 - \epsilon^{\text{MC}}} \cdot N_{\text{failed}}^{\bar{t}\bar{t},\text{MC}} + N_{\text{failed}}^{\text{non-}\bar{t}\bar{t},\text{MC}}. \quad (4.8)$$

The $f^{\bar{t}\bar{t}}$ normalization factor and the top jet mis-tag efficiency scale factor SF are measured in bins of the top jet p_T . Four bins are defined to ensure a sufficient data statistics: $300 < p_T < 400$ GeV, $400 < p_T < 500$ GeV, $500 < p_T < 600$ GeV and $600 < p_T < 1000$ GeV.

4.3.0.2 Data and MC Samples

The mis-tagging efficiency calibration is performed using the $\sqrt{s} = 13$ TeV pp collision data from 2015–2018 data-taking period, collected by the ATLAS experiment. This dataset corresponds to an integrated luminosity of $139.0 \pm 2.4 \text{ fb}^{-1}$. It is recorded under stable beam conditions with all relevant ATLAS detector subsystems fully operational.

The simulated samples used for this calibration include semi-leptonic $t\bar{t}$ bar, t-channel and s-channel single top, tW production single top, W/Z +jets, diboson and $t\bar{t}V$. The technical details are documented in the Table A.1 in Appendix A.1.

4.3.0.3 Object Selection

The objects reconstruction is described in Sec 3.4 and the object selections are described here,

Electrons Electron candidates are required to match an ID track and pass the *tight* identification as described in Ref.^[79]. Electron candidates in the calibration are required to satisfy $p_T > 28$ GeV.

Muons Muon candidates are required to satisfy $p_T > 28$ GeV and $|\eta| < 2.5$, and pass the *medium* identification as in Ref.^[81].

The lepton isolation criterion is implemented following the procedure outlined in Section 3.4.2. To reduce the mis-reconstructed leptons such as hadrons, converted electron or non-prompt leptons the `tight` isolation working point is applied. Furthermore, electron candidates are subjected to an additional criterion requiring that the transverse energy sum of topo-clusters is less than 6% if positioned within a cone of $\Delta R = 0.2$ surrounding the electron.

Besides these conditions, electron and muon candidates are required to match the primary vertex by ensuring the longitudinal impact parameter $z_0 \sin \theta$ fulfills $|z_0 \sin \theta| < 0.5$ mm, where θ represents the track's polar angle. For transverse impact parameter significance d_0/σ_{d_0} , calculated relative to the beam line position, the criteria are $|d_0/\sigma_{d_0}| < 5$ for electrons and $|d_0/\sigma_{d_0}| < 3$ for muons, with σ_{d_0} denoting the uncertainty in d_0 .

Efficiencies for lepton reconstruction, identification, trigger, and isolation in simulated events are adjusted to match the measurements obtained from data.

Small- R jets Small- R particle flow (PFlow) jets are reconstructed using the anti- k_T algorithm^[91] with a radius parameter $R = 0.4$. The energy of these jets is calibrated^[120] to account for pile-up effects. Jets are required to meet the conditions $p_T > 25$ GeV and $|\eta| < 2.5$. To suppress jets not originating from the hard-scatter process, the Jet Vertex Tagger (JVT) discriminant^[121] is applied for jets with $p_T < 60$ GeV and $|\eta| < 2.4$, leveraging tracking and vertexing information. The selected working point ensures approximately 96% efficiency for selecting hard-scatter jets. Any discrepancies in efficiency between simulation and data are corrected using scale factors.

Small- R jets are identified as b -jets (originating from b -quarks) using the DL1r algorithm, as detailed in Section 3.4.5.4. Corrections for differences between data and simulation are applied to account for the mis-tagging efficiency of non- b -jets passing the b -tagging algorithm.

Large- R jets Large- R jets are reconstructed using topological clusters calibrated with the LCW scheme (LCTopo)^[74], clustered via the anti- k_T algorithm with a radius parameter $R = 1.0$. Trimming, as outlined in Section 3.4.5.1, is applied. For this analysis, only trimmed

large- R jets with $p_T > 300$ GeV and $|\eta| < 2.0$ are included.

Variable-Radius (VR) track-jets Track-jets in this study are reconstructed from inner detector tracks, clustered using the variable-radius (VR) anti- k_T algorithm^[122]. In contrast to fixed-radius jets, the VR jet radius is inversely related to track-jet p_T , governed by a constant parameter $\rho = 30$ GeV, optimized to improve matching efficiency between the b -hadron direction and the jet axis^[123]. The radius is constrained to a minimum of $R_{min} = 0.02$ and a maximum of $R_{max} = 0.4$. VR track-jets are ghost-associated^[124] to the large- R jet and are required to meet $p_T > 7$ GeV, $|\eta| < 2.5$, and have a minimum of two track constituents. These associated VR track-jets, referred to as subjets, are used for truth labeling of large- R jets to determine their flavor composition when applying the $DXbb$ algorithm.

Overlap Removal To prevent double-counting and minimize the influence of non-prompt objects, overlaps among candidate objects are sequentially resolved. Initially, electron candidates located within $\Delta R = 0.01$ of a muon candidate are excluded to reduce contributions from muon bremsstrahlung. Subsequently, overlaps between electron and jet candidates are handled: if the axis of a jet lies within $\Delta R = 0.2$ of an electron, the jet is removed to prevent electrons from being double-counted as jets. If the electron is found within $\Delta R = 0.4$ of any remaining jet, the electron is removed, and the jet is retained.

For muons, overlaps with jets are resolved using the condition $\Delta R(\mu, \text{jet}) < 0.04 + 10 \text{ GeV}/p_T(\mu)$. If the jet has at least three tracks originating from the primary vertex, the muon is discarded; otherwise, the jet is removed, and the muon is retained.

4.3.0.4 Event Selection

Events are required to contain exactly one trigger-matched electron or muon with $p_T > 70$ GeV. To select a sample enriched in semileptonic $t\bar{t}$ events, the selection criteria summarized in Figure 4.6 are applied. The event must have $E_T^{\text{miss}} > 70$ GeV, at least one small- R jet with $p_T > 25$ GeV, and at least one large- R jet with $p_T > 300$ GeV.

To enhance the purity of the $t\bar{t}$ events, a tag-and-probe method is employed. Among all small- R jets in the event, the jet closest to the lepton must be tagged by the DL1r algorithm at the 77% signal efficiency working point. This jet is referred to as the tag-jet. The leading- p_T large- R jet in the event is defined as the probe-jet. The absolute value of the azimuthal angle

difference, $|\Delta\phi|$, between the tag-jet and the probe-jet is required to be greater than 1.0. Additionally, the invariant mass of the tag-jet and the lepton, denoted as m_{lj} , must be less than 150 GeV, as this selection is designed to target top-quark decays.

Only events containing both a tag-jet and a probe-jet are retained, defining the pre-tag event sample.

As shown in Figure 4.7a, $t\bar{t}$ events dominate the sample before applying the $X \rightarrow b\bar{b}$ requirement (pre-tag). A decreasing slope in the data-over-simulation ratio is observed along the p_T spectrum, attributed to mis-modeling of $t\bar{t}$ events in the MC simulation. This effect has also been observed in other ATLAS measurements with comparable $t\bar{t}$ event selection^[125]. It is considered by introducing $f^{t\bar{t}}$, as described in Section 4.3.0.1.

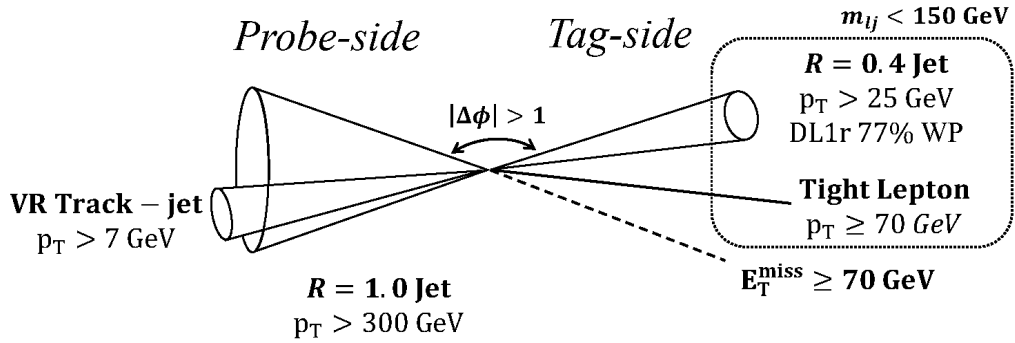


Figure 4.6 Summary of the event selection for the semileptonic $t\bar{t}$ calibration.

With the $X \rightarrow b\bar{b}$ tagger signal efficiency working point (WP) of 60%, the pre-tag events are further categorised into "Passed Signal Region" ($SR_{\text{passed}}^{\text{WP}}$), if the probe-jet passes the chosen WP. Otherwise the events are categorised into "Failed Signal Region" ($SR_{\text{failed}}^{\text{WP}}$).

4.3.0.5 Semileptonic $t\bar{t}$ calibration uncertainties

Two types of systematic uncertainties are evaluated: the theoretical *process modelling* and experimental *detector-related* uncertainties.

Theoretical uncertainties are evaluated by comparing nominal and alternative samples generated using different generators, showering models, or parameter settings, as described in Section 4.3.0.2. These uncertainties are assessed for $t\bar{t}$, tW -single-top, and W +jets event samples, with effects ranging from 4% to 15%. The detailed procedures are outlined below:

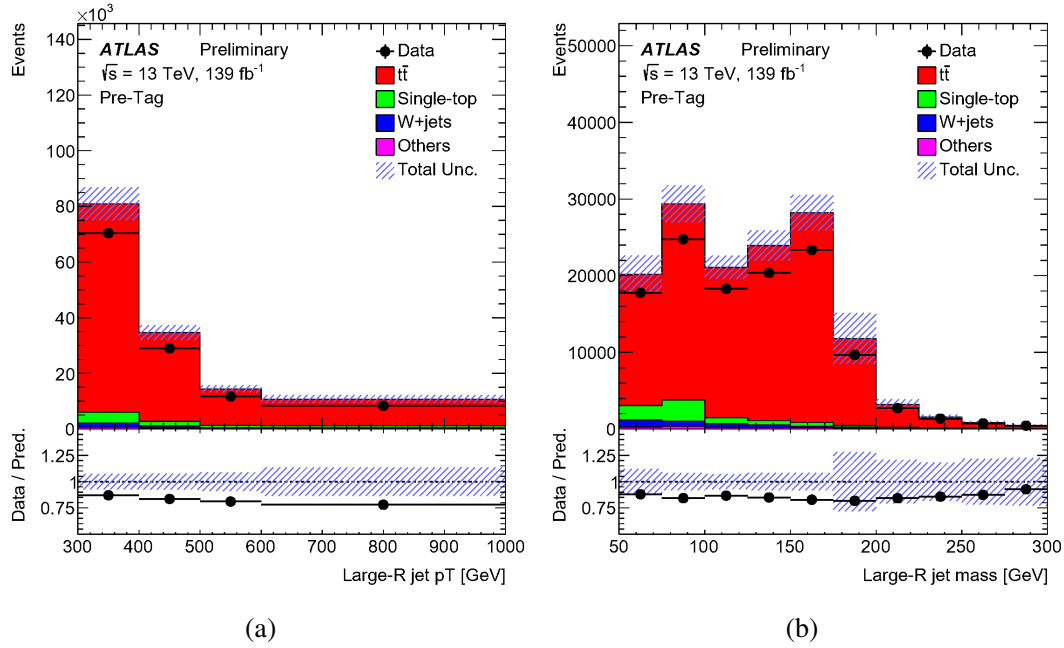


Figure 4.7 Data and MC simulated distributions of p_T (a) and mass of the probe jet (b) for the pre-tag selection. The ratio panel shows the data-to-MC ratio. The uncertainty band includes MC statistical and systematic uncertainties.

For the $t\bar{t}$ process, the dominant sources of systematic uncertainty arise from matrix element generation, hadronization, and QCD initial-state-radiation (ISR) and final-state-radiation (FSR). These are identified as the key contributors to modelling uncertainties.

Matrix Element (ME) and Parton Shower (PS): Assessed by comparing nominal with the alternative samples. Differences in tagging efficiency between these simulations result in an acceptance correction (MC/MC factor), while shape variations contribute less than 0.5% to the measured scale factor.

ISR: Estimated by varying the h_{damp} parameter, the μ_r and μ_f scales, and the Var3c up/down variations of the A14 tune^[126]. ISR effects introduce variations of 3–10% in the scale factor, primarily due to changes in the flavor composition of the $t\bar{t}$ simulation.

FSR: Evaluated by modifying the renormalization scale μ_r for parton-shower emissions by a factor of two in either direction. The impact on the scale factor is similar to that of ISR.

For the tW -single-top process, the primary uncertainty originates from the MC simulation's interference-removal scheme. Comparisons between diagram-subtraction (DR) and diagram-removal (DS) methods result in uncertainties ranging from 0.5–1.5%. Other sources, such as generator and QCD radiation variations, contribute minimally.

For the W +jets process, uncertainties due to higher-order QCD corrections are evaluated using generator-provided reweighting. Uncertainties from missing higher-order contributions are assessed by varying μ_r and μ_f scales by a factor of two, with the maximum variation taken as the uncertainty. These effects are typically below 0.5%.

Other process-modelling uncertainties, such as PDF choices and cross-section corrections, are also considered. Using the PDF4LHC recipe^[127], the $t\bar{t}$ PDF uncertainty is approximately 1–2%, while for other processes, the impact is negligible.

Experimental uncertainties are from the reconstruction of objects (such as electrons, muons, jets and E_T^{miss}), the b -tagging misidentification (e.g. c -, τ -, or light-flavor jets incorrectly tagged as b -jets), and modelling of the pile-up effect.

Jet uncertainties: Large- R jet energy and mass scale (JES, JMS) and resolution (JMR) uncertainties^[96] contribute about 1.5%. Small- R jet uncertainties^[120] add 1–2% to the scale factor.

Flavor tagging: Variations in b -tagging efficiency correction factors^[128-129] for b , c , τ , and light jets are included, but their impact on the scale factor is negligible.

Lepton and E_T^{miss} : Electron and muon uncertainties^[76,81] include variations in energy/momentum scale, resolution, reconstruction, identification, and isolation efficiencies. E_T^{miss} uncertainties due to the soft term energy scale and resolution^[130] are also included. Together with pile-up and luminosity uncertainties, these effects result in a scale factor uncertainty below 1%.

All uncertainties are treated as independent and uncorrelated across the calibrated p_T^{probe} bins. Each systematic source's effect is quantified by replacing nominal samples with systematically varied samples, rerunning the analysis, and computing the difference. The relative deviation from the nominal value is taken as the uncertainty, with the total uncertainty calculated as the quadrature sum of individual contributions.

4.3.0.6 Semileptonic $t\bar{t}$ Calibration Results

The modelling correction f^{fit} and scale factor SF are extracted using a binned likelihood fit^[21] performed simultaneously in the $\text{SR}_{\text{pass}}^{\text{WP}}$ and $\text{SR}_{\text{fail}}^{\text{WP}}$ regions. To enhance discriminating power, the fit is carried out on the probe-jet mass distribution. The binning of the mass is adapted for different regions and is detailed in Table 4.4.

Figures 4.8 and 4.9 show the post-fit distribution of the large- R jet mass in $\text{SR}_{\text{pass}}^{\text{WP}}$ and

Table 4.4 Summary of the binning used in different p_T^{probe} region.

Region	pT Region [GeV]	Observable	Binning [GeV]
SR^{pass}	$300 < p_T^{\text{probe}} < 400$	$m_{\text{large-}R}$	50 - 75 - 100 - 120 - 140 - 160 - 180 - 200 - 300
	$400 < p_T^{\text{probe}} < 500$		
	$500 < p_T^{\text{probe}} < 600$		50 - 75 - 100 - 120 - 140 - 160 - 180 - 200 - 240 - 300
	$600 < p_T^{\text{probe}} < 1000$		
SR^{fail}	$300 < p_T^{\text{probe}} < 400$	$m_{\text{large-}R}$	50 - 75 - 100 - 120 - 140 - 160 - 180 - 300
	$400 < p_T^{\text{probe}} < 500$		50 - 100 - 140 - 180 - 300
	$500 < p_T^{\text{probe}} < 600$		
	$600 < p_T^{\text{probe}} < 1000$		50 - 120 - 190 - 300

$\text{SR}_{\text{fail}}^{\text{WP}}$ regions, respectively. Good agreement is obtained between data and simulation after fitting.

The SF corresponding to a given systematic variation is determined by performing a fit to data, replacing the nominal sample (referred to as the nominal fit) with the alternative sample or alternative settings corresponding to the systematic variation (referred to as the alternative fit). The uncertainty is then evaluated as the difference between the SF obtained from the alternative fit and the nominal SF.

In the alternative fit, the large- R jet mass distribution is replaced by the alternative distribution, while the ϵ^{MC} parameter in Eq. 4.8 is fixed to its nominal value. As a result, the difference between the nominal value of ϵ^{MC} and its value in the alternative fit is propagated to the measured SF. This procedure is applied to all modelling uncertainties except for parton shower (PS) and hadronisation model systematics.

For PS and hadronisation model systematics, the alternative fit sets ϵ^{MC} to the value obtained from the alternative sample. Since PS and hadronisation models depend on the generator used in the analysis where the calibration will be applied, this dependency is accounted for during calibration application through the use of generator-dependent MC-to-MC SFs.

The measured mis-tag efficiency, ϵ_{data} , are compared to the efficiency predicted by the simulation, ϵ_{MC} , in Figure 4.10a. The scale factors are visualised in Figure 4.10b. They are compatible with unity within statistical uncertainties in each p_T bin.

The uncertainties on the SF are summarized in Table 4.5 and 4.6. The measurement achieves a precision of approximately 5% in the first p_T^{probe} bin (300–400 GeV) and less than 16% in the last p_T^{probe} bin. The calibration is primarily limited by systematic uncertainties,

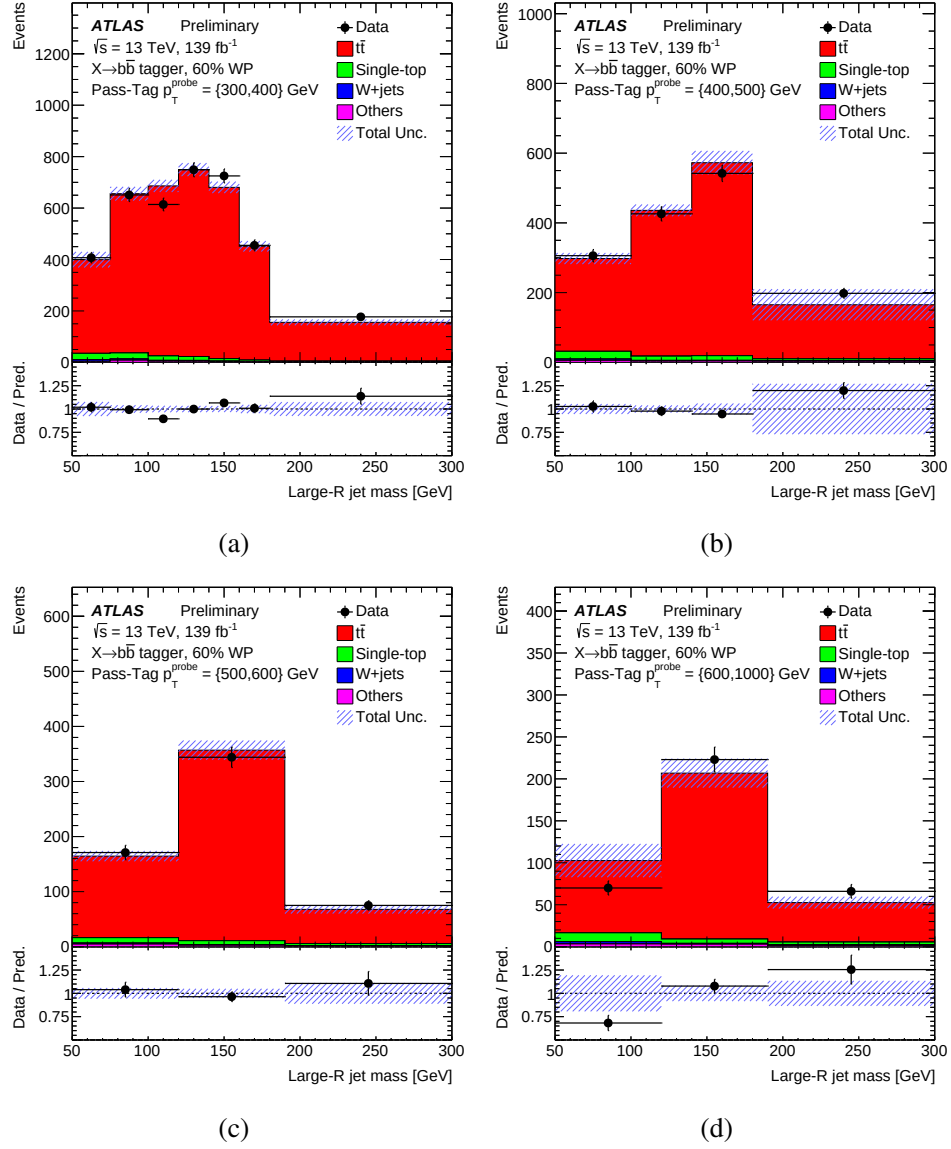


Figure 4.8 Post-fit distribution of the large- R jet mass in $\text{SR}_{\text{pass}}^{60\%}$ used for calibration of the top jet mis-tag efficiency with $X \rightarrow b\bar{b}$ tagger at 60% efficiency WP for $300 < p_T^{\text{probe}} < 400$ GeV (a); $400 < p_T^{\text{probe}} < 500$ GeV (b); $500 < p_T^{\text{probe}} < 600$ GeV (c) and $600 < p_T^{\text{probe}} < 1000$ GeV (d). The uncertainty band represents the systematic uncertainty.

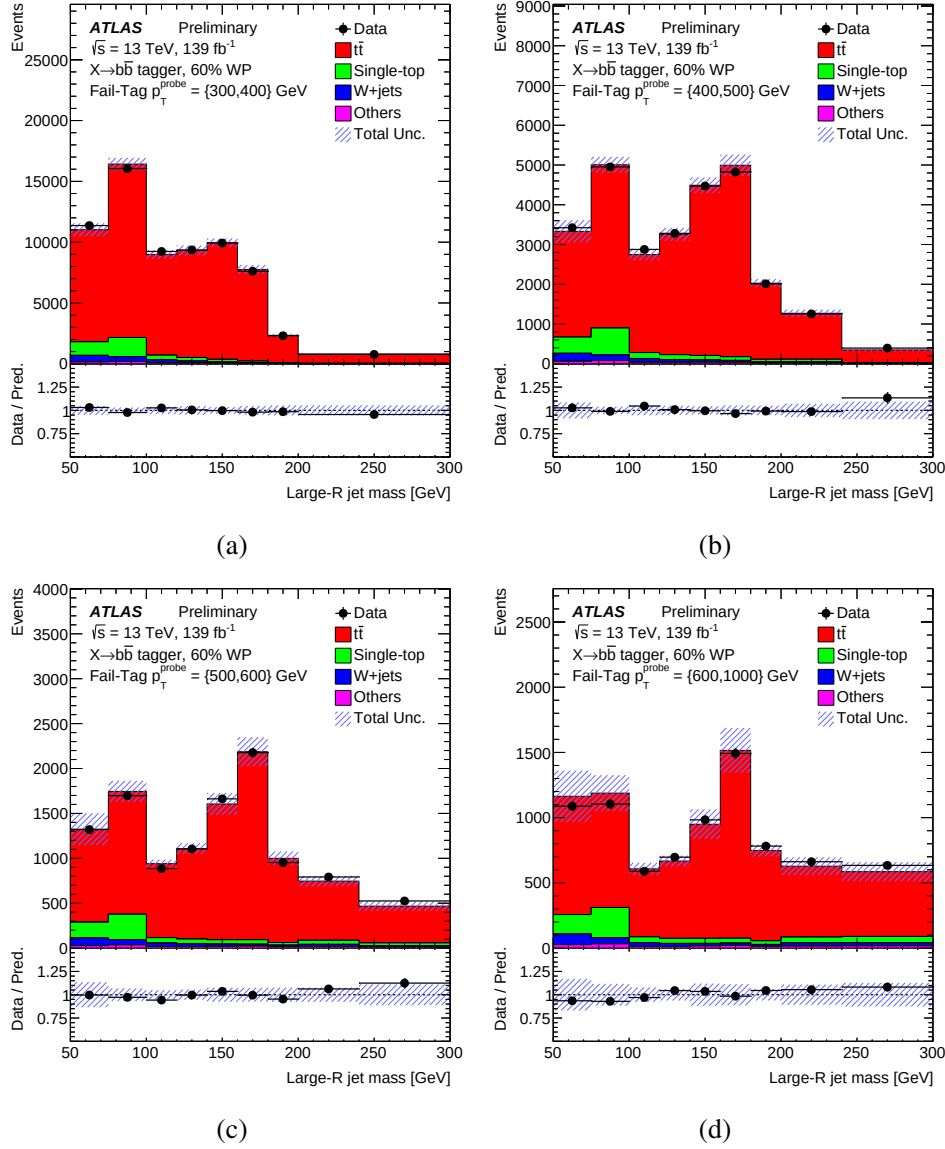


Figure 4.9 Post-fit distribution of the large- R jet mass in $\text{SR}_{\text{fail}}^{60\%}$ used for calibration of the top jet mis-tag efficiency with $X \rightarrow b\bar{b}$ tagger at 60% efficiency WP for $300 < p_T^{\text{probe}} < 400$ GeV (a); $400 < p_T^{\text{probe}} < 500$ GeV (b); $500 < p_T^{\text{probe}} < 600$ GeV (c) and $600 < p_T^{\text{probe}} < 1000$ GeV (d). The uncertainty band represents the systematic uncertainty.

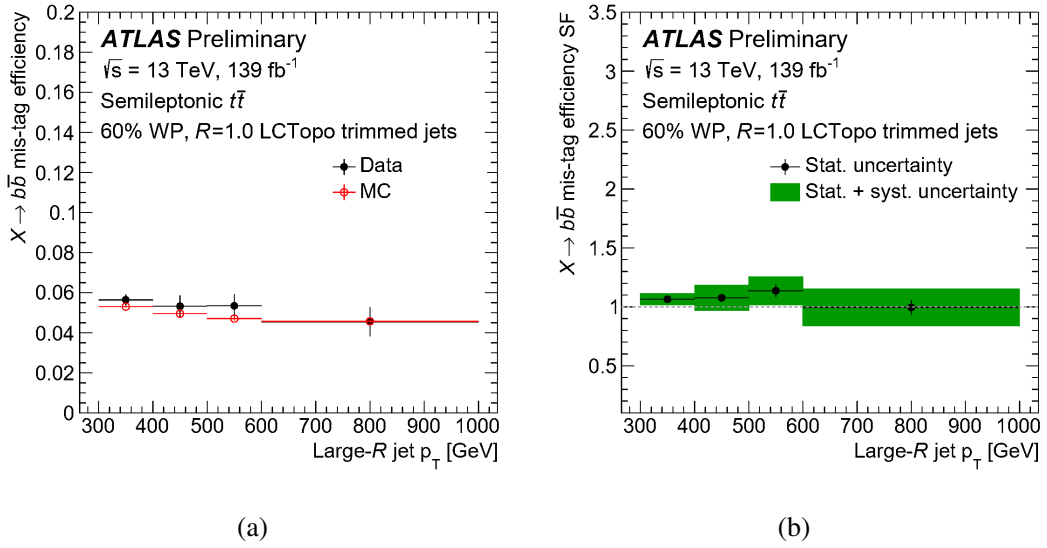


Figure 4.10 (a) The top jet mis-tag efficiency measured in data (full circles) and simulation (open circles), corresponding to the 60% signal jet tagging efficiency WP, as a function of jet p_T . The error bars correspond to total uncertainties for data and statistical uncertainties for simulation, respectively. (b) Data-to-simulation mis-tag efficiency scale factors as a function of the jet p_T . The statistical uncertainties and the total uncertainties are shown as error bars and shaded region, respectively.

particularly those arising from theory modeling, with $t\bar{t}$ modeling being the dominant source. In comparison, the statistical uncertainties range from 2% to 7% across the p_T^{probe} bins, from low to high p_T^{probe} .

This reflects the fact that the advanced machine learning-based b-tagging captures the underlying differences between theory models and generators, which are not inherent features of physical data. The MC/MC factor recipe, as described earlier, has already corrected for the major part of this effect arising from different central values of efficiency, though residual effects are still notable.

To address this, two major efforts are being developed for future applications. The first approach is to incorporate the uncertainty in the machine learning model to better capture and control this uncertainty in statistical applications, such as more refined treatment of related NPs. The uncertainty-aware machine learning^[131] is one promising effort in this direction. The second approach aims to reduce the dependence on MC in the training process, which inspires unsupervised training methods ultimately targeting training-on-data to fully mitigate theory uncertainties. This latter approach is also closely related to the ongoing study of

self-supervised learning, as introduced in Sec. 7.2.

The fitted $f^{t\bar{t}}$ values as a function of p_T are shown in Figure 4.11. After applying these corrections in each p_T bin, as shown in Figure 4.7a, the discrepancy between data and simulation is mitigated, as demonstrated in Figure 4.12.

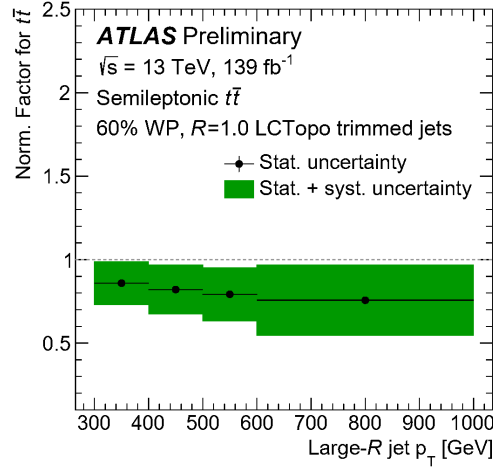


Figure 4.11 The fit values of normalisation correction $f^{t\bar{t}}$ in every p_T bin. The dark green area shows the systematic uncertainty and light green for total unc. respectively for left plot.

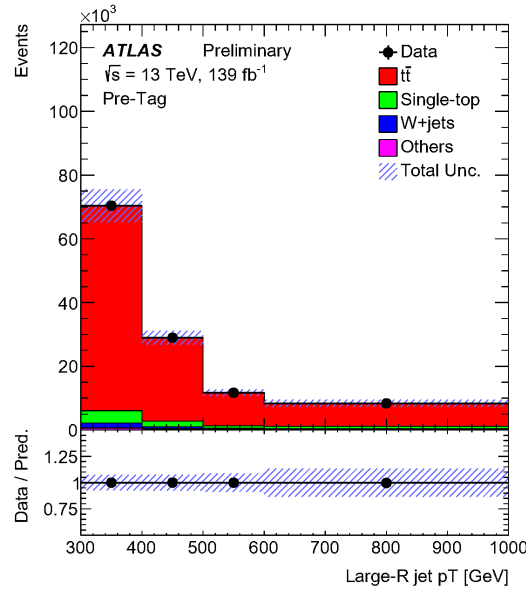


Figure 4.12 The post-fit p_T^{probe} distribution with pre-tag events. The shaded area shows the total uncertainty for MC samples.

Table 4.5 Uncertainties affecting the $t\bar{t}$ calibration in each p_T^{probe} bin. 60% efficiency working point of the DXbb tagging is studied and the contributions from different uncertainty components are summed in quadrature. Total uncertainty and the theory uncertainty are shown in this part of table.

p_T [GeV]	300–400	400–500	500–600	600–1000
Total Uncertainty	4.5%	10.0%	10.5%	15.7%
Stat Uncertainty	1.8%	2.9%	4.6%	6.0%
Syst. Uncertainty	4.1%	9.5%	9.5%	14.5%
$t\bar{t}$ Theory Unc.	3.9%	9.4%	8.8%	14.2%
<i>parton shower (Pythia8 v.s. Herwig7)</i>	<0.1%	0.2%	0.3%	0.2%
<i>FSR var.</i>	2.2%	7.5%	3.6%	9.3%
<i>ISR var.</i>	3.1%	5.5%	7.8%	10.5%
<i>generator (Powheg v.s. aMC@NLO)</i>	<0.1%	<0.1%	<0.1%	<0.1%
<i>P.D.F.</i>	1.0%	1.5%	1.9%	2.2%
<i>cross-section</i>	–	<0.1%	<0.1%	<0.1%
Single-top Theory Unc.	0.7%	0.9%	2.0%	2.3%
<i>Wt DR v.s. DS</i>	0.5%	0.7%	1.4%	1.5%
<i>parton shower (Pythia8 v.s. Herwig7)</i>	<0.1%	0.2%	0.7%	1.5%
<i>generator (Powheg v.s. aMC@NLO)</i>	0.4%	–	1.1%	0.2%
<i>cross-section</i>	0.3%	0.2%	0.3%	0.3%
W+jets scale variations	0.4%	0.3%	0.4%	0.5%
W+jets cross-section	<0.1%	<0.1%	0.1%	0.1%

Table 4.6 Uncertainties affecting the $t\bar{t}b\bar{b}$ calibration in each p_T^{probe} bin. 60% efficiency working point of the DXbb tagging is studied and the contributions from different uncertainty components are summed in quadrature. Detector related experimental uncertainty are shown in this part of table.

p_T [GeV]	300–400	400–500	500–600	600–1000
Small-R Jet Unc.	0.8%	1.1%	2.2%	1.6%
<i>JES (Detector)</i>	<0.1%	<0.1%	<0.1%	<0.1%
<i>JES (Flavour)</i>	0.3%	0.5%	0.7%	0.2%
<i>JER</i>	0.3%	0.4%	1.7%	0.7%
<i>JVT</i>	<0.1%	0.2%	0.3%	0.1%
<i>others</i>	<0.1%	<0.1%	<0.1%	<0.1%
<i>JES (Modelling)</i>	<0.1%	0.1%	0.1%	0.1%
<i>BJES</i>	<0.1%	<0.1%	0.1%	0.2%
<i>JES (Mixed)</i>	0.1%	0.1%	0.2%	0.1%
<i>JES (Statistics)</i>	<0.1%	0.1%	<0.1%	0.2%
<i>JES (η intercalib)</i>	0.4%	0.6%	1.0%	0.9%
Large-R Jet Unc.	0.4%	0.8%	1.4%	0.8%
<i>JMS/JMR</i>	0.3%	0.5%	1.2%	0.3%
<i>JES (Modelling)</i>	0.2%	0.5%	0.5%	0.4%
<i>JES (Statistics)</i>	<0.1%	0.3%	0.4%	0.2%
<i>JES (Mixed)</i>	<0.1%	0.3%	0.4%	0.5%
<i>JES (Detector)</i>	<0.1%	0.1%	0.2%	<0.1%
Flavour Tagging Unc.	0.1%	0.1%	0.1%	0.2%
<i>b-mistagging</i>	<0.1%	<0.1%	<0.1%	<0.1%
<i>c-mistagging</i>	<0.1%	<0.1%	<0.1%	<0.1%
<i>light-mistagging</i>	<0.1%	<0.1%	<0.1%	0.1%
<i>Flavour tagging extrapolations</i>	<0.1%	<0.1%	<0.1%	<0.1%
Others	0.3%	0.4%	0.4%	0.6%
<i>Lepton uncertainties</i>	0.1%	0.1%	0.2%	0.3%
<i>E_T^{miss} soft term</i>	<0.1%	0.1%	<0.1%	0.3%
<i>Pile-up modelling</i>	0.2%	0.4%	0.3%	0.5%
<i>Luminosity</i>	<0.1%	<0.1%	0.1%	0.1%

Chapter 5 Search for Dark Higgs with ATLAS Full Run2 Data

5.1 Overview

Multiple astrophysical observations^[17,132], discussed in Section 2.2, provide strong evidence for the existence of dark matter (DM). Efforts to identify potential DM candidates are actively ongoing across direct and indirect detection experiments, as well as within collider experiments^[133-139].

If DM particles interact weakly with Standard Model (SM) matter, they could be produced at the Large Hadron Collider (LHC), where their presence would manifest as a missing transverse momentum signal, E_T^{miss} . Since DM particles are not directly observable, their detection relies on identifying an additional visible object, X , produced alongside the DM particles. This visible object may result from initial-state QCD, weak, or electromagnetic radiation, giving rise to signatures such as mono-jet^[140-142], mono- Z/W ^[143-145], and mono-photon^[146-148] final states. Additionally, the visible object could be a SM Higgs boson, leading to a mono-Higgs signature^[149-150].

The origin of dark matter mass necessitates a mechanism, with theoretical models offering compelling targets for collider-based searches. This analysis explores final states with b -jets and missing transverse energy (E_T^{miss}) to investigate the production of DM candidates alongside a dark Higgs boson, using the model described in Section 2.2.3. In the signal, E_T^{miss} correlates with the transverse momentum of the dark Higgs boson. At lower E_T^{miss} , the b -jets from the Higgs decay are well-separated and reconstructed as small-radius jets. As E_T^{miss} increases, the dark Higgs acquires a higher Lorentz boost, causing the b -jets to merge into a single jet, necessitating reconstruction using a large-radius jet. To address this, the analysis employs both "resolved" and "merged" reconstruction methods, applying the resolved approach for $E_T^{\text{miss}} < 500$ GeV and the merged approach for $E_T^{\text{miss}} \geq 500$ GeV.

The strategy for this analysis builds on the robust framework established by ATLAS^[149], with significant modifications to optimize the search for a low-mass dark Higgs boson. These enhancements include improvements in jet reconstruction and tagging, background estimation, signal modeling, event selection, and systematic uncertainty evaluation. The study focuses on the 0-lepton channel, while the 1- and 2-lepton channels serve as control

regions to constrain dominant backgrounds, such as top-pair production ($t\bar{t}$) and W, Z bosons associated with jets. Specifically, the analysis incorporates three channels: 0, 1, and 2 leptons. The 0-lepton channel defines the primary "Signal Region" (0L), while the 1- and 2-lepton regions ('Control Regions', 1L and 2L) are used to constrain the main backgrounds. Detailed descriptions of the analysis, along with additional technical information, are provided in subsequent sections and the appendix.

5.2 Signal Model

The dark Higgs model incorporates six parameters that vary, as outlined in Table 2.1 and Section 2.2.3, resulting in different scenarios under the applied constraints of this analysis. Four parameters are treated as free: the three mass parameters m_s, m_χ , and $m_{Z'}$, along with the coupling parameter g_χ . Meanwhile, the coupling constant g_q is fixed at 0.25, and the mixing angle θ is set to 0.01. The value of g_q is based on recommendation from the LHC Dark Matter Benchmark study^[151], while the choice of θ aligns with theoretical recommendations provided in Ref.^[36].

The mixing angle between the dark Higgs boson and the SM Higgs boson is not treated as a free parameter, as its specific value does not influence the relevant phenomenology. It is assumed that $\theta = 0.01$ is sufficiently large to ensure that the dark Higgs boson undergoes prompt decay, consistent with Ref.^[36].

In the low-mass region for the dark Higgs boson ($m_s < 160$ GeV), the primary decay mode is $s \rightarrow b\bar{b}$. This decay channel, combined with the E_T^{miss} signature from DM particles, is the focus of this analysis.

The parameter space is constrained by relic density requirements, as specific parameter combinations reproduce the DM freeze-out relic density^[152], aligning with cosmological observations^[17]. Within this framework, it is hypothesized that the $\chi\chi \rightarrow s\bar{s}$ interaction would have ceased once the Universe reached thermal equilibrium. Following the rapid inflationary phase, dark matter would have dispersed sufficiently to halt further interactions.

To explore the full phase space defined by the four free parameters, three interpretations are proposed for the mono- s ($b\bar{b}$) analysis. These interpretations are summarized in Table 5.1, with further details provided below.

The first interpretation, Scheme1, explores scenarios with varying dark Higgs mass, m_s ,

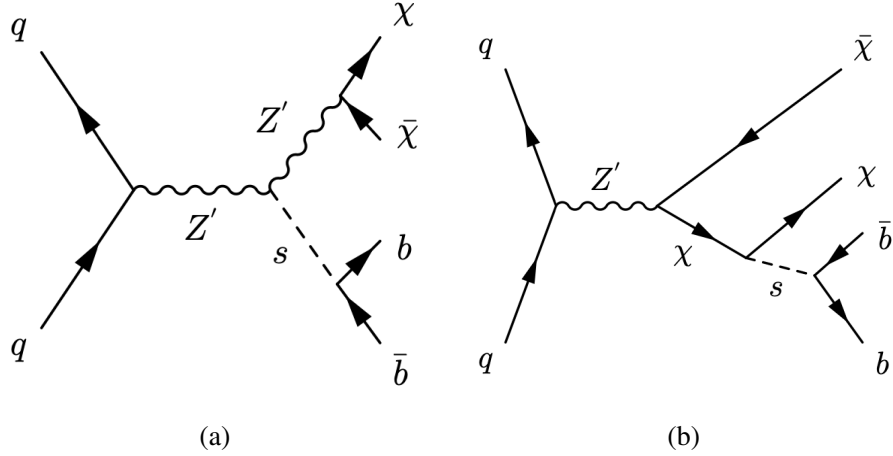


Figure 5.1 Processes leading to a dark Higgs signal with E_T^{miss} due to DM particles χ and decay of the dark Higgs to $b\bar{b}$ -quarks^[36].

Table 5.1 Dark Higgs Signal Interpretation Schemes. In Scheme 1, the observed DM relic abundance will only be reproduced for specific values of the three masses. While in Scheme 2 and 3, the coupling g_χ is set to the specific value to reproduce the observed DM relic abundance for each mass combination. ROI means Range Of Interest.

	m_s/GeV	$m_{Z'}/\text{GeV}$	m_χ/GeV	g_χ
Scheme 1	ROI	ROI	200	1
Scheme 2	ROI	ROI	900	relic-coherent
Scheme 3	70	ROI	ROI	relic-coherent

and Z' mass, $m_{Z'}$, while keeping the DM mass and the coupling parameter g_χ fixed. This interpretation complements the mono- $S(VV)$ analyses^[153-154], which focus on higher dark Higgs masses. The phenomenology of the model is not strongly dependent on the DM mass, provided that the relevant interactions are kinematically accessible and the mass hierarchy remains similar, i.e., $m_s \lesssim m_\chi < m_{Z'}$. Since Scheme 1 serves as the benchmark for all search channels targeting the dark Higgs boson, the DM mass is set to 200 GeV, consistent with the other mono- S studies. The signal points associated with Scheme1 are summarized in Fig. 5.2.

The other two interpretations focus on the coupling parameter g_χ , which is adjusted to ensure compatibility with the observed relic density as described in Section 2.2.2, rather than being fixed at 1. In these interpretations, each signal point satisfies the cosmological relic density constraint $\Omega h^2 = 0.1200 \pm 0.0012$ ^[17].

The second interpretation, Scheme2, examines the $m_s - m_{Z'}$ plane with a fixed DM mass

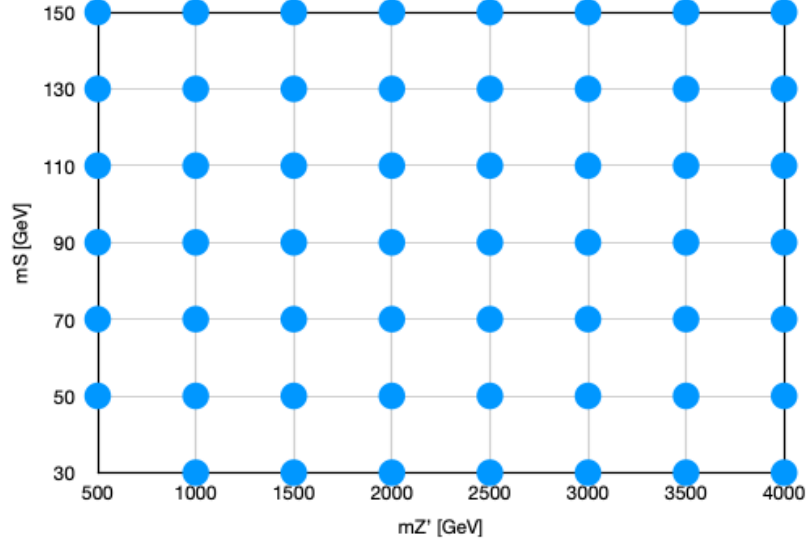


Figure 5.2 The signal points for scheme 1. The x axis stands for the $m_{Z'}$ with the unit of GeV. The y axis stands for the m_S with the unit of GeV.

of 900 GeV. This parameter choice, while extending beyond the range explored in Scheme1, remains within the perturbative limit. For each signal point, g_χ is scanned to compute relic density-compatible values using madDM^[155]. The values of g_χ and the corresponding cross-sections are shown in Fig. 5.3. The specific signal points used in Scheme2 are summarized in Fig. 5.4, with these points strategically located around the predicted exclusion region, as depicted in the middle panel of Fig. 5.7.

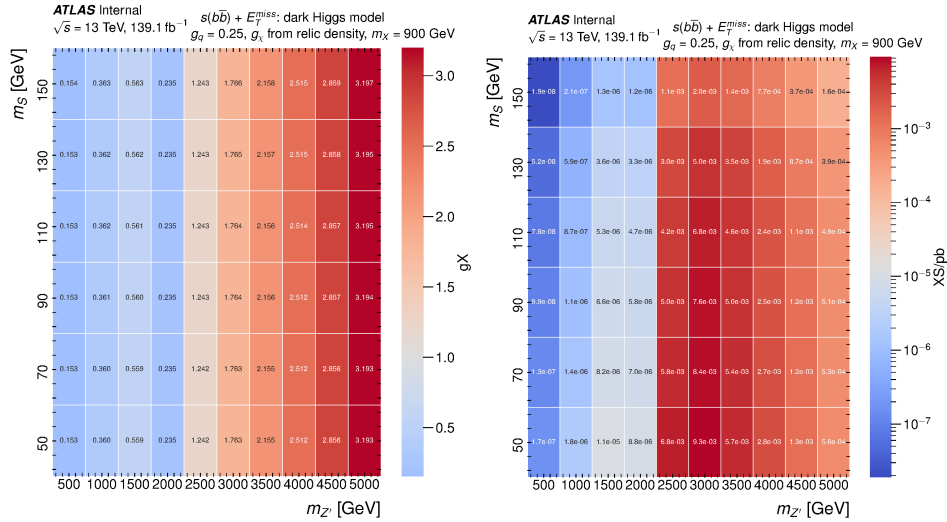


Figure 5.3 Relic density coherent g_χ values (left) and cross-section (right) of the signal points for interpretation scheme 2

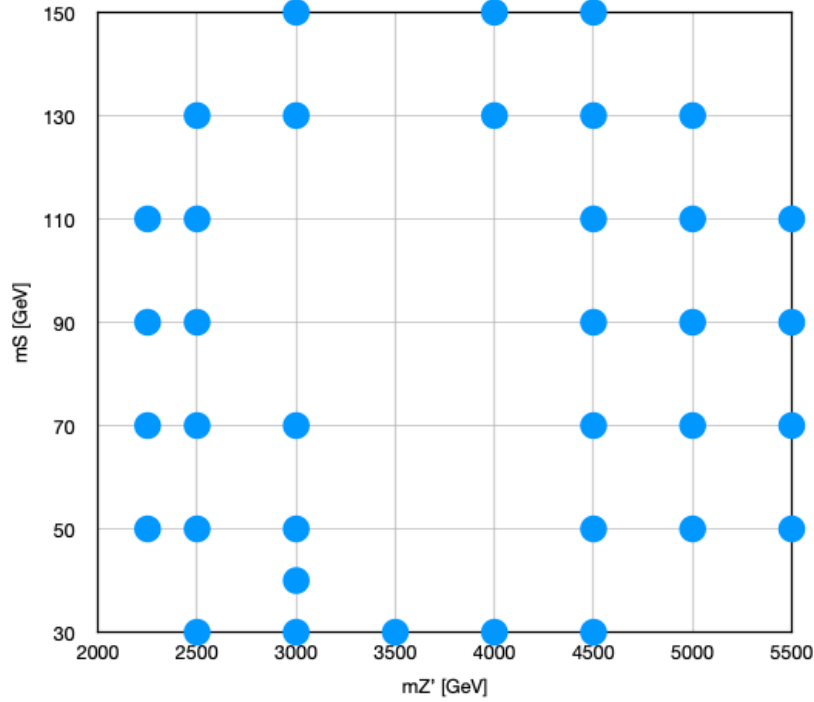


Figure 5.4 The signal points for scheme 2. The x axis stands for the $m_{Z'}$ with the unit of GeV. The y axis stands for the m_s with the unit of GeV. The m_χ is fixed to 900 GeV, and g_χ is compatible with relic density.

The third interpretation, Scheme 3, explores the m_χ - $m_{Z'}$ parameter space to provide another intersection of the multi-dimensional parameter space, aiming to fully explore the model. The dark Higgs mass is fixed at 70 GeV, a value found to have good sensitivity in the exclusion of $m_{Z'}$ in the pre-study of Scheme2, and serves as a benchmark point. In this scenario, g_χ is adjusted at each signal point to ensure relic density compatibility. The resulting g_χ values and their corresponding cross-sections are shown in Fig. 5.5. The signal points used in Scheme3 are detailed in Fig. 5.6, focusing on regions near the exclusion curve, as illustrated in the rightmost panel of Fig. 5.7.

A fast analysis is conducted to estimate signal limits and guide the signal request strategy. Signals are generated using MadGraph and interfaced with Pythia for parton showering and hadronization. MadAnalysis Simplified Fast Simulation^[156] is utilized to simulate detector effects, apply analysis selections, and compute acceptance. Background estimation is based on the mono- $h(b\bar{b})$ analysis using the full ATLAS analysis chain^[149]. The results are summarized in Fig. 5.7.

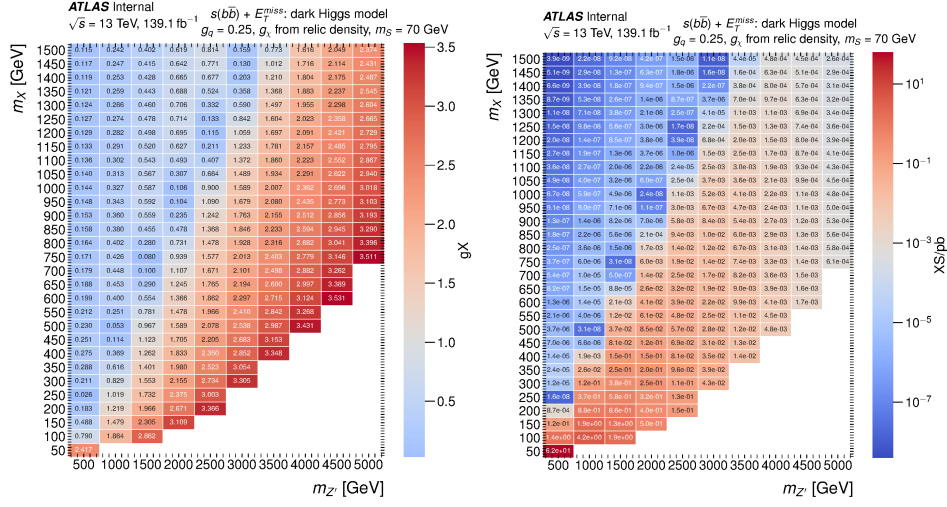


Figure 5.5 Relic density coherent g_χ values (left) and cross-section (right) of the signal points for interpretation scheme 3. The g_χ value should be smaller than $\sqrt{4\pi}$ to ensure the perturbative limit. The g_χ value in the blank area will violate such a requirement.

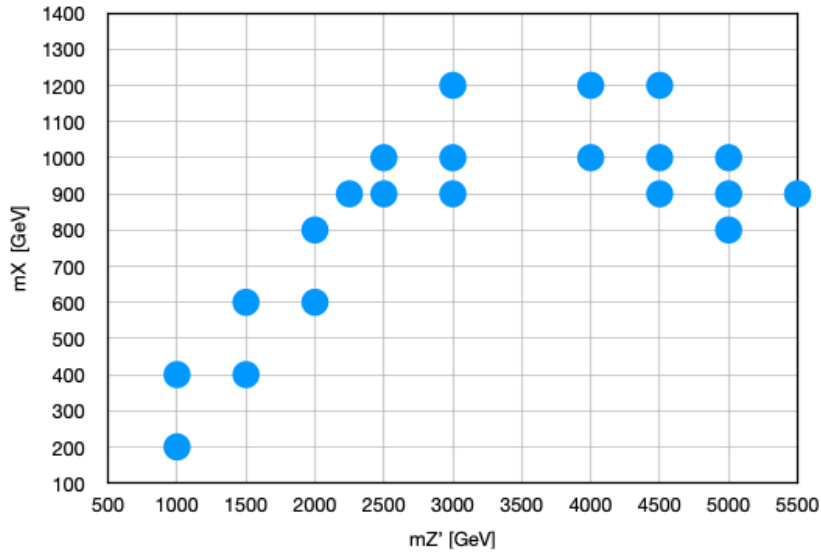


Figure 5.6 The signal points for scheme 3. The x axis stands for the $m_{Z'}$ with the unit of GeV. The y axis stands for the m_χ with the unit of GeV. The m_s is fixed to 70 GeV, and g_χ is compatible with relic density.

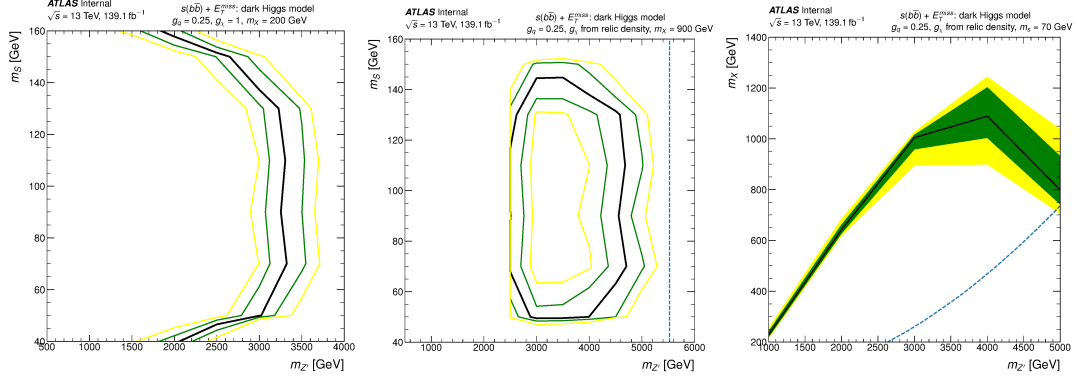


Figure 5.7 Exclusion curve for scheme 1 (left), 2 (middle) and 3 (right). The blue dotted line represents the Z' -DM coupling perturbative limit.

5.3 Data and MC

5.3.1 Data Samples

In the analysis, the full Run-2 dataset of pp collisions at a centre-of-mass energy of 13 TeV, collected during the 2015-2018 data-taking period, is used. The Good-Run-List (GRL) and the corresponding luminosities are summarized in Appendix A.2. The total integrated luminosity amounts to 140.0 fb^{-1} [157].

Lowest un-prescaled E_T^{miss} triggers are used for analysis regions where targeting events 0 lepton or 1 muon, while un-prescaled single lepton triggers are used for 2-lepton regions.

Detailed options for the triggers used are provided in Appendix A.3. During the 2018 data-taking period, the lowest E_T^{miss} trigger, HLT_xe110_pufit_xe65_L1XE50, was only available for part of the year (from period C5 onward). To simplify the analysis, the trigger named HLT_xe110_pufit_xe70_L1XE50 was used for the entire 2018 dataset. The E_T^{miss} trigger efficiency calibration is based on the analysis performed in a similar E_T^{miss} phase space [149], and the same efficiency scale factors and associated systematic uncertainties are applied in this analysis.

5.3.2 Simulated Samples

The simulated samples (MC) is summarized in Table 5.2.

5.3.2.1 Dark Higgs Signal

The signal samples are generated by calculating the hard scattering process at leading order (LO) using MADGRAPH5_aMC@NLO 2.9.3.atlas [158], based on the UFO model

Table 5.2 Samples used for the evaluation of the top-pair theory uncertainties.

Process	Generator	Systematic effect
ttbar	POWHEG + PYTHIA 8	Nominal
		μ_R, μ_F , PDF
	AMcAtNLO + PYTHIA 8 POWHEG + HERWIG 7	FSR
		ISR up
		Matrix element (matching)
		Parton shower
single top	POWHEG + PYTHIA 8	Nominal
	Diagram Removal	
	AMcAtNLO + PYTHIA 8	ME (matching)
	POWHEG + HERWIG 7	PS, hadron., UE
	POWHEG + PYTHIA 8 Diagram Subtraction	$t\bar{t}$ -single top interf.
V+jets	SHERPA 2.2.11 0,1,2j @ NLO + 3,4,5j @ LO	Nominal
		μ_R, μ_F , PDF
	MADGRAPH + PYTHIA 8 FxFx N_p -sliced, 0-4j @ LO	NLO merging (CKKW)
		Resummation (QSF)
		ME/merging/ Parton shower
V+jets T-Channel	SHERPA 2.2.11	Nominal
		μ_R, μ_F , PDF
		NLO merging (CKKW) Resummation (QSF)
Diboson	SHERPA 2.2.11 $q\bar{q} \rightarrow VV$	Nominal (with μ_R, μ_F , PDF)
	0,1j @ NLO + 2,3j @ LO	
	SHERPA 2.2.2 $gg \rightarrow VV$	
	0,1j @ LO	
	POWHEG + PYTHIA 8	hadron./UE/ Parton shower
	POWHEG + HERWIG++	CKKW/QSF
VH	POWHEG + PYTHIA 8	Nominal
	POWHEG + HERWIG 7	μ_R, μ_F , PDF Parton shower
monoSbb	MADGRAPH + PYTHIA 8	Nominal μ_R, μ_F , PDF

described in Ref.^[36]. These samples are interfaced with PYTHIA 8.245p3.lhcb7^[159] to simulate parton showers and the underlying event. The generation allows one additional jet, with the CKKW-L merging scheme^[160] employed to prevent overlaps between the matrix element and parton shower. The merging procedure uses a matching scale of 40 GeV.

The NNPDF3.0 parton distribution function (PDF) set with $\alpha_S = 0.13$ (NNPDF30_nlo_as_0118)^[161] and the A14 tune for PYTHIA (A14tune)^[162] are applied. Renormalization and factorization scales follow the default settings of MADGRAPH5_aMC@NLO. Bottom and charm quark decays are modeled using EVTGEN v1.7.0^[163].

To simulate multiple pp interactions within a bunch crossing, as well as those occurring before or after the hard scattering process, inelastic pp collisions are generated with PYTHIA 8 using the A3 tune and the NNPDF2.3LO PDF set^[164]. These interactions are overlaid with the signal samples. A pile-up reweighting factor, based on the observed average number of interactions per bunch crossing in the data, is applied. All events are processed using the ATLAS detector simulation, based on Geant4^[165].

5.3.2.2 V+jets SHERPA v2.2.11

QCD V+jets processes, illustrated in the left and middle panels of Fig. 5.8, are simulated using SHERPA v2.2.11^[166-167]. Matrix elements are computed at NLO for up to 2 jets and at LO for up to 5 jets, using Comix^[168] and OpenLoops^[169-171]. These are matched with the SHERPA parton shower^[172] following the MEPS@NLO prescription^[173-176], with SHERPA-tuned parameters. The generation uses the NNPDF3.0NNLO PDF set^[161], incorporating NLO virtual EW corrections^[170-171]. The nominal prediction includes both NLO EW and QCD corrections.

Additional EW contributions from t-channel V+jets processes^[177], simulated with SHERPA v2.2.11 and computed at LO for 2 or 3 jets, are also included in the analysis. These contributions are significant primarily in the highest E_T^{miss} regions.

5.3.2.3 $t\bar{t}$

Top-pair production, depicted in the right panel of Fig. 5.8, is simulated using the POWHEGBOX^[178-182] v2 generator at the NLO precision with NNPDF3.0NLO PDF set. The h_{damp} parameter is set to $1.5m_{\text{top}}$ ^[183], and renormalization and factorization scales are defined as $\sqrt{m_{\text{top}}^2 + p_T^2}$. Parton showers and hadronization are simulated using PYTHIA 8.230 with the A14 tune, while EVTGEN v1.6.0 models bottom and charm hadron decays.

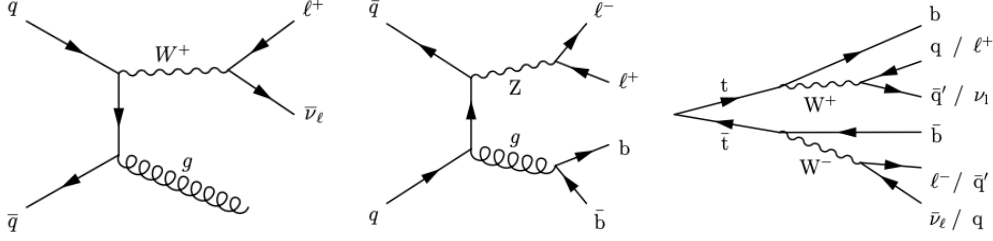


Figure 5.8 Diagrams for W +jets, Z +jets, and $t\bar{t}$ processes.

The $t\bar{t}$ production cross-section at NLO is corrected to NNLO in QCD, including NNLL soft-gluon resummation, using TOP++ 2.0^[184]. PDF and α_S uncertainties are evaluated with PDF4LHC^[185], MSTW2008 NNLO^[186-187], CT10 NNLO^[188-189], and NNPDF2.3 5f FFN^[190], with scale uncertainties combined in quadrature.

All-hadronic $t\bar{t}$ events are negligible due to the high E_T^{miss} selection. Non-all-hadronic $t\bar{t}$ samples, including dileptonic and semi-leptonic decays, are used. Inclusive and E_T^{miss} -filtered samples are combined to improve statistics in high- E_T^{miss} regions. Events with $E_T^{\text{miss}} < 100$ GeV come from inclusive samples, while those with $E_T^{\text{miss}} > 200$ GeV are drawn from filtered samples. For E_T^{miss} between 100 and 200 GeV, both sources are used with halved weights.

5.3.2.4 Single top

The single-top tW process is simulated using POWHEGBOX v2 at NLO in the five-flavor scheme with NNPDF3.0NLO PDF set. Renormalization and factorization scales are set to m_{top} , and interference with $t\bar{t}$ is managed using the diagram removal scheme^[191]. Parton showers, hadronization, and hadron decays are modeled similarly to the tW process.

Inclusive cross-section corrections for t-channel and s-channel single-top production use the same methods, with consistent details across both processes.

5.3.2.5 Diboson

Diboson production is simulated with SHERPA v2.2.11 for $q\bar{q}$ -initiated processes and SHERPA v2.2.2 for loop-induced gg processes. Matrix elements and additional jets are matched with the SHERPA parton shower using the MEPS@NLO method^[168,172].

5.3.2.6 Standard Model $Vh(b\bar{b})$

Production of $q\bar{q} \rightarrow Wh/Zh$ is modeled using POWHEGBOX v2 at the NLO precision with the relevant PDF sets and showering models. Cross-sections are calculated with NLO

and NNLO corrections.

5.4 Physics Object

The general description of the reconstruction and calibration are detailed in Section 3.4 and this section focus on analysis specific setup.

Electrons and muons are classified as either *baseline* or *signal* leptons. Baseline objects are selected using looser criteria compared to signal objects, resulting in higher acceptance. This selection is particularly advantageous for computing the missing transverse momentum, E_T^{miss} , and ensures a high efficiency for lepton vetoes within the signal region. Conversely, signal objects are defined with stricter selection criteria, providing higher purity than baseline objects. As a result, signal objects are employed to identify leptons in the single-muon and dilepton control regions.

5.4.1 Electrons

The same pseudo-rapidity requirement is applied for baseline and signal electrons, $|\eta| < 2.47$, while the p_T thresholds are 7 GeV and 27 GeV, respectively. Both baseline and signal electrons share the same track-to-vertex association requirement of $|d_0^{\text{BL}}(\sigma)| < 5$. The `LooseAndBLayerLLH` identification and `FCLoose` isolation criteria are applied for both types of electrons. For signal electrons with $p_T > 200$ GeV, the `FCHighPtCaloOnly` isolation criterion is applied instead.

5.4.2 Muons

Baseline muons are required to meet the `Loose` selection and `FCLoose` isolation criteria, while signal muons must satisfy the `Medium` selection and `TightTrackOnly-VarRad` isolation criteria. Common requirements for both baseline and signal muons include $|\eta| < 2.5$, $d_0/\sigma(d_0) < 3$, and $|z_0 \sin \theta| < 0.5$ mm. Signal muons have two different p_T thresholds: the leading signal muon must have $p_T \geq 25$ GeV, while the sub-leading signal muon must have $p_T > 7$ GeV.

5.4.3 Tau-leptons

In all signal and control regions the τ -leptons are vetoed. And the `very loose` working point is used for their reconstruction.

The impact of these selections on the mono- $s(b\bar{b})$ signal is detailed in Appendix A.4. This selection, combined with the extended τ veto described in Sec. 5.5.2, removes less than 3% of signal events.

Table 5.3 Tau selection criteria.

Feature	Requirement
Charge	$ Q = 1$
Asso. Track	1 or 3 tracks
Transverse momentum	$p_T > 20 \text{ GeV}$
τ energy scale (TES)	MVA TES
Pseudorapidity	$ \eta < 2.5$
Electron rejection	BDT-based algo.
Muon rejection	Overlap removal in $\Delta R < 0.2$ and $p_T > 2 \text{ GeV}$. No Calo-tagged Muons.
Jet rejection	RNN-based (veryLoose) algo.

5.4.4 Small-R jets

Small-R jets are categorized as *central* or *forward* jets based on their pseudorapidity (η) range. Central jets are defined by $|\eta| < 2.5$ and are exclusively used to reconstruct the two candidate jets originating from the $s \rightarrow b\bar{b}$ decay in the resolved region as described in Sec. 5.5.2.1. To eliminate jets resulting from pileup interactions, the jet-vertex-tagger (JVT) algorithms^[192] are applied. Forward jets, on the other hand, are defined as those within the range $2.5 < |\eta| < 4.5$.

The calibration and reconstruction of small-R jets employ the anti- k_t algorithm with a radius parameter $R = 0.4$, and Particle Flow (PFlow) inputs are used as constituents. The detailed settings of the small-R jets are summarized in Table 5.4.

5.4.5 LCTopo Large-R jets

Large-radius jets are utilized to reconstruct the boosted $s \rightarrow b\bar{b}$ decays. The settings of the large-R jets used in the analysis are summarized in Table 5.5.

5.4.6 Re-clustered (RC) large-R jets

In this analysis, low-mass large- R jets (mass $< 50 \text{ GeV}$) are investigated, where LCTopo/UFO large- R jet calibrations are not yet available. Jet re-clustering provides a versatile method for constructing large- R jets from calibrated small- R jets. This approach inherently propa-

Table 5.4 Reconstruction criteria for small- R jets.

Feature	Requirement
Input constituent	PFlow
Algo.	Anti- k_t ($R=0.4$)
CalibArea tag	00-04-82
Calibration config.	JES_JMS_MC16Recommendation_Consolidated_PFlow_July2019_Rel21
Calibration sequence (MC)	JetArea_Residual_EtaJES_GSC
Selection requirements	
Observable	Requirement
p_T	> 20 GeV (central) / > 30 GeV (forward)
$ \eta $	< 2.5 (central) / $2.5 < \eta < 4.5$ (forward)
JVT	Tight working point, only applied to central jets with $20 < p_T < 60$ GeV and $ \eta < 2.4$

Table 5.5 Large- R jet reconstruction criteria.

Feature	Requirement
Input constituent	LCTopo
Algo.	anti- k_t ($R=1.0$)
Grooming algo.	Trimming
R_{trim}	0.2
Trimmed sub-jets p_T fraction	0.05
CalibArea tag	00-04-82
Calibration config. for data	JES_MC16recommendation_FatJet_Trimmed_JMS_comb_3April2019
Calibration sequence (Data)	EtaJES_JMS_Insitu_InsituCombinedMass
Calibration config. for MC	JES_MC16recommendation_FatJet_Trimmed_JMS_comb_17Oct2018
Calibration sequence (MC)	EtaJES_JMS
Selection requirements	
Observable	Requirement
p_T	> 200 GeV
$ \eta $	< 2

gates calibrations and uncertainties from small- R jets to large- R jets, allowing analyses to tailor them for specific purposes. By utilizing jet re-clustering, ATLAS enhances large- R jet calibrations using the well-understood small- R jets and their systematic uncertainties, while also providing greater flexibility for analysis.

The inputs for re-clustering are small- R jets with $R = 0.4$, constructed using the anti- k_t algorithm^[91] applied to EM-scale topological clusters^[74] and tracks from the hard-scatter primary vertex, processed with the FastJet algorithm^[193-194].

The workflow for reclustered jets involves reclustering small- R jets using the anti- k_t algorithm with $R = 1.0$ to form large- R jets, which are then trimmed. All systematic uncertainties from AntiKt4EMPFLOW jets, including jet mass scale (JMS) uncertainties, are propagated to the reclustered large- R jets.

Table 5.6 Re-clustered Large- R jet configuration

property	configuration
InputJet	AntiKt4EMPFLOW
InputJetPtMin	20.0 GeV
Algorithm	anti- k_t
Radius	1.0
GroomingAlg	trim
TrimPtFrac	0.05
TrimSubjetRadius	0.2
SoftDropZCut	0.1
SoftDropBeta	0.0
SoftDropR0	1.0

5.4.7 Variable-radius track jets

The Variable Radius (VR) track jets are reconstructed from the tracks in ID using the anti- k_t algorithm. These tracks are required to meet stricter quality criteria compared to standard tracking. To mitigate pileup jets, only tracks with $p_T > 0.5$ GeV and $|z_0 \sin \theta| < 3$ mm are used as jet inputs^[123]. Here, z_0 represents the longitudinal impact parameter, evaluated relative to the primary vertex. To address mismodelling effects, simulated events are reweighted based on a comparison between data and simulation in dileptonic $t\bar{t}$ events^[104,195].

The p_T dependent jet radius^[122] is used for the VR track jets:

$$R(p_T) = \frac{30 \text{ GeV}}{p_T} \quad (5.1)$$

The parameters, $R_{\min} = 0.02$ and $R_{\max} = 0.4$, define the minimum and maximum effective size of the track jets, respectively^[123]. As the radius decreases with increasing track jet p_T , VR track jets achieve improved reconstruction efficiency for boosted decays compared to fixed-radius jet as demonstrated in Ref.^[196]. To determine the flavour composition of the calibrated large- R jet, VR track jets are associated with the initial ungroomed large- R jet using the ghost-association algorithm^[124,197].

5.4.8 B-tagging strategy

The baseline tagging strategy in the resolved and merged regions is summarised in Fig. 5.9. This strategy combines the best available b-tagging algorithms in ATLAS for both single and double b-jets, leveraging the advantages of novel techniques such as $DXbb$, developed and detailed in Section 4.

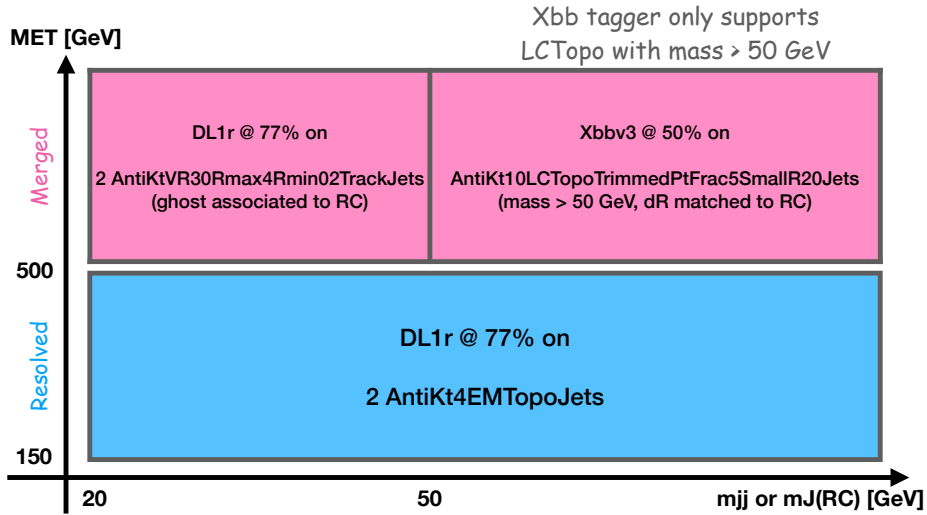


Figure 5.9 The tagging strategy is divided by the resolved region ($E_T^{\text{miss}} < 500$ GeV) and merged region ($E_T^{\text{miss}} > 500$ GeV) and the merged region is further divided by the RC large- R jet mass $m_J(RC) = 50$ GeV. The tagger, working point and the tagging objects are listed.

5.4.8.1 Single b-tagging

In the resolved region, the b -tagging is performed on the central jets (`AntiKt4EMPFLOW`). In the merged region, where $m_J < 50$ GeV and large- R b -tagging is not available, single- b tagging is performed using the leading two associated VR track jets. Each jet is assigned a classification of 0, 1, or 2 b -tags. For both jet collections, the `DL1r` discriminant with the

77% b -tagging efficiency working point is employed^[100].

The b -tagging settings used in the analysis are summarized in Table 5.7.

Table 5.7 b -tagging selection criteria.

Feature	Requirement
Jet defination	AntiKt4EMPFflow / AntiKtVR30Rmax4Rmin02
Algo.	DL1r
Working Point (WP)	Fixed Eff = 77%
CDI(Calib.)	2020-21-12TeV-MC16-CDI-2021-04-16_v1
Jet defination	AntiKt10LCTopoTrimmedPtFrac5SmallR20Jets
Algo.	$DXbb$
Working Point (WP)	Fixed Eff = 50%
CDI(Calib.)	Customized. See Sec. 4.2 and Sec. 4.3

5.4.8.2 Double b -tagging

Large-radius (large- R) jets are reconstructed to capture the entire scalar boson decay, while smaller-radius track-based jets (sub-jets) are used to resolve and identify the individual b -hadrons. At high p_T , the two jets become highly merged, making the reconstruction of sub-jets and single- b tagging challenging.

The novel $DXbb$ tagger is utilized in most of the merged-region phase space, as described in Chapter 4. The tagger is trained using LCTopo large- R jets with masses above 50 GeV, $50 < p_T < 3000$ GeV, and $|\eta| < 2.0$. In this analysis, a different large- R jet definition, the reclustered large- R jet (RC-jet), is used to access both the low-mass ($m_J^{\text{leading}} < 50$ GeV) and high-mass ($m_J^{\text{leading}} > 50$ GeV) ranges. Tagging information is attached to the RC-jet using $DXbb$, with the dR -matched LCTopo large- R jet as input when $m_J^{\text{leading}} > 50$ GeV. Otherwise, the fallback single- b tagging method, as described in the previous section, is employed.

The matching and mis-matching efficiencies are carefully studied under various jet kinematics. The dR distribution is shown in Fig. 5.10. The experimental systematic uncertainties affecting dR , primarily arises from jet reconstruction, are summed in quadrature for the most conservative estimate, as shown by the dashed lines in the figure. For inclusive and accurate matching, the dR is required to be within 1.0.

The matching efficiency, defined as the fraction of events where at least one LCTopo jet is matched to the leading RC-jet, is shown in Fig. 5.11 with the uncertainty impact shown by the dashed lines.

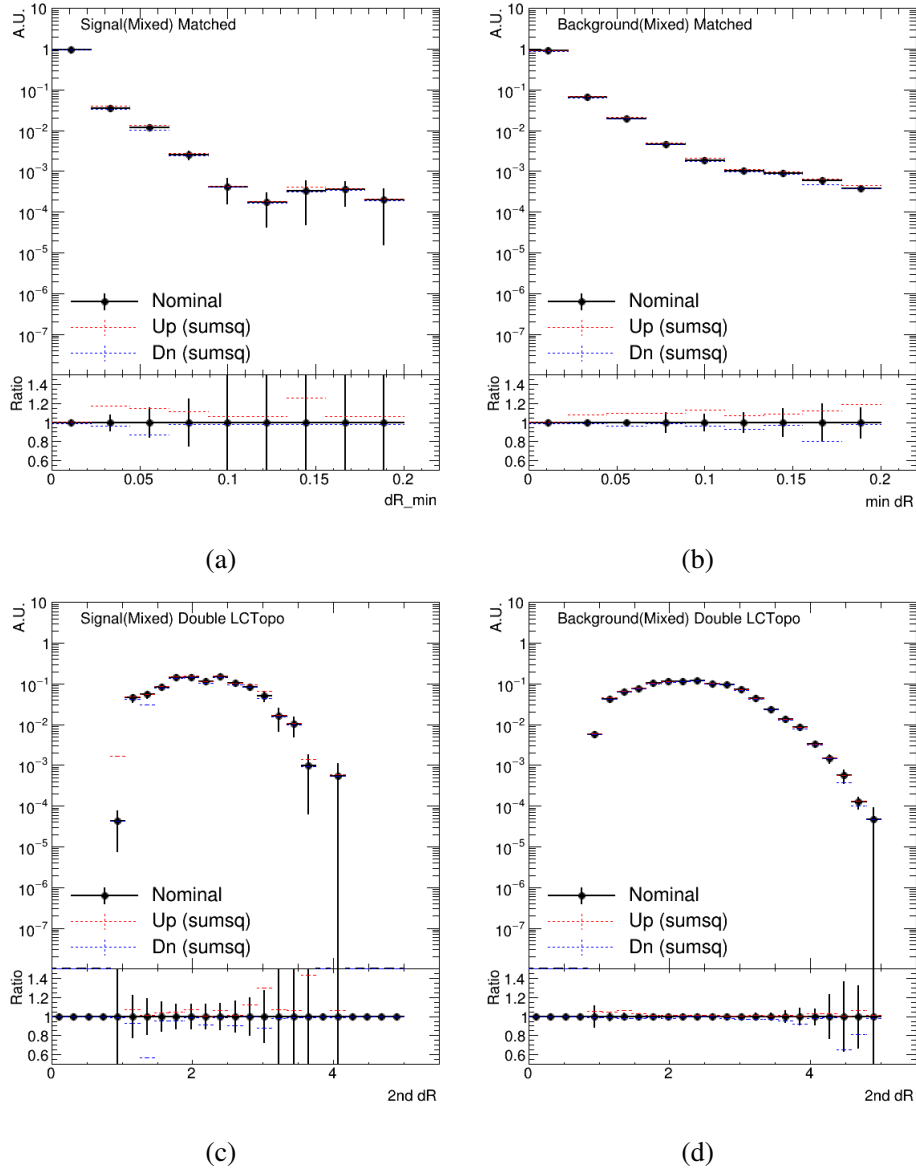


Figure 5.10 dR between leading RC jet and closet/sub-closet LCTopo jet. Reconstruction-related uncertainties are propagated and summed in quadrature, with the impact shown by the red and blue dashed lines.

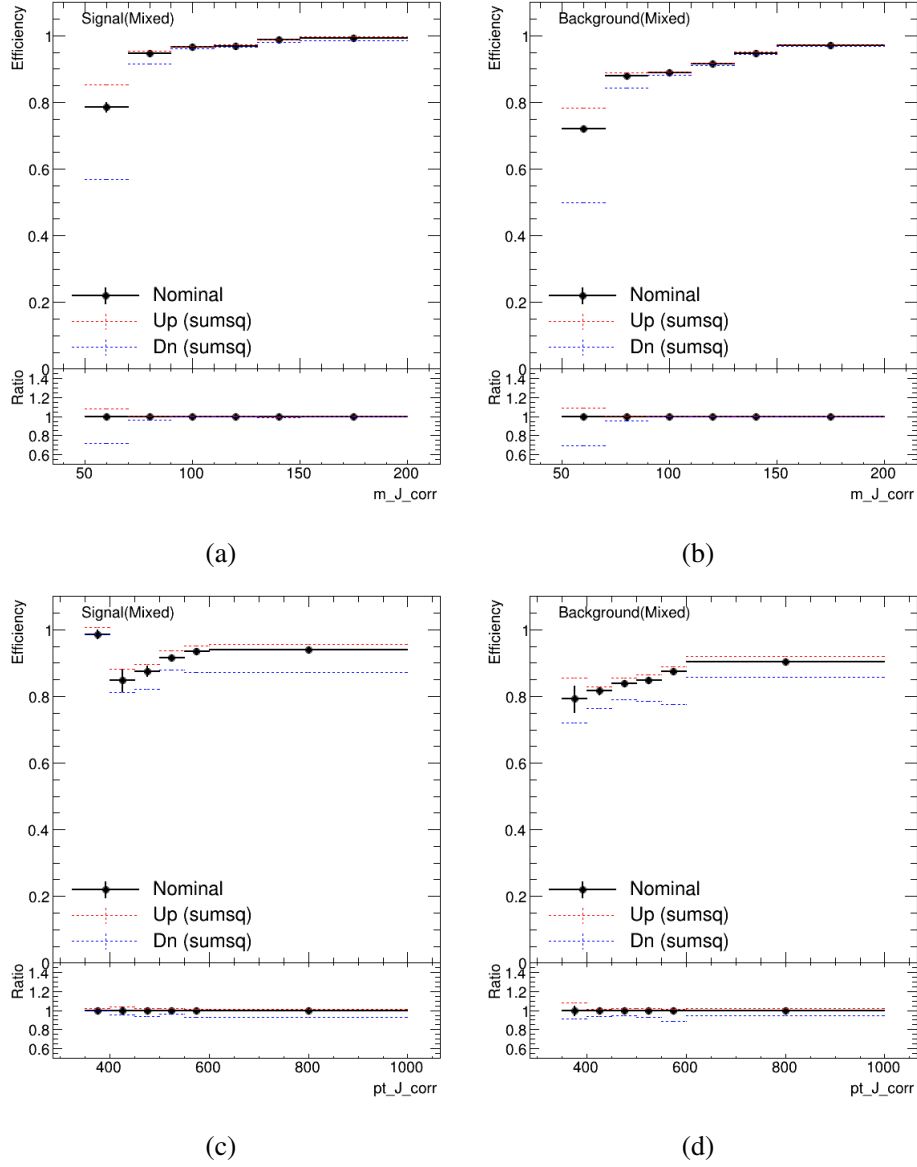


Figure 5.11 dR matching efficiency studied with the events passing analysis selections of SR+CR1+CR2, except the requirement of tagging. Reconstruction-related uncertainties are propagated and summed in quadrature, with the impact shown by the red and blue dashed lines.

To study the uncertainty of dR matching acceptance, the experimental uncertainties are propagated and the kinematics distribution of dR -match jet is compared. As illustrated in Fig. 5.12, the propagated uncertainties are summed in quadrature and the variation of jet mass and p_T is shown in dashed lines. The study concludes that the effect is negligible and no additional uncertainty is added in the analysis.

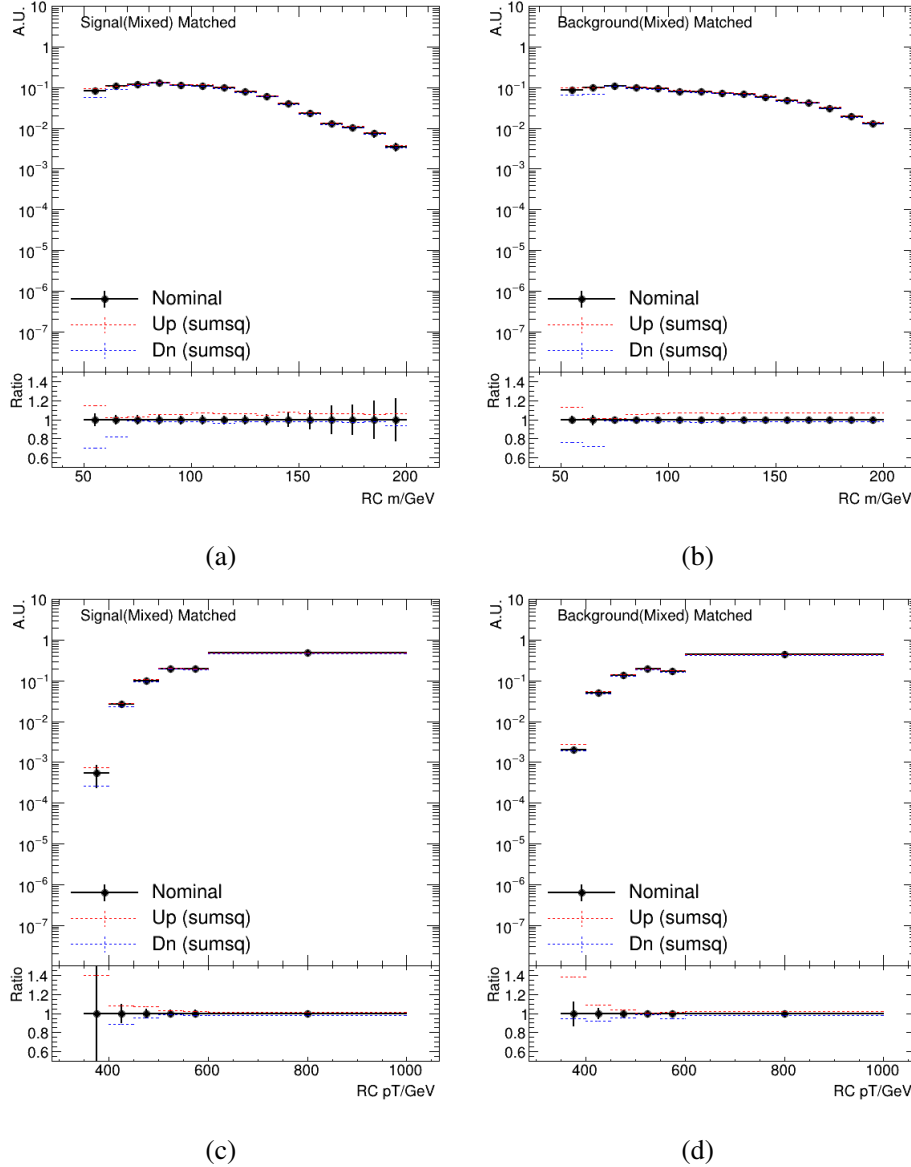


Figure 5.12 Distribution of the mass and p_T of dR -matched jet in signal(mixed of all mass) and background(total) samples. Reconstruction-related uncertainties are propagated and summed in quadrature, with the impact shown by the red and blue dashed lines. The variation are pure acceptance effect.

To summarize, the dR -matching demonstrates consistently high efficiency and accuracy, enabling the effective utilization of the powerful $DXbb$ tagger in this analysis.

5.4.9 Missing transverse momentum

Missing transverse momentum (E_T^{miss}) is reconstructed using the Track-based Soft Term (TST) approach, as described in Section 3.4.5.3. Neither τ -leptons nor photons are included in the $\vec{E}_T^{\text{miss}}$ calculation for this analysis. Jets with $|\eta| > 2.4$ are required to have $p_T > 30$ GeV, corresponding to the criteria of the tight E_T^{miss} working point.

5.4.9.1 Choice of E_T^{miss} proxy

In the signal region, a direct E_T^{miss} cut is applied, while in the control regions, $E_{T, \text{lep. invis.}}^{\text{miss}}$ is used as a proxy. In the 1-lepton muon control region (CR1mu), which consists of events containing exactly one muon and no electrons, the leading signal muon is treated as invisible, and the E_T^{miss} value is recalculated excluding the muon's contribution. In the 2-lepton channels, contributions from the two signal electrons or muons are excluded from the E_T^{miss} calculation. Specifically, in the 2-lepton muon control region, consisting of events with exactly two muons and no electrons, the leading two signal muons are treated as invisible. Similarly, in the 2-lepton electron control region, which contains events with exactly two electrons and no muons, the leading two signal electrons are treated as invisible.

The use of $E_{T, \text{lep. invis.}}^{\text{miss}}$ provides the advantage of aligning the kinematics of the 2-lepton control regions more closely with those of the signal region. Additionally, $E_{T, \text{lep. invis.}}^{\text{miss}}$ accounts for potential E_T^{miss} contributions arising from resolution effects and mis-reconstructions.

5.4.10 Object-based E_T^{miss} significance $\mathcal{S}$

The object-based E_T^{miss} significance ($\mathcal{S}$), as described in Section 3.4.5.3, is employed to distinguish events with real E_T^{miss} , arising from neutrinos or weakly interacting exotic particles, from events where E_T^{miss} originates due to measurement limitations and resolution effects. This variable is particularly effective at suppressing QCD backgrounds, as demonstrated in Ref.^[196]. The calculation of $\mathcal{S}$ incorporates the expected resolutions of all objects contributing to the $\vec{E}_T^{\text{miss}}$ reconstruction and their directional correlations. In the 1-lepton and 2-lepton control regions, the E_T^{miss} significance is computed using the same lepton treatment as $E_{T, \text{lep. invis.}}^{\text{miss}}$, as outlined in Section 5.4.9.1.

5.4.11 Overlap removal

The reconstruction of the same energy deposits in the detector as multiple objects is resolved using the standard overlap removal procedure as,

Table 5.8 Overlap removal

Remove	Against	Criteria
Electron	Electron	$p_{T,1} < p_{T,2}$, shared track
Tau	Electron	$\Delta R < 0.2$
Tau	Muon	$\Delta R < 0.2$
Muon	Electron	Calo-Muon, shared ID track
Electron	Muon	Shared ID track
Jet	Electron	$\Delta R < 0.2$
Electron	Jet	$\Delta R < \min(0.4, 0.04 + 10 \text{ GeV}/p_T(e))$
Jet	Muon	ghost-associated or $\Delta R < 0.2$ $N_{\text{Track}} < 3$
Muon	Jet	$\Delta R < \min(0.4, 0.04 + 10 \text{ GeV}/p_T(\mu))$
Jet	Tau	$\Delta R < 0.2$
Fat-jet	Electron	$\Delta R < 1.0$

ΔR is computed using rapidity. Table 5.8 summarizes the priority order applied to resolve the identities of overlapping objects.

5.5 Event Selection and Categorization

As introduced in the Overview section 5.1 multiple regions are defined in the analysis and they are further divided according to the E_T^{miss} , to achieve better reconstruction of signal with different topology and control of background with different composition, so that better analysis sensitivity. The signal topology with different E_T^{miss} is summarized in Fig. 5.13 and the final categorization used in analysis is summarized in Fig. 5.14. The event selections, in each region, are described in the following.

5.5.1 Event Cleaning for Data

The event cleaning is performed for all the data taken from the detector in all the analysis regions. Data events must be part of the runs listed in the GRLs as described in Section 5.3. The veto is designed to remove the bad or corrupted events such as LAr noise burst, data corruption, tile corrupted events, SCT recovery procedure for single event upsets, incomplete events, events with cosmic muons or with badly measured muons.

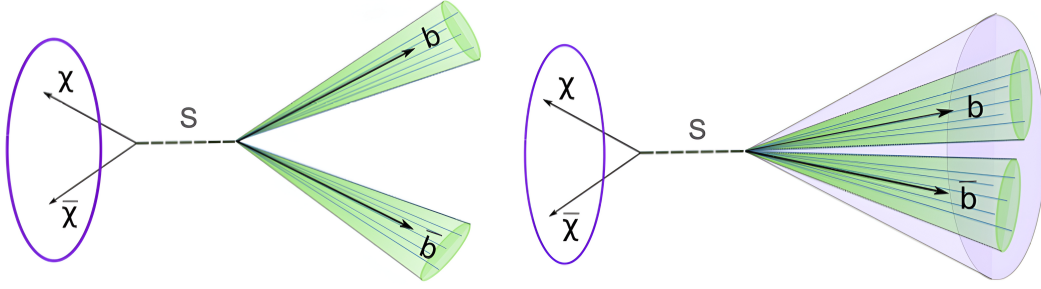


Figure 5.13 Two small-R jets or one large-R jet are used to reconstruct the $S \rightarrow b\bar{b}$ decay in the resolved regions (left) and merged regions (right) respectively.

SR / CR	SR	1 muon CR	2L CR
MET / METproxy [GeV]	> 750	> 500	> 500
	500-750		
	350 - 500	350 - 500	350 - 500
	200 - 350	200 - 350	200 - 350
	150 - 200	150 - 200	150 - 200
Fitted variable	m_{jj} / m_J	muon charge	Yield

Figure 5.14 Definition of Analysis Regions

Events must include a primary vertex with a minimum of two associated tracks. The primary vertex is identified as the one with the highest Σp_T^2 , where the sum considers all tracks with transverse momentum $p_T > 0.5$ GeV that are linked to the vertex.

5.5.2 Common Selections for Signal and Control Regions

The common selections are designed based on the previous study^[149] and are listed below and the first rows in Table 5.9.

Loose/Bad jet veto: to remove non-collisional backgrounds

$E_T^{\text{miss proxy}} > 150\text{GeV}$: E_T^{miss} or $E_{T, \text{lep. invis.}}^{\text{miss}}$ is used in signal or control regions

Tau veto: Event with baseline τ -lepton are rejected. And extended selection is applied to further suppresses W +jets, single-top, and $t\bar{t}$ backgrounds. The calculation uses reconstructed jets as input, employing small-R jets in the resolved region or reclustered large-R jets in the merged region. A jet is identified as a tau candidate if it meets both

of the following criteria:

1. Track multiplicity within the jet cone satisfies $1 \leq N_{\text{trk}} \leq 4$.
 2. Angular separation between the jet and E_T^{miss} satisfies $\Delta\phi \leq 22.5^\circ$.
- $\min_{j \in \{1,2,3\}} \Delta\phi(E_T^{\text{miss}}, j) > 20^\circ$: the E_T^{miss} vector often aligns with a jet in fake E_T^{miss} in multijet events. To mitigate this background, events failing to satisfy $\min \Delta\phi(E_T^{\text{miss}}, j) > 20^\circ$, calculated over the three leading jets, are rejected.
- $0.7 < \frac{E_T^{\text{miss}}}{p_T} < 1.3$: back to back topology and reduces contributions from $t\bar{t}$ and W +jets events.

The selections which are specific to resolved and merged regions are described below.

5.5.2.1 Selections in Resolved Region

In the resolved region, the dominant background process is $t\bar{t}$ production. To suppress this background, the variables $m_T^{b,\text{min}}$ and $m_T^{b,\text{max}}$ are utilized with the requirements $m_T^{b,\text{min}} > 170$ GeV and $m_T^{b,\text{max}} > 200$ GeV. These variables are defined as:

$$m_T^{b,\text{min/max}} = \sqrt{2p_T^{b,\text{min/max}} E_T^{\text{miss}} (1 - \cos \Delta\phi(\vec{p}_T^{b,\text{min/max}}, \vec{E}_T^{\text{miss}}))} \quad (5.2)$$

where $p_T^{b,\text{min}}$ and $p_T^{b,\text{max}}$ represent the p_T of the b -jet that is nearest to (denoted as min) or farthest from (denoted as max) $\vec{E}_T^{\text{miss}}$ in ϕ , respectively.

In the signal region, resolved event selections include an additional requirement on the object-based E_T^{miss} significance, imposing $S > 12$ to further reduce multi-jet background contributions. For E_T^{miss} and $S(b\bar{b})$ recoil, events must satisfy $0.7 < E_T^{\text{miss}}/p_T(jj) < 1.3$, as introduced in Sec. 5.5.2.

The number of small-R jets in the event also helps discriminate between signal and $t\bar{t}$ background. To this end, a cut of $N(\text{central small-R jets}) \leq 4$ is applied.

The invariant mass of the scalar candidate jets, m_{jj} , reconstructed from the two b -tagged small-R jets, serves as the final discriminating variable in the fit. The fit range is defined as $20 \text{ GeV} < m_{jj} < 270 \text{ GeV}$.

In practice, no events survive below $m_{jj} = 35, 40$, and 50 GeV for low ($[150, 200] \text{ GeV}$), medium ($[200, 350] \text{ GeV}$), and high ($[350, 500] \text{ GeV}$) E_T^{miss} bins, respectively. Consequently, the fit ranges are adjusted to $m_{bb} \in [35, 270], [40, 270],$ and $[50, 270] \text{ GeV}$.

For both m_{jj} and $p_{T(jj)}$, the muon-in-jet correction described in Ref. [1612.01656] is applied.

A summary of some variables used for event selection is shown in Fig. 5.15 and clear separation between various signals and background is observed.

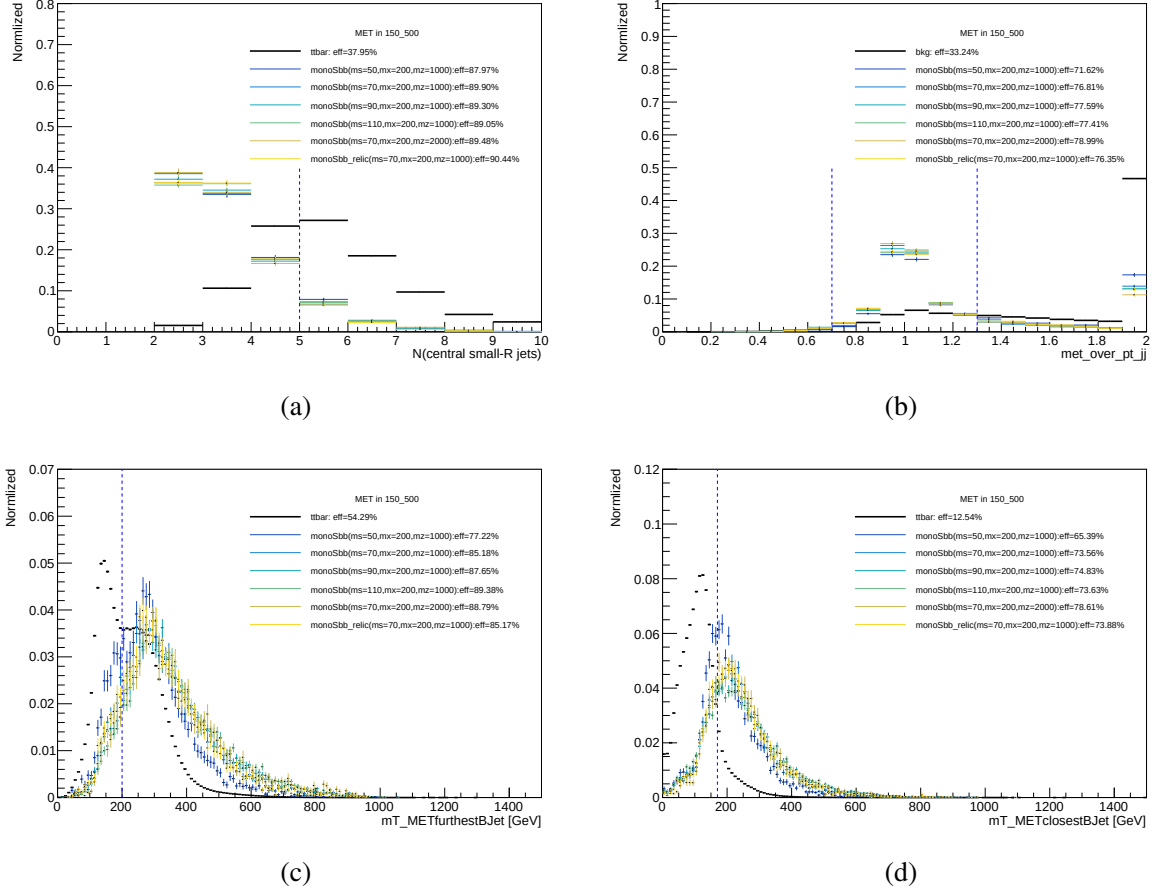


Figure 5.15 The distribution of a) small-R jets multiplicity, b) $E_T^{\text{miss}}/p_T(jj)$, c) $m_T^{b,\text{max}}$ and d) $m_T^{b,\text{min}}$ in the resolved region without apply these cuts. For each variable, the selected signal distributions are compared with the one for either $t\bar{t}$ or all backgrounds. The blue dashed line stands for the cut value on the variable.

5.5.2.2 Selections in Merged Region

In the merged region at least one central RC large radius jet is required and the highest p_T large radius jet is treated as the reconstructed Higgs candidate. To ensure that the majority of the decay products are contained in the RC large radius jet, a $2m_J/p_T(J) < 0.6$ cut is applied for the merged topology. For E_T^{miss} and $S(b\bar{b})$ recoil, the events are required to have $0.7 < E_T^{\text{miss}}/p_T(J) < 1.3$. The impact of these two cuts on one selected signal and Z+bb are shown in Fig. 5.17. Some of variables used for event selection, and their justification, has

been summarised in the Fig. 5.16

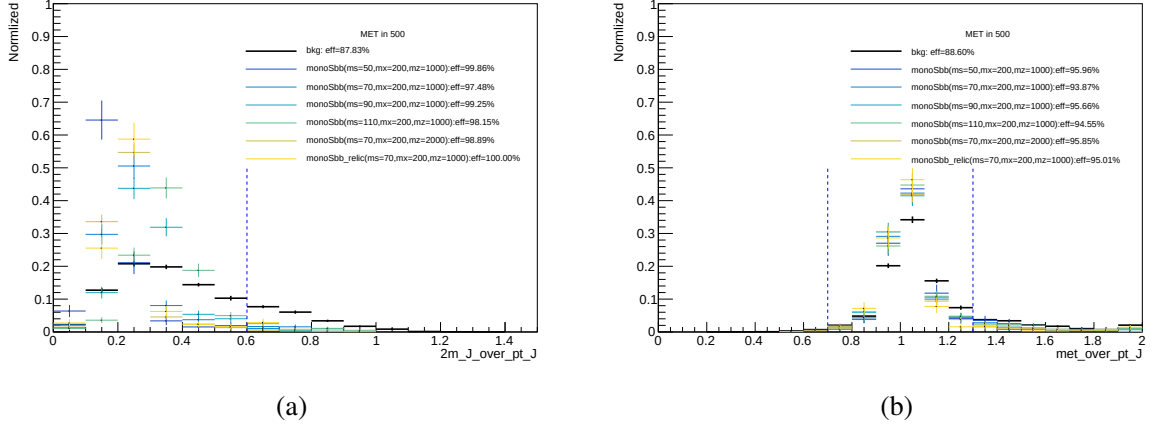


Figure 5.16 The distribution of a) $2m_J/p_T(J)$ and b) $E_T^{\text{miss}}/p_T(J)$ in the merged region without applying these cuts, for either variable, the selected signal distributions are compared with the one for all backgrounds. The blue dashed line stands for the cut value on the variable.

The final discriminant variable in the fit is the reconstructed mass of the dark Higgs candidate, the m_J . Events are required to be within $20 \text{ GeV} < m_J < 270 \text{ GeV}$ for the fit.

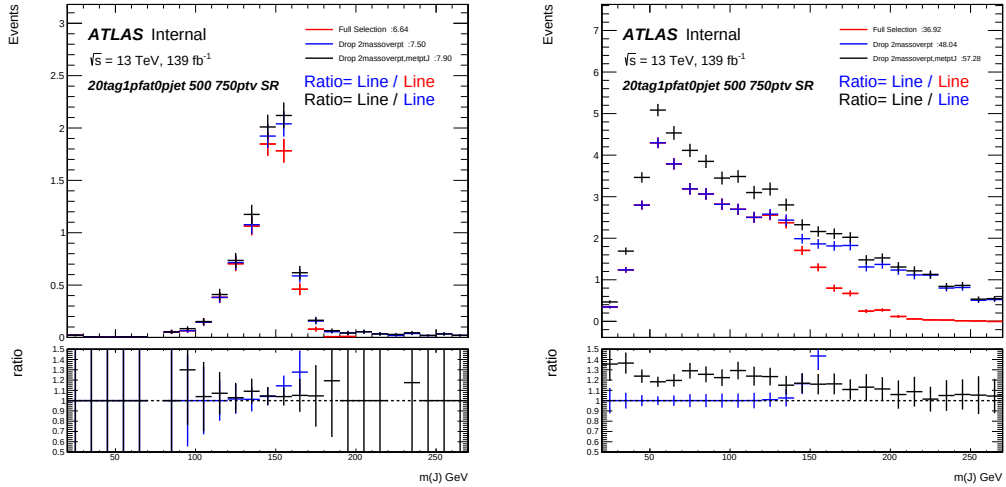


Figure 5.17 The impact from $2m_J/p_T(J) < 0.6$ and $0.7 < E_T^{\text{miss}}/p_T(J) < 1.3$ on monoSbb $m_Z'=3000 \text{ GeV}$, $m_X=200 \text{ GeV}$, $m_S=150 \text{ GeV}$ (left) and Z+bb in 0 lepton $500 < E_T^{\text{miss}} < 750 \text{ GeV}$; These two cuts remove 16% singal meanwhile 36% Z+bb.

Events containing any additional b-tagged VR track jet not associated with the RC large-R jet are vetoed in this region to suppress contributions from top-quark events.

The selections of the resolved and merged region are summarized in Table 5.9.

Table 5.9 Event selections in the signal and control regions. The resolved and merged topologies are displayed in separate columns, with some selections shared between them.

Cut	Resolved	Merged
Trigger	0/1-lepton SR/CR: unprescaled E_T^{miss} trig. w/ lowest threshold 2-lepton CR: unprescaled single-lepton trig. w/ lowest threshold	
Lepton multiplicity	0-lepton SR: veto event with baseline electron or muon 1-lepton CR: event with exactly one signal μ 2-lepton CR: 2 baseline e or μ , exactly 2 signal e or μ with opposite sign	
Z mass window	2-lepton CR only: $ m_Z - m_{\ell\ell} < 10 \text{ GeV}$	
τ vetoes	veto on baseline τ leptons & extended τ -veto	
$\min_{j \in \{1,2,3\}} \Delta\phi(E_T^{\text{miss}}, j)$	$2 \leq N_{\text{small-R jets}}^{\text{central}} \leq 4$	$N_{\text{large-R jets}}^{\text{central}} \geq 1$
Jet multiplicity	$N_{\text{small-R jets}}^{b\text{-tagged}} = 2$	leading large-R jet $D_{\text{Xbb-tagged}}(m_J > 50 \text{ GeV})$
b -tag multiplicity		$N_{\text{asso.VRtk,jets}}^{b\text{-tagged}} = 2$ ($m_J < 50 \text{ GeV}$)
Non-associated b -jet veto	-	$N_{\text{non-asso.VRtk,jets}}^{b\text{-tagged}} = 0$
E_T^{miss} significance	0-lepton SR: $S > 12$ 1-lepton CR: $S_{\text{lep, invis.}} > 12$ 2-lepton CR: $S_{\text{lep, invis.}} > 12$ & $S < 5$	—
Top-mass proxy	$m_T^{b,\text{min}} > 170 \text{ GeV}$ $m_T^{b,\text{max}} > 200 \text{ GeV}$	—
E_T^{miss} and $S(b\bar{b})$ recoil	$0.7 < E_T^{\text{miss}}/p_T(j) < 1.3$	$0.7 < E_T^{\text{miss}}/p_T(J) < 1.3$
Boosted decay	-	$2m_J/p_T(J) < 0.6$
E_T^{miss}	$150 < E_T^{\text{miss}} < 500 \text{ GeV}$	$E_T^{\text{miss}} > 500 \text{ GeV}$

5.5.3 Dedicated selection in Control regions

Control regions are defined to constrain various background contributions. These control regions are orthogonal to the signal regions and target W/Z +jets and $t\bar{t}$ processes which constitute the dominant backgrounds in the signal regions. The orthogonality is ensured by inverting the lepton veto.

5.5.3.1 1-lepton channel (1L)

The W +jets background in the SR is from the leptonic decay and the $t\bar{t}$ background is from the semileptonic one. For both background, events enter the signal region if the leptons fail to be identified or be outside from the detector acceptance. They are mainly contributed from the τ decay channel.

The 1-muon control region is designed to constrain these backgrounds using data. Using muons instead of electrons or τ -leptons has the advantage that the signal region kinematics can be imitated very well, as single-muon events can be selected using the same E_T^{miss} triggers as for the signal region, since muons passing through the inner detector deposit little energy in the calorimeters. This leads to the muon's momentum contributing to the trigger level calculation of E_T^{miss} , which is entirely calorimeter based. Events in this control region are required to have exactly one signal muon and no additional baseline leptons. To mimic events in the signal region, in which the muon is not detected, $E_{T, \text{lep. invis.}}^{\text{miss}}$ is used in the 1-muon region instead of E_T^{miss} . Also all other E_T^{miss} dependent variables, like the E_T^{miss} significance and $m_T^{b, \text{min/max}}$ are calculated with $E_{T, \text{lep. invis.}}^{\text{miss}}$. Apart from that the same event selection as in the signal region is used, as described above.

The 1-electron control region is studied by assuming it has same statistics as 1-muon control region, and the relative fraction is same for each component. The improvement on the limit and error of the signal strength is marginal. Considering the 1-electron region will suffer the multi-jet backgrounds, this region is not considered for this round.

5.5.3.2 2-lepton channel (2L)

The 2-lepton control region is designed to estimate the Z +jets background. Within the signal region, the production of $Z(\rightarrow \nu\nu)$ + jets contributes significantly to the background, as it shares the same decay topology as $Z(\rightarrow \ell\ell)$ + jets. This similarity arises because the Z boson's momentum is independent of its decay products. Consequently, the normalization

of $Z(\rightarrow \nu\nu) + \text{jets}$ events can be inferred using a $Z(\rightarrow \ell\ell) + \text{jets}$ control region.

The lowest unprescaled single lepton triggers are used as described in Appendix A.3. Exactly 2 electrons or 2 muons are required. Events with further baseline leptons of any flavor are discarded. Two leptons must satisfy the signal lepton requirements. The trigger matching is required. At least one of the lepton must have a sufficiently high p_T to fire the trigger.

The signal muons are required to have $p_T > 25 \text{ GeV}$ and signal electrons need to have $p_T > 27 \text{ GeV}$. The second lepton does not need to be a signal lepton in order to increase the acceptance of $Z\text{jets}$ events. The selected leptons are required to be of opposite charge and to have an invariant mass fulfilling $|m_Z - m_{\ell\ell}| < 10 \text{ GeV}$. This suppresses backgrounds without a resonant lepton-pair around the Z -boson mass, such as $t\bar{t}$ events.

The E_T^{miss} significance $\mathcal{S}$ is used as a powerful variable to distinguish events with genuine E_T^{miss} , from events with "fake" E_T^{miss} originating from such as mis-identified object or imprecise reconstruction, as described in Section 5.4. In $Z(\rightarrow \mu\mu) + \text{jets}$ events no real E_T^{miss} is expected, while for $t\bar{t}$ events real E_T^{miss} is present in the event due to the two escaping neutrinos. Therefore, to further reduce the $t\bar{t}$ background a cut of $\mathcal{S} < 5$ is applied.

For the remaining event selection the same cuts as in the signal region are applied, with the only difference that in the cuts on E_T^{miss} and all E_T^{miss} dependent variables $E_{T, \text{lep. invis.}}^{\text{miss}}$ is used. Thereby the kinematics of $Z(\rightarrow \nu\nu) + \text{jets}$ events can be imitated.

5.6 Systematic Uncertainty

The analysis considers both the theoretical and experimental systematics.

Systematic uncertainties are mainly from the reconstruction of different physics objects, predictions for signal and background processes. These uncertainties influence the yields of signal or background within designated regions and affect the shape of the fit discriminant, m_s .

5.6.1 Experimental Systematics

The E_T^{miss} trigger response in simulations is subject to uncertainties, which are quantified through a specific calibration procedure detailed in Ref.^[198]. Two types of uncertainties are identified: METTrigStat and METTrigSyst. The former represents the 1σ statistical

uncertainty from the trigger scale factor fit, while the latter accounts for uncertainties arising from the background composition.

Uncertainties for electrons, muons, jets, E_T^{miss} , and lepton triggers are determined based on performance studies, as described in Section 3.4.

To address uncertainties in the jet energy scale (JES) and jet energy resolution (JER) for small-R jets, the `CategoryReduction_SimpleJER` scheme is utilized. This approach employs 29 nuisance parameters for JES and 8 for JER. b -tagging uncertainties are parameterized using eigenvector variations under the `medium` reduction scheme, leading to 4, 3, and 6 eigenvector variation nuisance parameters for b -jets, c -jets, and light-flavor jets, respectively.

The `CategoryReduction_SimpleJER` scheme is used to estimate the uncertainty from AntiKt4EMPFLOW jet which is the input for large-R jet reclustering, which includes the one from jet energy scale (JES), resolution (JER) and JMS (Rtrk based).

The uncertainty from the DL1r VR algorithm which is used for low mass ($m_J < 50\text{GeV}$) large-R jet tagging is derived based on the recommendations^[104].

The uncertainty of data/MC scale factor of Xbb tagging in merged region for high mass ($m_J > 50\text{GeV}$) large-R jet is derived from the calibrations introduced in Section 4, according to the formula 5.6.

$$\kappa \equiv \frac{\epsilon_{data}}{\epsilon_{MC}} \quad (5.3)$$

$$\alpha \equiv \frac{\epsilon_{MC}}{\epsilon_{MC'}} \quad (5.4)$$

$$\epsilon_{data} = \epsilon_{MC} * \kappa = \epsilon_{MC'} * \kappa * \alpha \quad (5.5)$$

$$\frac{\delta(\epsilon_{data})}{\epsilon_{data}} = \frac{\delta(\kappa)}{\kappa} \quad (5.6)$$

The ϵ denotes the Xbb tagging efficiency and MC denotes the Monte Carlo simulation with specific generator and parton showering. κ is the data/MC scale factor which calibrates the tagging efficiency of MC to data. The value and uncertainty of κ is taken from the calibrations. Different calibrations are applied based on the physics process and flavor composition of large-R jet. For signal, V +jets, $VHbb$, Diboson process, the scale factor from Zbb calibration as introduced in Section 4.2 is applied when the leading large-R jet contains two b -quark. For the $t\bar{t}b\bar{a}$ and single top process, the scale factor is taken from

ttbar calibration as introduced in Section 4.3. The difference of MC efficiency between the samples used in analysis and calibration is corrected with MC/MC scale factor α , mainly originating from the different parton showering used.

5.6.2 Theory Systematics

- **Missing higher orders calculation of matrix elements (ME):** estimated by varying the renormalisation and factorisation scales (μ_R and μ_F) independently by a factor of 2. Variations such as $(\mu_R, \mu_F) = (\frac{1}{2}, 2)$ and $(\mu_R, \mu_F) = (2, \frac{1}{2}) \times \mu_{\text{central}}$ are excluded to avoid large logarithmic corrections.
- **Choice of PDFs and α_s :** Estimated following the PDF4LHC prescription^[127].
- **Merging-scale uncertainties:** evaluated by varying the scale up and down by a factor of 2 for the samples with different jet multiplicity in ME such as $V+1, 2, \dots$ jets
- **Resummation scale uncertainties:** an additional uncertainty associated with the energy cut-off in the parton shower (PS)^[199] for SHERPA samples.
- **Matching uncertainties:** uncertainties related to the matrix element/parton shower (ME/PS) matching procedure and are assessed by comparing POWHEG and MG5AMC samples.
- **Parton shower/hadronisation uncertainties:** evaluated by comparing samples generated with different generators, such as PYTHIA 8 and HERWIG 7.
- **Eigentune uncertainties:** related to the ATLAS tuning programme^[162].

5.7 Statistical Study

5.7.1 Likelihood definition

The binned likelihood function is constructed as the product of following Poisson probability terms,

$$\mathcal{L}(\mu, \vec{\theta}, \vec{\gamma}) = \prod_{i \in \text{bins}} \text{Pois}(N_i | \mu s_i(\vec{\theta}) + \gamma_i b_i(\vec{\theta})) \times \prod_{\theta \in \vec{\theta}} \frac{1}{\sqrt{2\pi}} e^{-\theta^2/2} \times \prod_{i \in \text{bins}} \text{Gauss}(\beta_i | \gamma_i \beta_i, \sqrt{\gamma_i \beta_i}) \quad (5.7)$$

where μ parameter is the signal strength and $s_i(b_i)$ the expected signal(background) yield in bin i .

The systematic uncertainties are implemented with the nuisance parameters (NP) θ ,

which change the prediction of the signal and background in each bin, according to different source. They are parameterized by Gaussian priors.

The limited MC statistics causes the fluctuation and it is modelled with γ -parameters and the yield of each bin could be modified by $b_i(\vec{\theta}) \rightarrow \gamma_i b_i(\vec{\theta})$ during the fitting. γ itself follows the Gaussian and $\beta_i = 1/\sigma_{\text{rel}}^2$ where σ_{rel} is the relative statistical uncertainty of the expected (MC simulated) total background yield.

The maximize likelihood method is used to obtain the μ and σ_μ with respect to all parameters. And the test statistic could be built to measure the compatibility between the background-only model and the observed data, with the definition as log-likelihood ratio,

$$q_\mu = 2 \ln \left(\frac{\mathcal{L}(\mu, \hat{\hat{\theta}}, \hat{\hat{\gamma}})}{\mathcal{L}(\hat{\mu}, \hat{\hat{\theta}}, \hat{\hat{\gamma}})} \right), \quad (5.8)$$

where $\hat{\mu}$ and $\hat{\hat{\theta}}$ are the parameters that maximise the likelihood at the same time, and $\hat{\hat{\theta}}$ are the values of nuisance parameter that maximise the likelihood for a given μ . The test statistic could also be used to derive exclusion intervals with CL_s method^[200]

5.7.2 Fit variables and event categories

The maximum likelihood fitting of data and MC templates (histograms) is performed across all the regions, including the 0/1/2 lepton regions and the different E_T^{miss} bins.

The definition of signal regions and control regions are described in Fig. 5.14 and Sec. 5.5.3.

In the resolved and merged regions within the 1L and 2L channels, $E_{T, \text{lep. invis.}}^{\text{miss}}$ binning is employed instead of the E_T^{miss} binning used in the 0-lepton channels and a single merged region is defined for 1L and 2L channels with $E_{T, \text{lep. invis.}}^{\text{miss}} > 500$ GeV due to limited statistics. This mimics the kinematics of semileptonic $t\bar{t}$ and W +jets events in the 0L region, where one lepton is undetected. The Z +jets background is constrained by fitting the event yield in a region containing exactly two electrons or muons (CR 2L).

In the SR the fitting is performed on the invariant mass of the dark Higgs-boson candidate (m_s). In the resolved regions this variable is constructed from the two leading b -jets and in merged regions from the mass of the leading large- R jet. The binning chosen for m_{bb}/m_J is detailed in Table 5.10. These choices are based on, and updated from, the previous study

presented in Ref.^[149].

To distinguish between W +jets and $t\bar{t}$ contributions, a separation based on the muon charge is applied. In $t\bar{t}$ events, the muon charge is generally distributed equally, whereas the production of W +jets is biased towards positively charged W -bosons due to the LHC being a pp collider. Therefore for the 1L channel, the muon charge is employed as the fit variable. As a result, each E_T^{miss} bin is divided into two bins based on the muon charge (positive and negative).

In the 2L channel, a single bin yield is used for each $E_{T, \text{lep. invis.}}^{\text{miss}}$ bin. This coarse binning enhances the robustness of the fitting procedure while maintaining sensitivity. With this binning, the control regions effectively constrain the background normalization without significant loss of precision.

Table 5.10 Binning of the final fitting observable in SR.

E_T^{miss} bin [GeV]	m_{jj} or m_J binning
150-200	[35,40,45,...,270] (5 GeV/bin)
200-350	[40,45,50,...,270] (5 GeV/bin)
350-500	[50,60,70,...,270] (10 GeV/bin)
500-750	[20, 50, 70, 90, 110, 130, 150, 180, 270]
750-inf	[20, 50, 90, 180, 270]

5.7.3 Merging of fit templates

Some of the background MC templates have low statistics, making it difficult for the fit to constrain them individually. To address this, templates corresponding to similar physical processes (e.g., Zbb , Zbc , etc.) are combined into a single template for the fit. The following templates are utilized:

- $Zhf = Z+bb/bc/bl/cc$
- $Whf = W+bb/bc/bl/cc$
- Zcl
- Wcl
- Zl
- Wl
- $t\bar{t}$
- single top = single-top Wt + t -channel + s -channel

- diboson = $WW+WZ+ZZ$
- $VH(b\bar{b})$ (SM Higgs)

The above merging scheme was inherited from the mono- $H(b\bar{b})$ ^[149] and also follows the fit model developed for the SM $VH(b\bar{b})$ search^[201]. The merging strategy considers the similarity of the distribution of different sub-process, as well as modelling of flavor composition with Sherpa 2.2.11^[202].

5.7.4 Implementation of $DXbb$ Correction

The uncertainties of $DXbb$ tagging on $V+hf$ (heavy flavor) are constrained by the control region as Zhf from 2 lepton region and Whf from 1 muon region respectively. Two scale factors in merged region are applied on Whf and Zhf respectively to propagate the correction from the corresponding CR to the SR. Since the SF includes not only the correction on the $DXbb$ tagging but also the modelling, so the SF is applied on Whf and Zhf separately as the fact that the modelling correction could be different for the two.

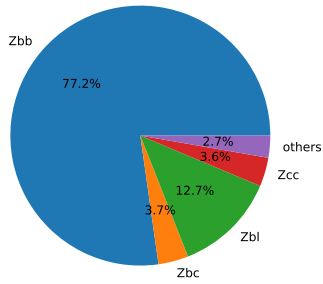
As the tagging performance is different w.r.t the flavour combination for the large- R jets, there is a further study on the flavour fraction of the Whf and Zhf in SR and CR respectively as shown in Fig 5.18. The flavour fractions is almost identical between SR and CR, so one SF for all flavours is enough. Meanwhile the modelling uncertainty on the relative ratio between the $Z+bb$ and other heavy flavours (like $Z+bc$) could provide some freedom to accommodate this difference.

5.7.5 Nuisance Parameters

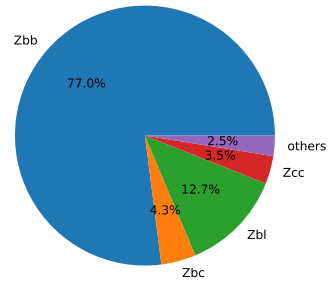
The nuisance parameters are set for each systematic source as described in Section 5.6. For theory uncertainty, three types of implementations are considered according to the impact from the variation of theory, such as normalization (cross-section of MC samples), shape of the m_{bb} distribution and the acceptance where events could be categorized into different region due to the uncertainty.

Several treatment of the nuisance parameters are performed to stabilize the fitting and reflect the real effect from the systematic uncertainty source, such as symmetrization, smoothing and pruning. All the processings are not tend to change the real impact of uncertainty thus through checks and validations are performed to ensure no artifact resulted. One example of the JET and Flavour Tagging systematics is shown in Fig. 5.19. The smoothing effect can

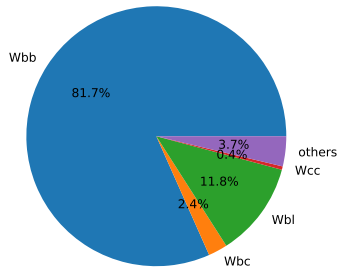
Flavour Fraction of Z+jets in 0L Merged Region



Flavour Fraction of Z+jets in 2L Merged Region



Flavour Fraction of W+jets in 0L Merged Region



Flavour Fraction of W+jets in 1L Merged Region

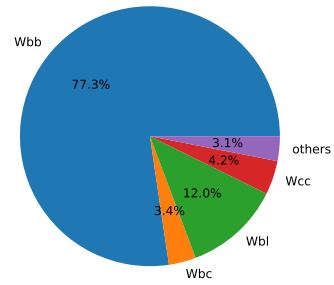


Figure 5.18 The flavour fraction of the large-R jet from Zhf (top) and Whf (bottom) comparison between SR (left) and 1L or 2L CR (right). Only the agreement for W+cc is not that perfect due to an insufficient statistics of W+cc in the SR merged regions, which is only 40 events.

be found from the comparison between the unsmoothed curves (dashed) and the smoothed curves (solid) and the fluctuation is removed.

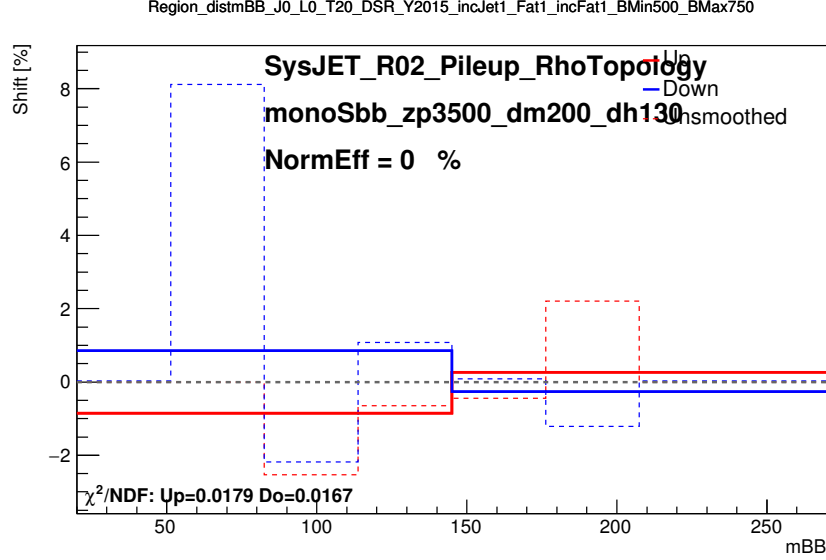


Figure 5.19 The variation in SR of one JET systematics for a signal process (Top). The dashed lines represent the systematics shape before the smoothing and the solid lines represent the systematic shape after smoothing.

The NPs as well as other parameters used in the subsequent study are indicated by the keywords summarized below, with detailed tables provided in Appendix A.5.

- Experimental Uncertainty (lepton and photon recon.): "EL"/"EG"/"MUON"/"TAUS";
- Experimental Uncertainty (jet and MET recon.): "JET"/"MET";
- Experimental Uncertainty (trigger and pileup): "METTrig" and "PRW";
- Theory Uncertainty (migration between MET Regions): "Sysmet";
- Theory Uncertainty (migration between Lepton regions): "Syslepton";
- Theory Uncertainty (variation of histogram shape): "SysZ", "SysW", "Systtbar", etc ("Sys"+process);
- Normalization (floating): "norm_" e.g. "norm_Zhf";
- Normalization (Gaussian prior): "..Norm" e.g. "VVNorm" and "LUMI"(luminosity);

5.8 Result and Interpretation

The results are described in this section. The pseudo-data (named Asimov dataset^[200]) which is made from the MC samples is firstly used as a final check of the analysis and no excess or "new physics" is expected to found in with this dataset. And after passing the check, the real data replace the pseudo-data and the search for dark Higgs is performed in the real ATLAS detector.

5.8.1 Results on Asimov dataset

5.8.1.1 Asimov fit: Post-fit discriminant

The distribution of the post-fit discriminant is shown for SR, 1-lepton CR and 2-lepton CR respectively, as shown in Figure 5.20, 5.21, and 5.22. A specific signal point with $m_s = 130$ GeV, $m_{Z'} = 3500$ GeV and $g_\chi = 1.0$ is shown. The signal is scaled in the SR by a certain factor in each region for visual convenience.

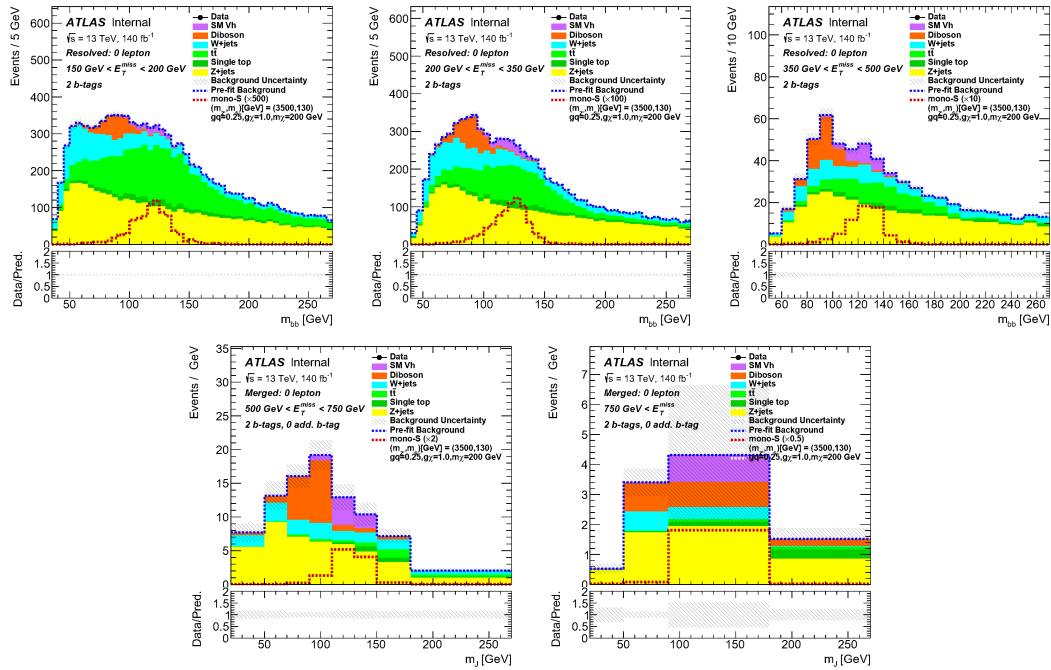


Figure 5.20 Post-fit mass distributions of Dark Higgs candidates in various E_T^{miss} regions within the 0-lepton channel. The uncertainty band incorporates both statistical errors and theoretical systematic uncertainties accounted for in the fit. To enhance visibility on the plot, the signal curve in each E_T^{miss} bin is scaled by a factor specified in the legend. This scaling factor corresponds to the ratio of signal to background.

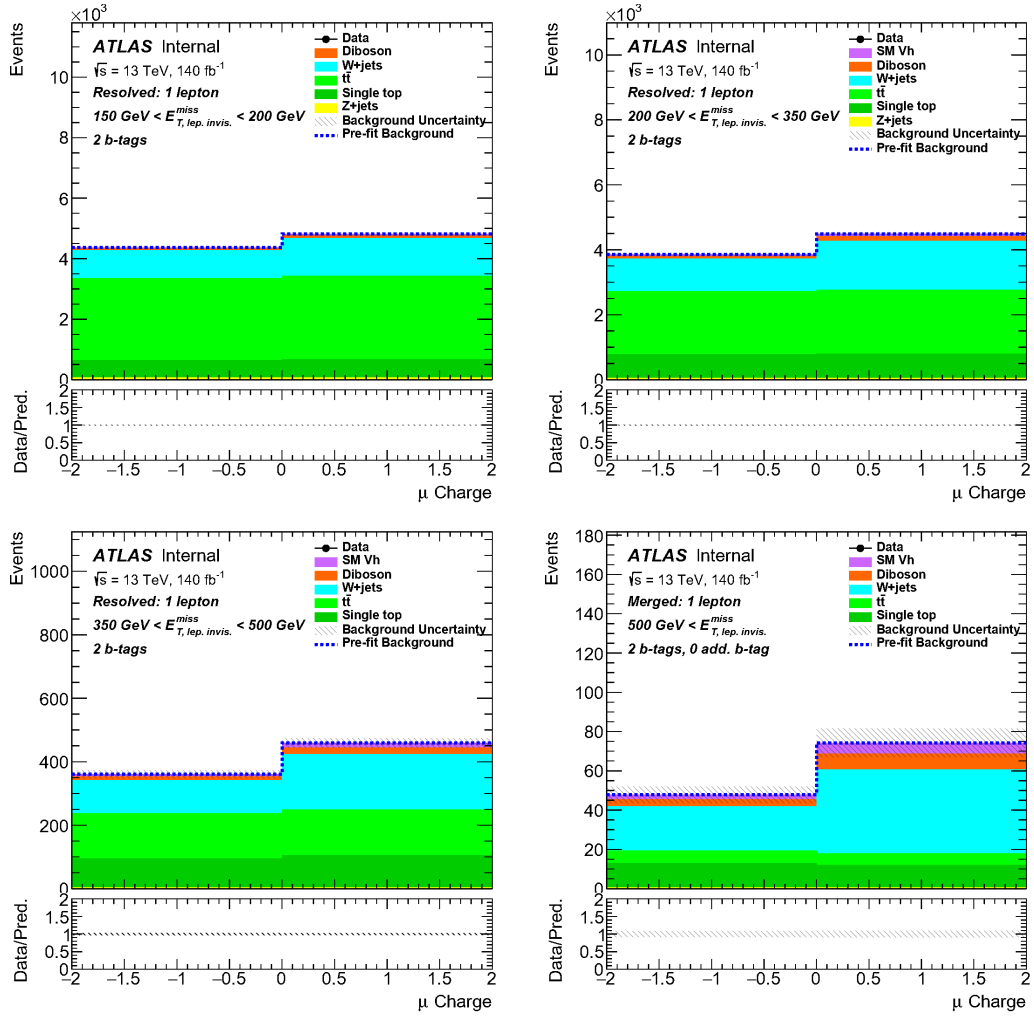


Figure 5.21 Post-fit distributions of the muon charge difference across various proxy E_T^{miss} regions in the 1-lepton channel. The uncertainty band includes statistical errors and theoretical systematic uncertainties incorporated in the fit.

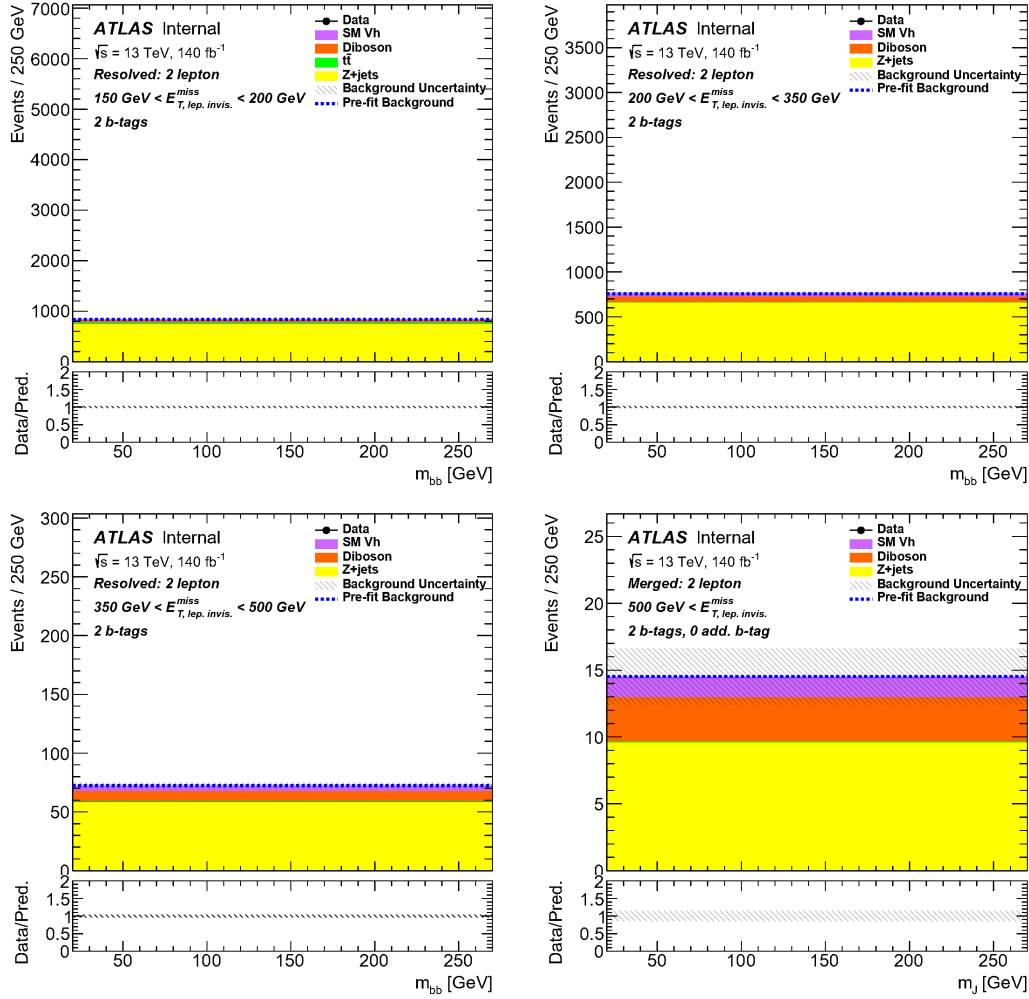


Figure 5.22 Post-fit yields across different proxy E_T^{miss} regions in the 2-lepton channel. The uncertainty band represents the statistical errors and theoretical systematic uncertainties accounted for in the fit.

5.8.1.2 Asimov fit: Rankings of the NP impact

The rankings of the NP are shown for three signals: 1) $m_s = 130$ GeV, $m_{Z'} = 3500$ GeV and $m_\chi = 200$, which is the default signal in fit studies 2) $m_s = 50$ GeV, $m_{Z'} = 3000$ GeV and $m_\chi = 200$ 3) $m_s = 150$ GeV, $m_{Z'} = 2500$ GeV and $m_\chi = 200$ in Fig. 5.23, 5.24 and 5.25 respectively. They reflect how large the impact from different uncertainty source (NP) should be on the parameter of interest (POI), here is the signal strength. Since pseudo-data is used, all the NPs should be fitted to the expected value and this study also serves as a good sanity check.

The background uncertainty with different m_J distribution has different impact on signal mass point. Z+jets process has a wide distribution of m_J thus affect almost all the mass point, while Diboson peaks around 90 GeV and VH around 125 GeV so the signal with close m_s is highly affected by its uncertainty.

The leading NP (*DXbb_Res_2b*) is the signal calibration uncertainties of *DXbb* tagging. It is directly applied on the signal ($m_s = 130$), Diboson and SM VHbb process as the leading large- R there are basically originated from similar decay topology. It is followed by the uncertainties on the main background: W+jets, diboson, VHbb, and Z+jets, also the experimental systematics of JES.

5.8.1.3 Asimov fit: Pull and constraint of the NP

The NP pulls study checks the how the pull of NP and how the constraint of prior is preferred by the data. Since the pseudo-data is used, there should be no any pulled NP. The process used in the analysis will have constrain power tighter than the prior of some NPs, so the slightly constrained ones are expected even with the pseudo-data. For example the nominal MC will prefer the generator it is generated and the uncertainty compared to alternative generator is generally large and constrained by the fitting.

The NP pulls are shown here in the categories of following and the expected behavior is concluded.

- b-tagging as in Fig 5.26;
- relative acceptance as in Fig 5.27;
- small-R jet (top) and input jet for the Re-clustered Large-R jet as in Fig 5.28;
- normalization as in Fig. 5.29;
- ttbar and single top processes and the E_T^{miss} as in Fig 5.30.

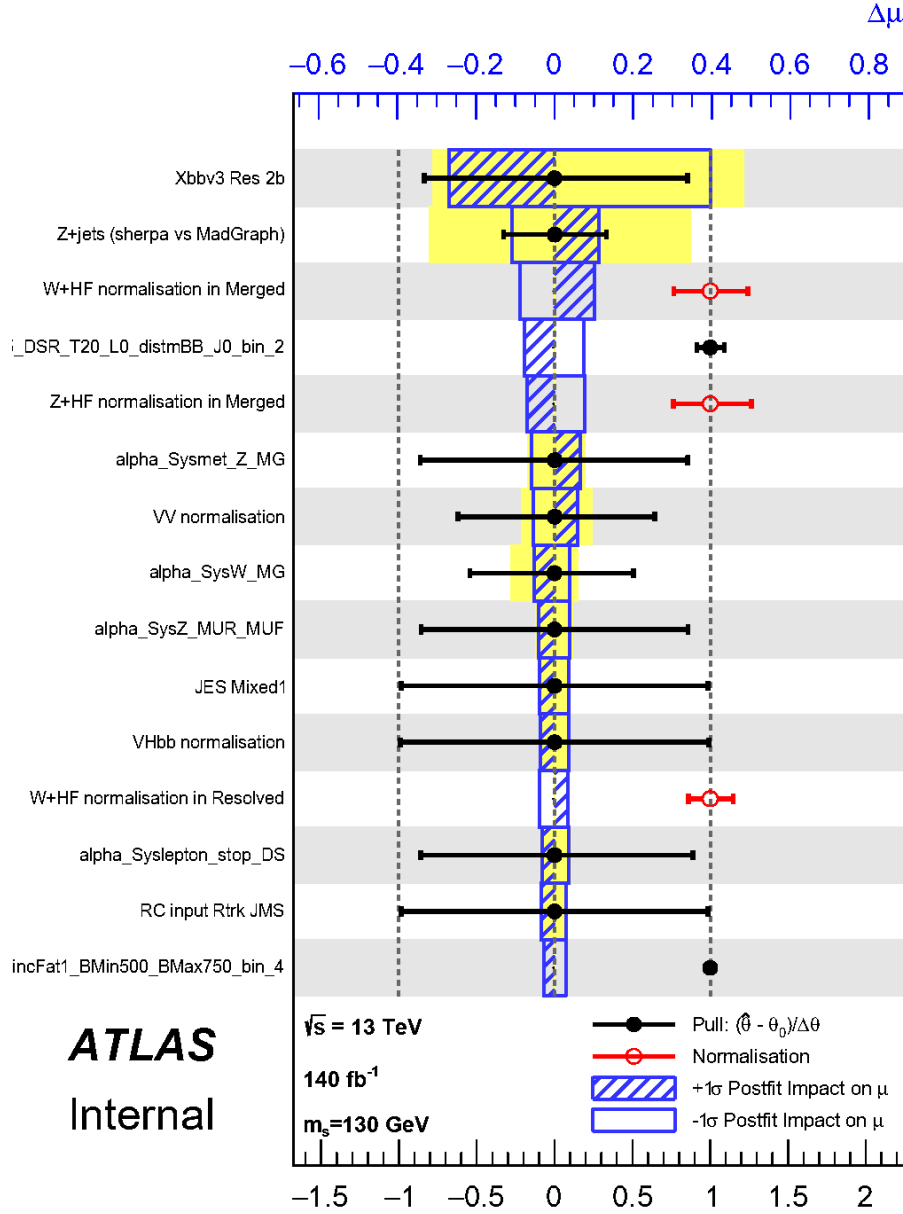


Figure 5.23 NP rankings on the signal strength of a specific signal point with $m_s = 130$ GeV, $m_{Z'} = 3500$ GeV and $g_\chi = 1.0$ is shown. The floating normalisation is colored in red. Since this is the asimov fit, the best fitted value of such NPs is 1. Gamma NPs, which account for the limited statistics of MC events in each histogram bin, are labeled with the suffix "_bin_n", with a nominal value of 1. Yellow band represents the prefit impact.

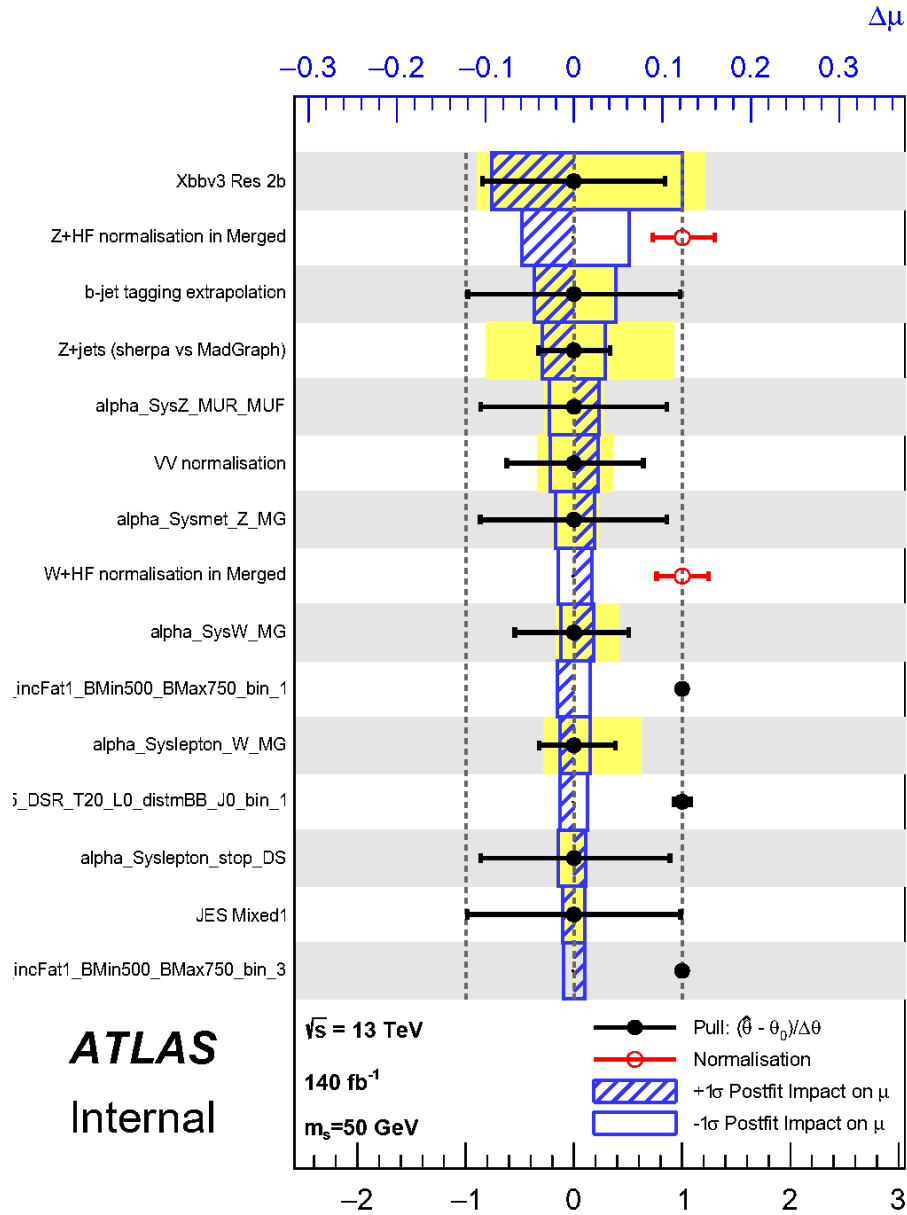


Figure 5.24 NP rankings on the signal strength of a specific signal point with $m_s = 50$ GeV, $m_{Z'} = 3000$ GeV and $g_\chi = 1.0$ is shown. The floating normalisation is colored in red. Since this is the asimov fit, the best fitted value of such NPs is 1. Gamma NPs, which account for the limited statistics of MC events in each histogram bin, are labeled with the suffix "_bin_n", with a nominal value of 1. Yellow band represents the prefit impact.

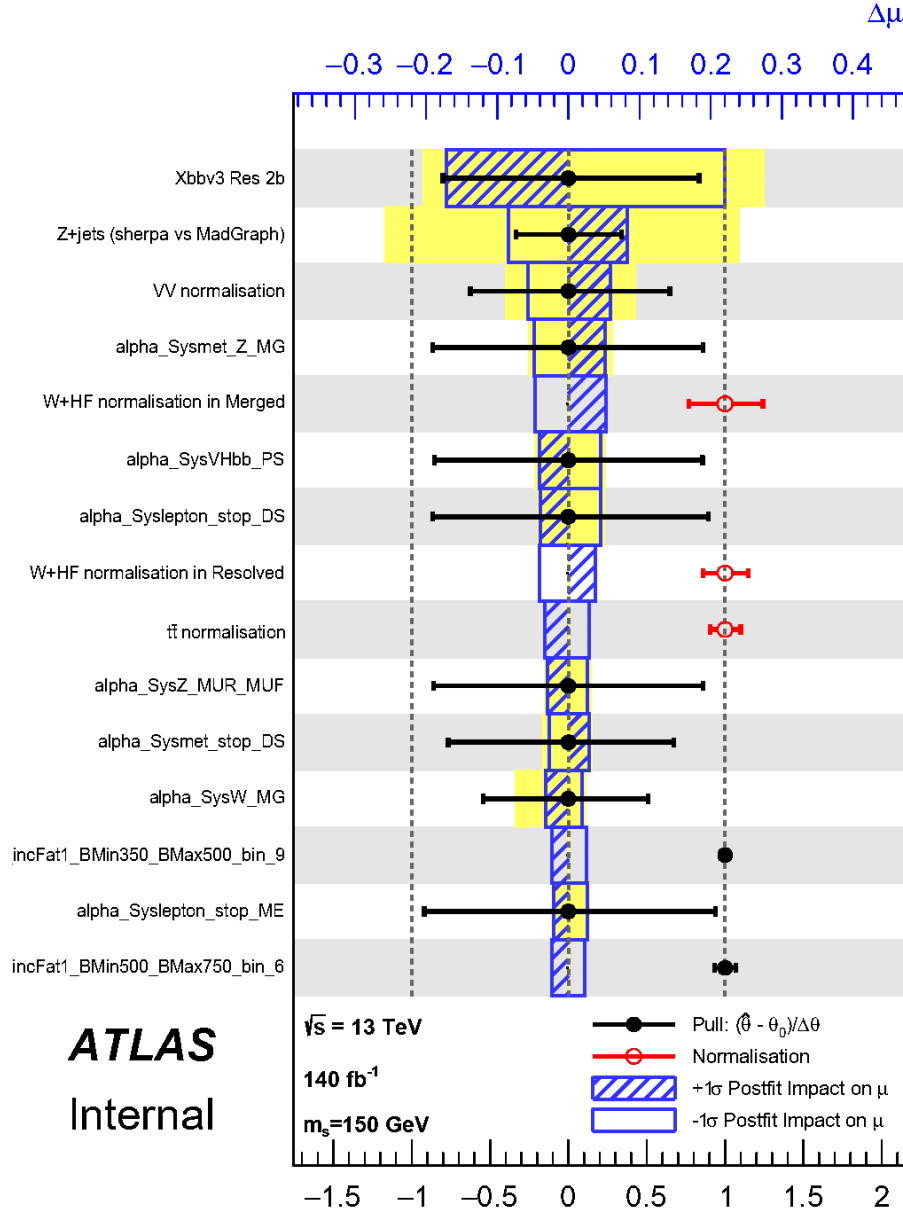


Figure 5.25 NP rankings on the signal strength of a specific signal point with $m_s = 150$ GeV, $m_{Z'} = 2500$ GeV and $g_\chi = 1.0$ is shown. The floating normalisation is colored in red. Since this is the asimov fit, the best fitted value of such NPs is 1. Gamma NPs, which account for the limited statistics of MC events in each histogram bin, are labeled with the suffix "_bin_n", with a nominal value of 1. Yellow band represents the prefit impact.

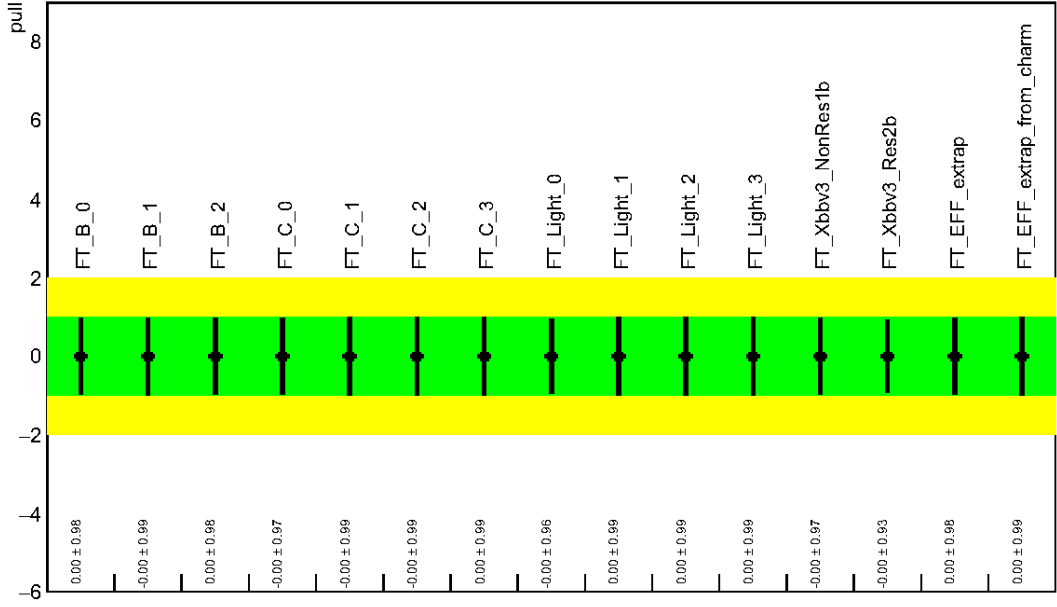


Figure 5.26 NP pulls for the systematics related to the b-tagging.

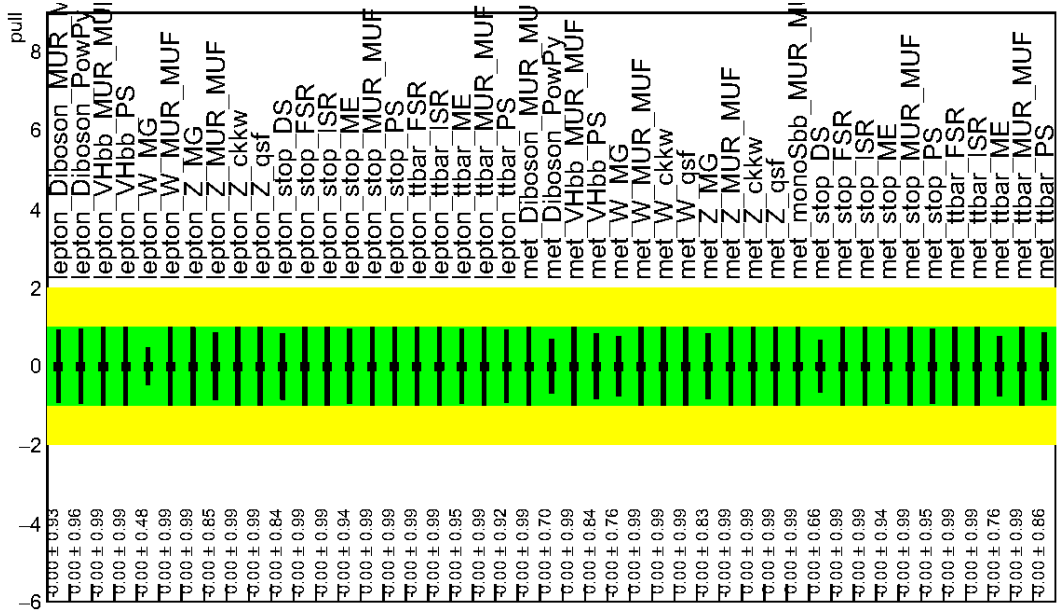


Figure 5.27 NP pulls for the systematics related to the region migration effect.

5.8.1.4 Asimov fit: correlation of the NP

The correlation between NPs infers the physics behind the processes and the systematic uncertainties. The check of NP correlation is vital to understand the analysis with large

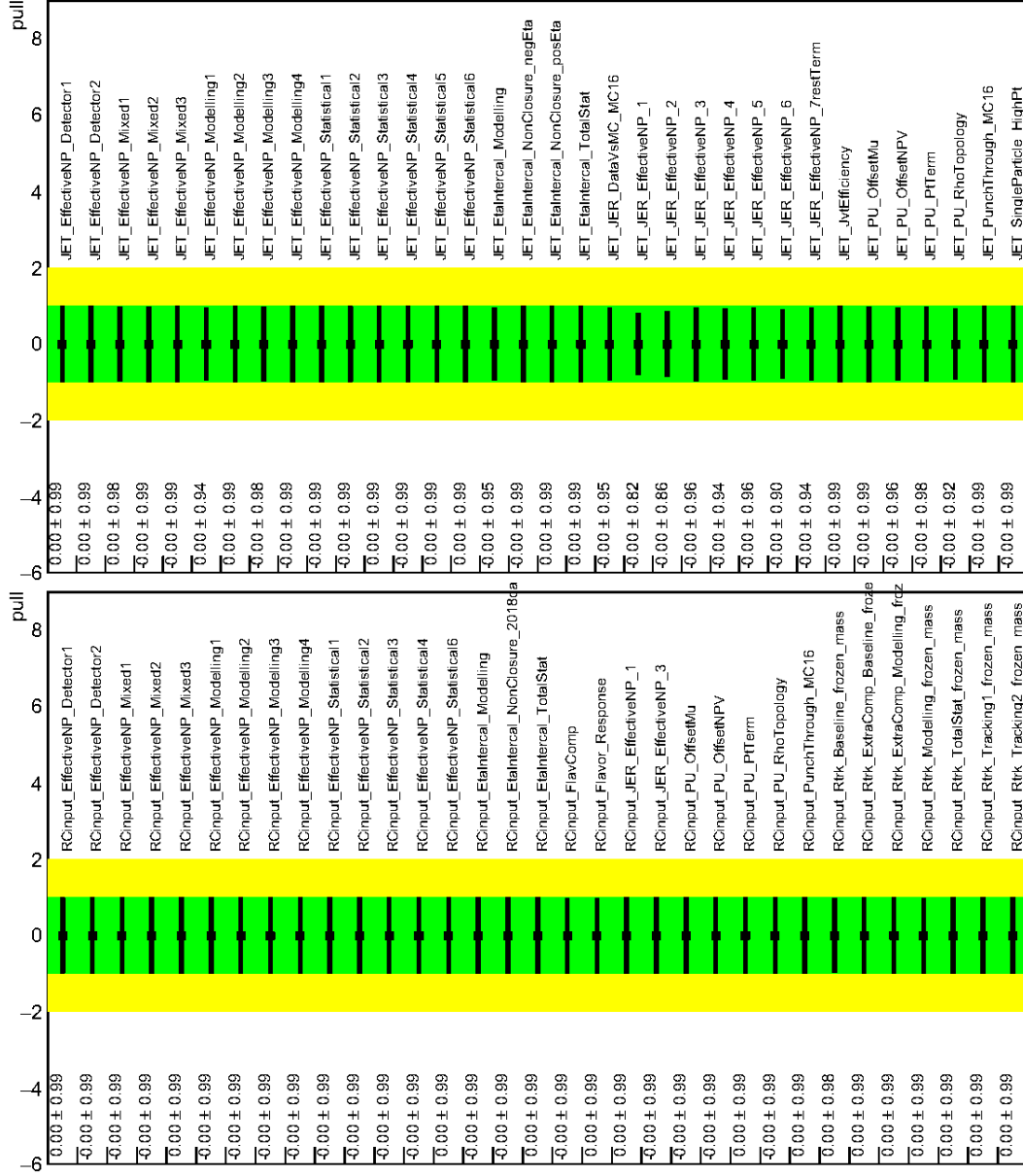


Figure 5.28 NP pulls for the systematics related to small-R jet (top) and input jet for the Re-clustered Large-R jet (bottom).

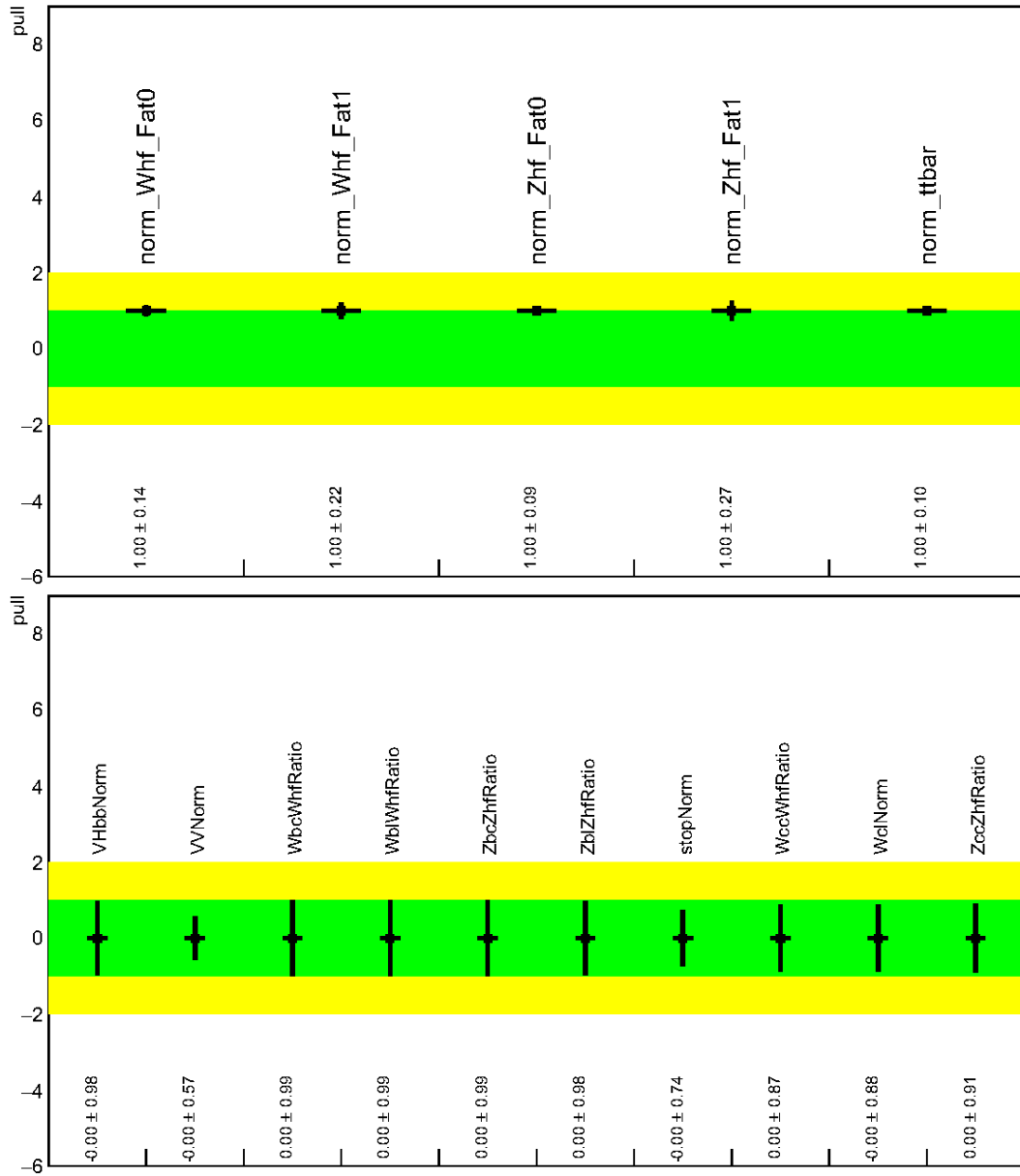


Figure 5.29 NP pulls for the systematics related to floating normalization for Zhf and Whf in resolved or merged regions and $ttbar$ (top) and normalization of the rest backgrounds (bottom). For the top plot, they are all NP for floating normalization, no priori sets on them. "Fat0" and "Fat1" represent the normalization in resolved or merged regions for W +jets and Z +jets respectively. Value of 1 means the fit prefers the normalisation from the prediction. Since this is the asimov fit, so the postfit values are still 1. In the fit model, the priori on the norm. of diboson (VV) and single top (stop) are conservative, and the processes are sensitive in the fit model given the sizable contribution to the background, so there are some constrains on them.

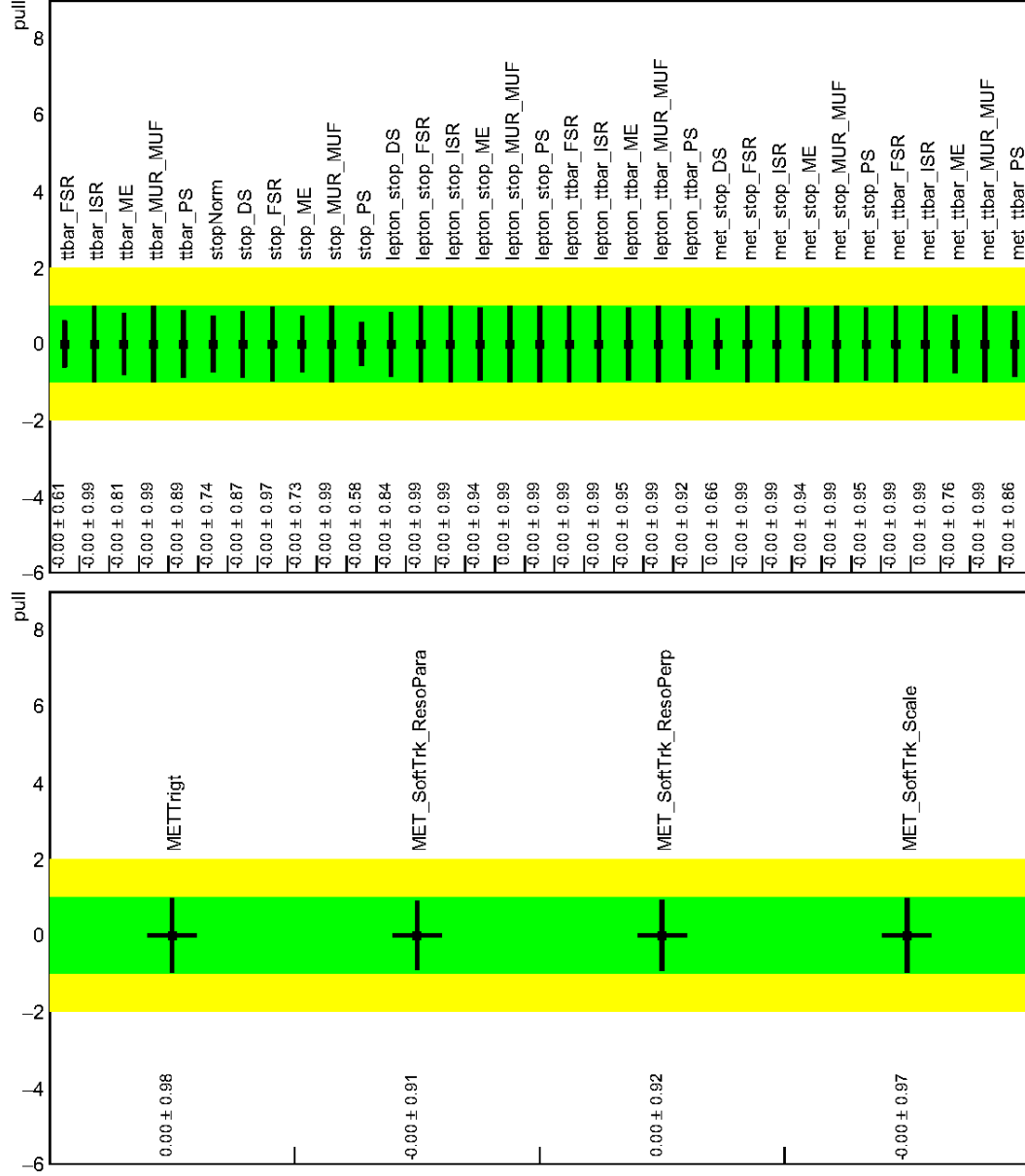


Figure 5.30 NP pulls for the systematics related to ttbar and single top processes (top) and the E_T^{miss} (bottom).

amount of systematic impact and ensure the consolidation of analysis.

The strong correlation and anti-correlation is found among the systematics applied on the same process, like the ones related to $t\bar{t}b\bar{a}r$, Z +jets and W +jets. And some cross processes correlation exists between W +jets and single top, $t\bar{t}b\bar{a}r$ (in 1 lepton regions), W +jets and Z +jets (in signal regions) due to the indirect impact such as two process are highly correlated if the sum is constrained by one region. The results are shown in the Fig. 5.31 following with the detailed study in Appendix A.6

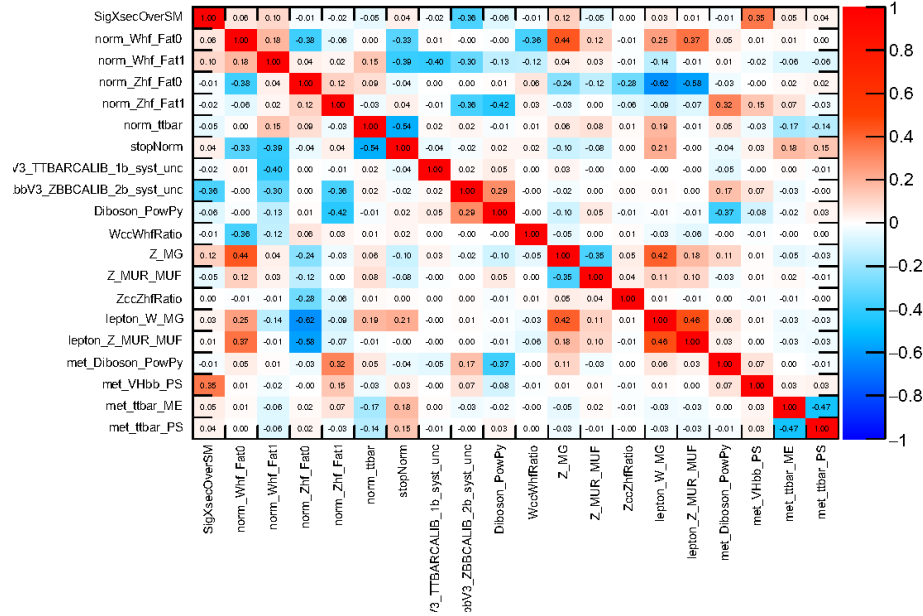


Figure 5.31 Correlation matrix for high correlation NPs. High correlation means the NP has the correlation above 0.25 with at least one other NP.

5.8.1.5 Asimov fit: Limits and Contour

The limit setting with the method mentioned in Section 5.7 on the pseudo-data yields the *expected* result which reflects the optimal sensitivity assuming the data is well described by the known SM simulation. The expected limit at 95% C.L. with the uncertainty is obtained with the available signal samples for all interpretation schemes. The expected limits and exclusion contours which introplate the tested points are shown as the left figures in Figures 5.32, 5.33 and 5.34 for interpretation schemes 1, 2 and 3 as described in Section 5.2 respectively.

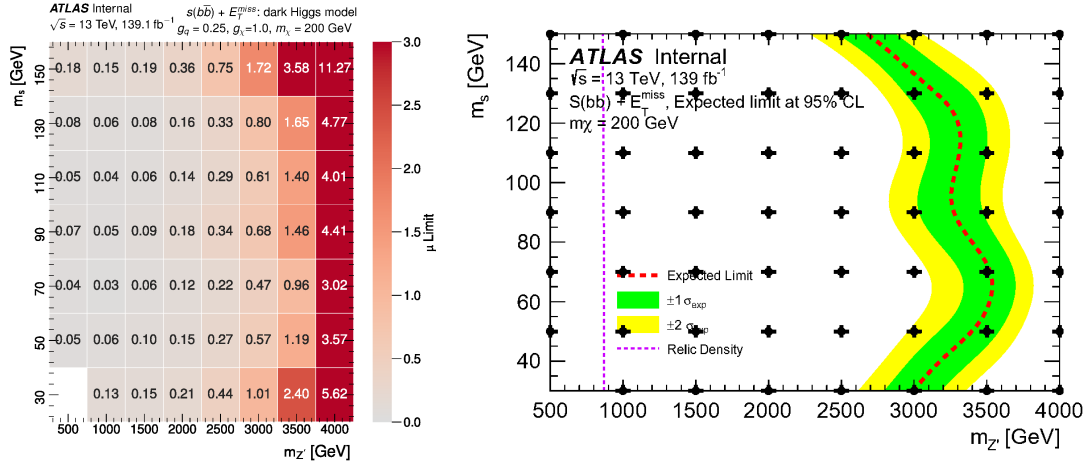


Figure 5.32 The expected limit (left) and exclusion contour (right) for interpretation strategy 1: m_s vs $m_{Z'}$ with $m_\chi = 200\text{GeV}$ and $g_\chi = 1.0$. The black crosses represent the signal points used in the search. The left area of the red dashed line is excluded. The pink dashed line corresponds to the signal parameter values that are consistent with a DM density of $\Omega h^2 = 0.12$ and a standard thermal history, as computed in MadDM^[155], and the parameter space in the right side is constrained by the relic density.

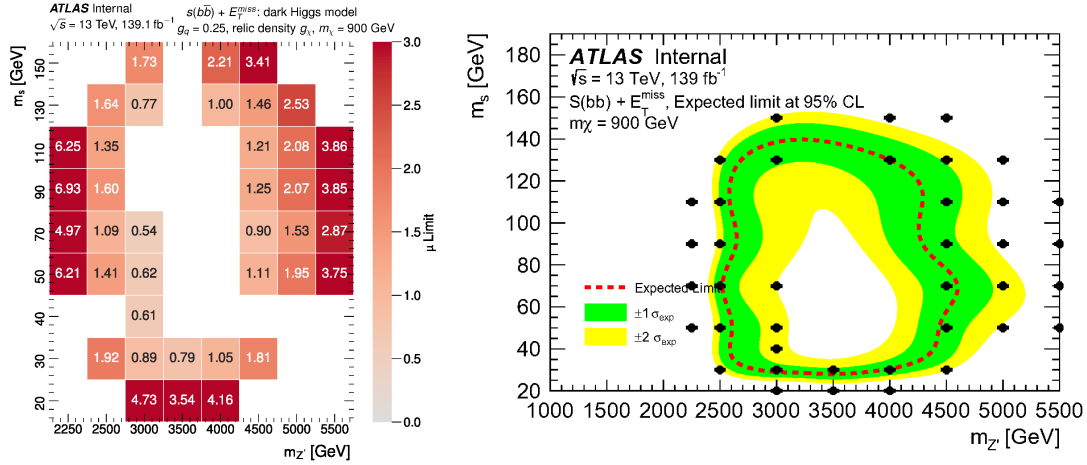


Figure 5.33 The expected limit (left) and exclusion contour (right) for interpretation strategy 2: m_s vs $m_{Z'}$ with $m_\chi = 2700\text{GeV}$ and g_χ value compatible with the relic density. The black crosses represent the signal points used in the calculation. The inner area of the red dashed contour is excluded by current analysis.

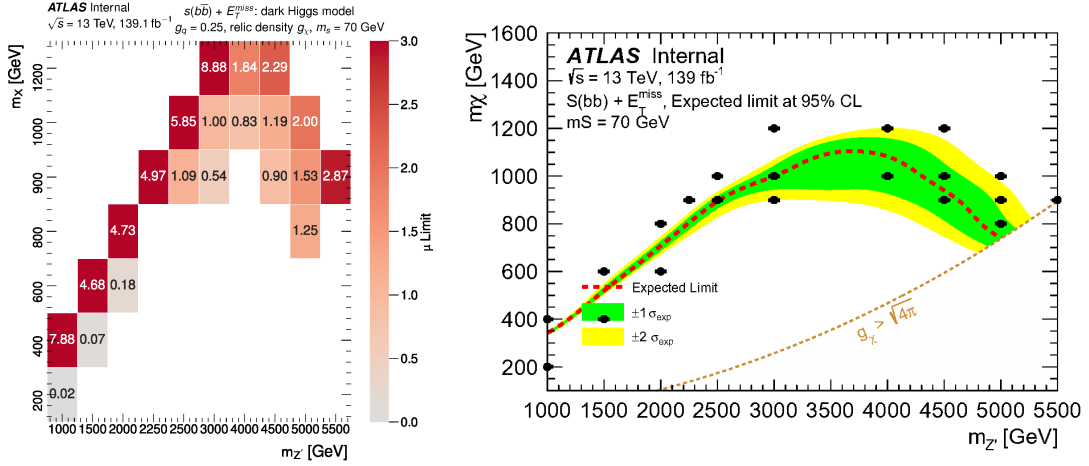


Figure 5.34 The expected limit (left) and exclusion contour (right) for interpretation strategy 3: m_χ vs $m_{\chi'}$ with $m_s = 70\text{ GeV}$ and g_χ value compatible with the relic density. The black crosses represent the signal points used in the calculation. The area below the red dashed line is excluded by current analysis. The dashed line in the bottom right shows the limit of the parameters in the perturbative calculation.

5.8.2 Results on Data

The result of the search for dark Higgs boson decaying into $b\bar{b}$ on the real data is presented as following.

The fitting converge well across all the analysis regions on the data and the distribution of the post-fit yield and discriminant for SR, 1-lepton CR and 2-lepton CR respectively are shown in Figure 5.35 and 5.36.

The similar checks as studied for the Asimov dataset are performed, including NP ranking, pulls, and correlation studies.

The NPs ranking is depicted in Figures 5.37, 5.38, and 5.39, respectively. These signals span a wide range of cross-sections, so the NP impacts are scaled differently, as indicated on the top axes of the figures.

Since the background templates exhibit m_J -dependent shapes—e.g., Z+jets dominate across the full range, Diboson contributions peak around 90 GeV, and VH contributions dominate near 125 GeV—the top-ranking NPs vary with the signal m_s . For example, the third signal is more sensitive to VH backgrounds than the others.

The leading NP (*Xbbv3_Res_2b*) corresponds to Xbbv3 tagging calibration uncertainties derived from the $Z \rightarrow b\bar{b}$ calibration. This uncertainty directly affects the signal ($m_s = 130$

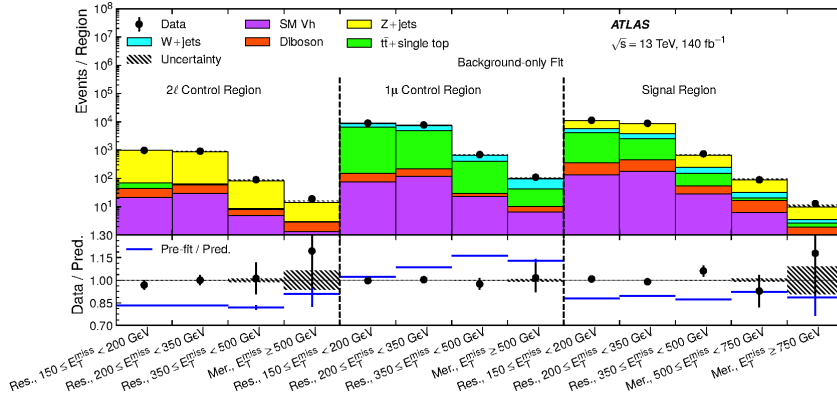


Figure 5.35 Data and predicted SM background yields following a simultaneous background-only fit across each resolved (Res.) and merged (Mer.) SR and CR E_T^{miss} category. The lower panel displays the ratio of data to the SM expectation, with lines representing the ratios of pre-fit to post-fit background predictions. The shaded regions indicate the total uncertainty in the background predictions.

GeV), Diboson, and SM VHbb processes. Following this are uncertainties associated with the main backgrounds: W+jets, Diboson, VHbb, and Z+jets, as well as experimental systematics, particularly JES.

The NP pulls are shown in the following figures following same categorization as the study with Asimov data: Fig. 5.40, 5.41, 5.42, 5.43, 5.44.

The relative importance of impact from different uncertainty source is summarized in Table 5.11 where clearly the large impact from normalization and modelling of Z+jets process, $t\bar{t}$ process and b-tagging are shown, as well as the statistical uncertainty indicating the search is still limited by the lacking of data especially in high E_T^{miss} phase space. The large impact of the b-tagging accompany its powerful performance and the future development will further reduce the uncertainty to further boost the search sensitivity for DM.

As no significant excess of data is seen above the predicted yield of SM background processes, the exclusion contours at 95% confidence level (CL) for the dark Higgs model with $b\bar{b}$ final states is set. The results are presented in Fig. 5.47 and dark Higgs boson with m_s below 150 GeV is thoroughly serched.

In the scenario 1, the $m_{Z'}$ is excluded up to 3.4 TeV with fixed coupling and 200 GeV DM particle. This well completes the searches for high mass dark Higgs^[153-154] and extends the excluded mass range down to 30 GeV as shown in Fig. 5.48. The comparsion is performed

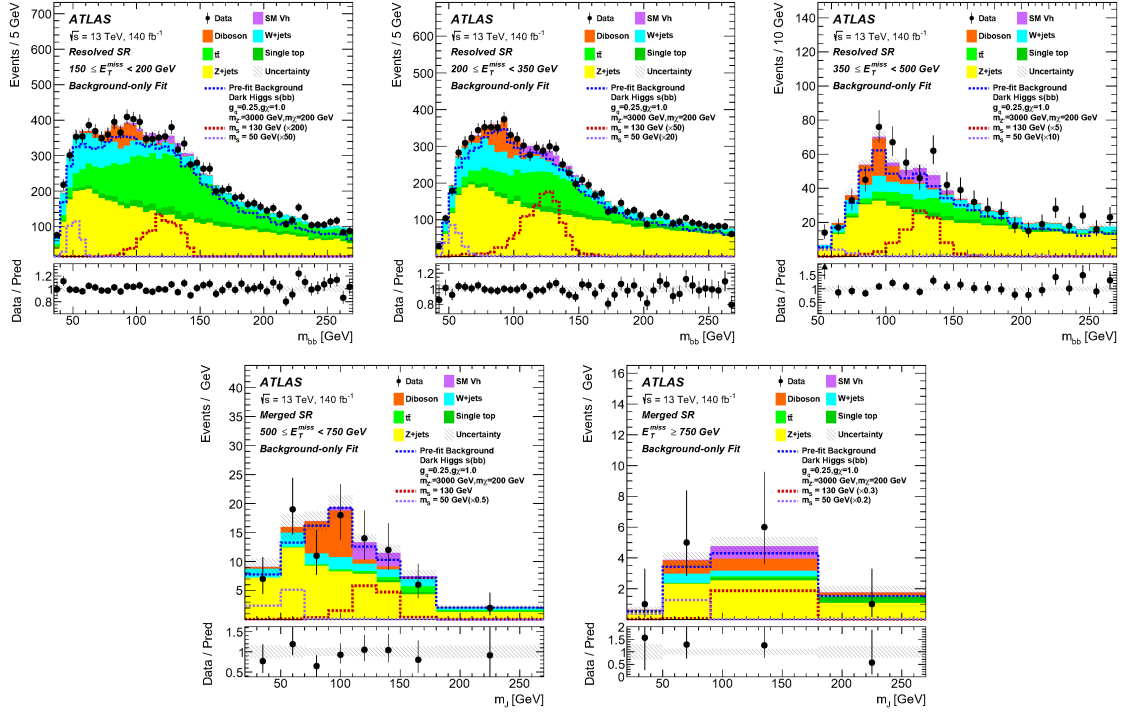


Figure 5.36 The m_{bb} distributions for data and SM expectations in the different E_T^{miss} regions for the resolved (top row) and merged (bottom row) topologies after a background-only simultaneous fit to data. The shaded area represents the total uncertainty in the predicted yields. Two signal distributions are overlaid, multiplied in each E_T^{miss} region by a scale factor indicated in the legend for visibility. The lower panels show the ratios of the data to the MC predictions.

with recast a previous analysis with similar phase space^[203] without the novel techniques and optimization studied in this search and the large improvement is clear to see, as shown in Fig. 5.46.

In scenario 2 and 3, relic density compatible parameters are used as described in Section 5.2 and with 900 GeV DM particle, the $m_{Z'}$ is excluded between 2.5 TeV and 4.5 TeV and the lower $m_{Z'}$ is mainly constrained by the relic abundance requirement which leads to a very small coupling and cross-section to be further excluded at collider. For the most sensitive case where the dark Higgs mass is 70 GeV, the $m_{Z'}$ is excluded up to perturbative theory limit with DM particle mass up to 700 GeV which shows again the good sensitivity in this search channel and the advancement from novel methods such the $DXbb$ boosted tagging.

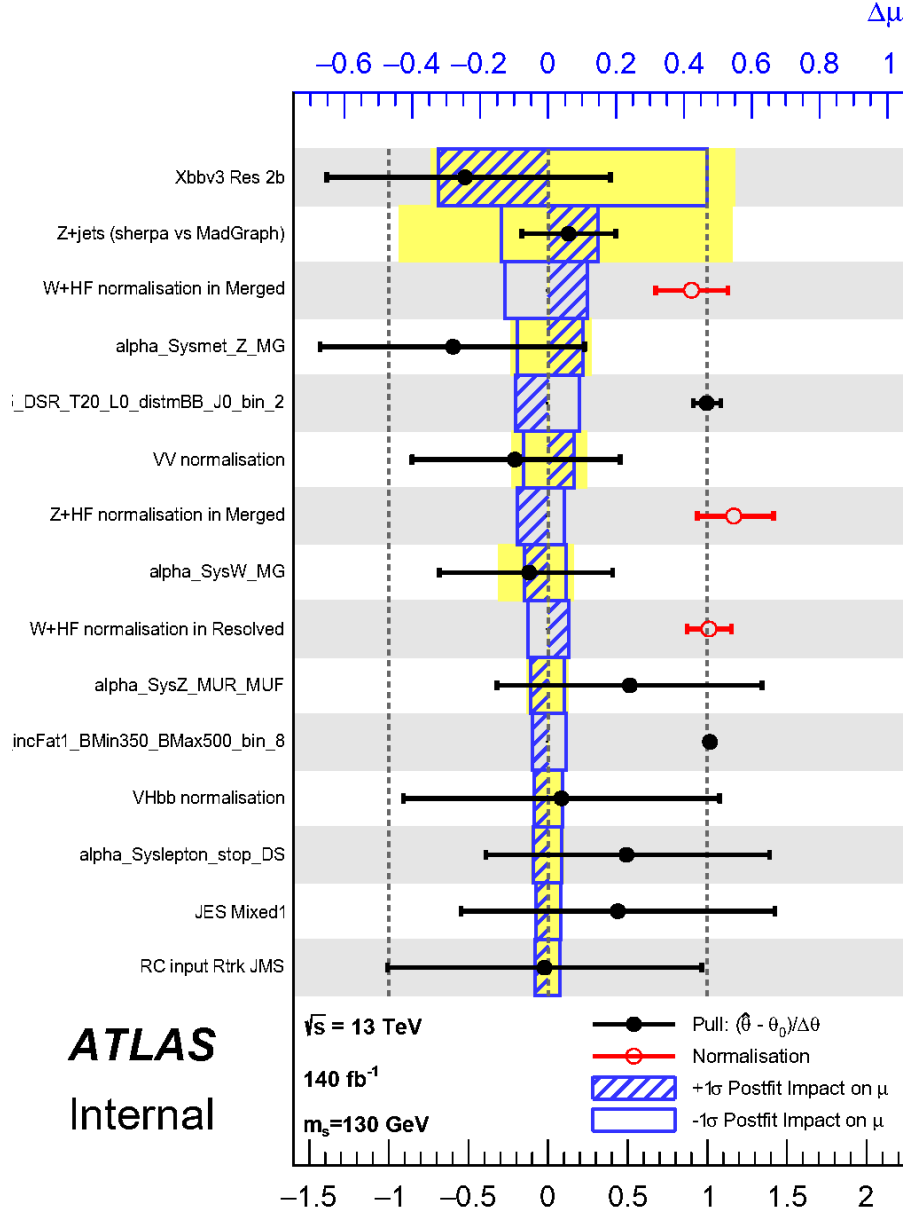


Figure 5.37 NP rankings for the signal strength of a specific signal point with $m_s = 130$ GeV, $m_{Z'} = 3500$ GeV, and $g_\chi = 1.0$. The floating normalization parameters are highlighted in red. Gamma NPs, which account for the limited statistics of MC events in each histogram bin, are labeled with the suffix "_bin_n", with a prefit value of 1. Yellow band represents the prefit impact.

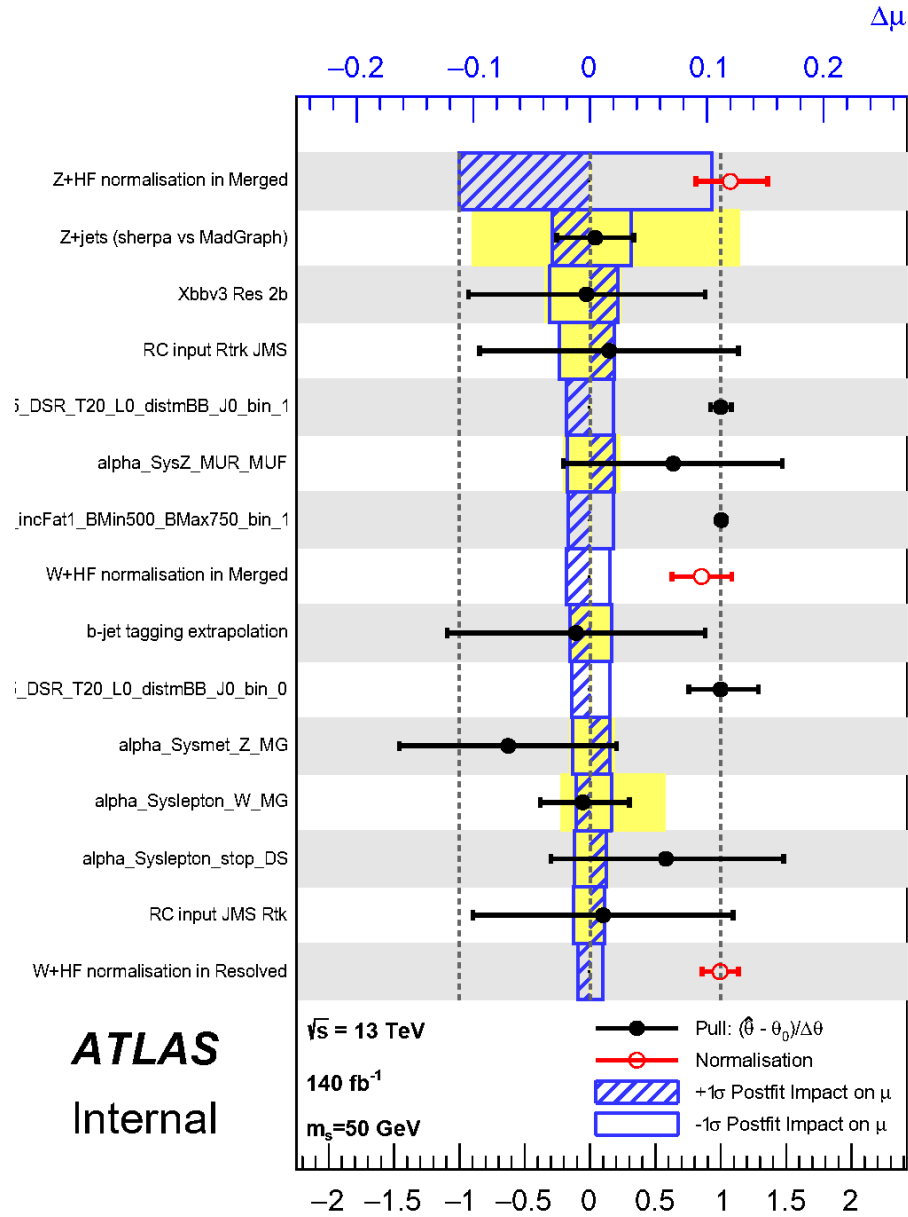


Figure 5.38 NP rankings for the signal strength of a specific signal point with $m_s = 50 \text{ GeV}$, $m_{Z'} = 3000 \text{ GeV}$, and $g_\chi = 1.0$. The floating normalization parameters are highlighted in red. Gamma NPs, which account for the limited statistics of MC events in each histogram bin, are labeled with the suffix "_bin_n", with a prefit value of 1. Yellow band represents the prefit impact.

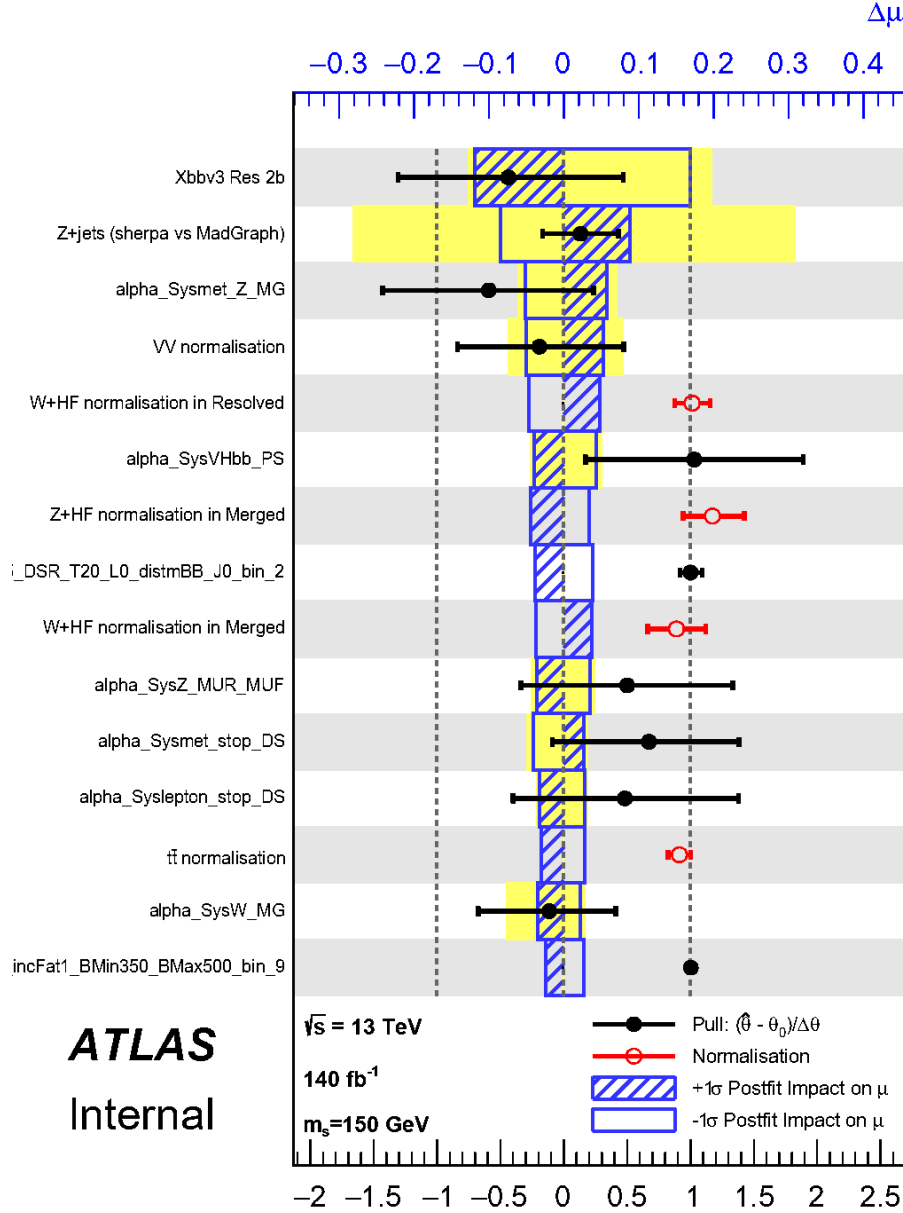


Figure 5.39 NP rankings for the signal strength of a specific signal point with $m_s = 150 \text{ GeV}$, $m_{Z'} = 2500 \text{ GeV}$, and $g_\chi = 1.0$. The floating normalization parameters are highlighted in red. Gamma NPs, which account for the limited statistics of MC events in each histogram bin, are labeled with the suffix "_bin_n", with a prefit value of 1. Yellow band represents the prefit impact.

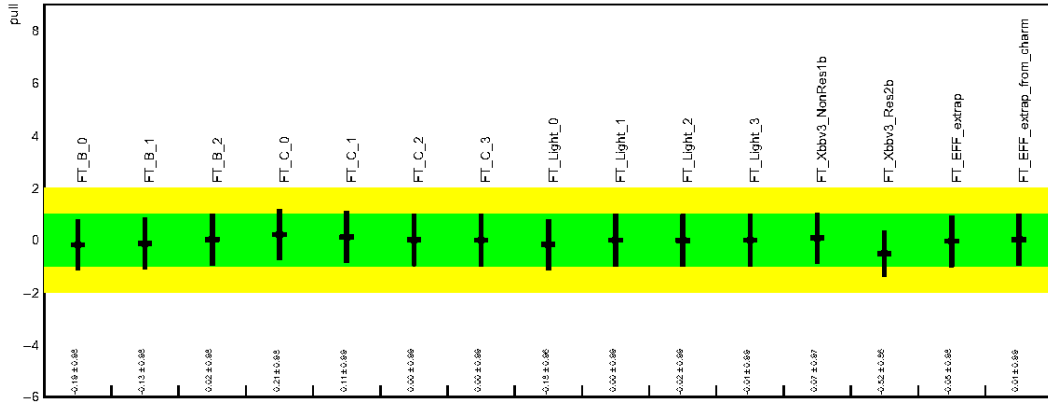


Figure 5.40 NP pulls for systematics related to b-tagging.

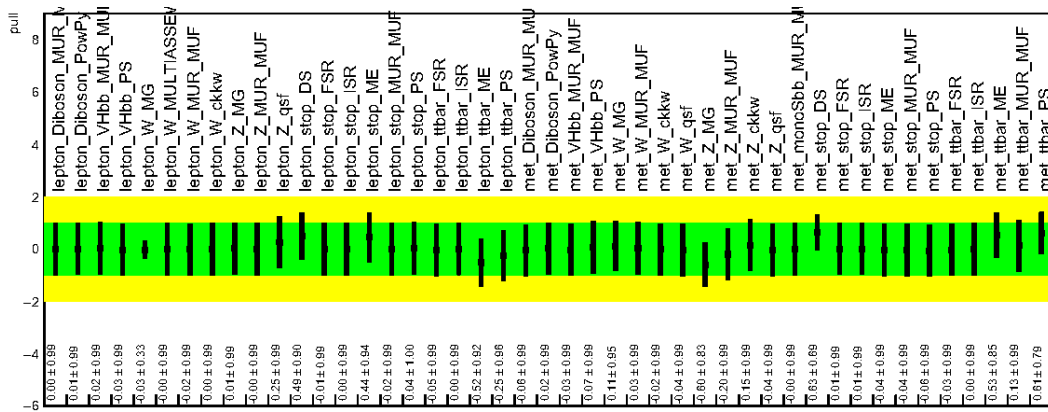


Figure 5.41 NP pulls for systematics related to relative acceptance.

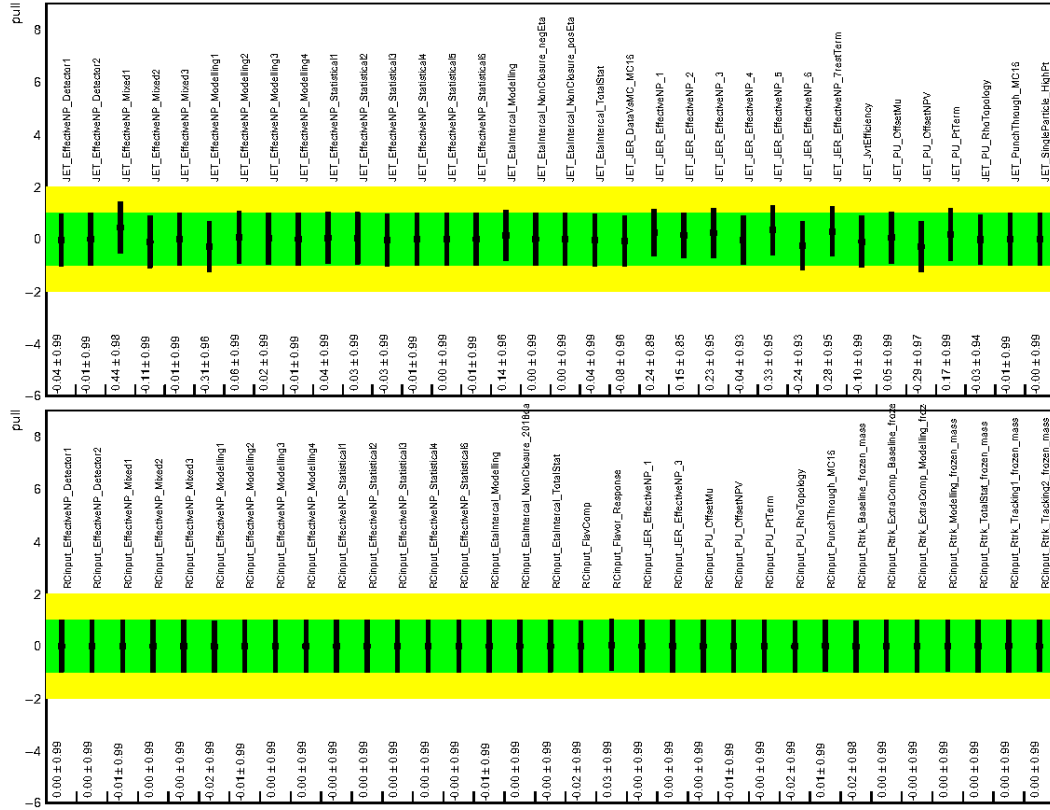


Figure 5.42 NP pulls for systematics related to small-R jets (top) and reclustered large-R jets (bottom).

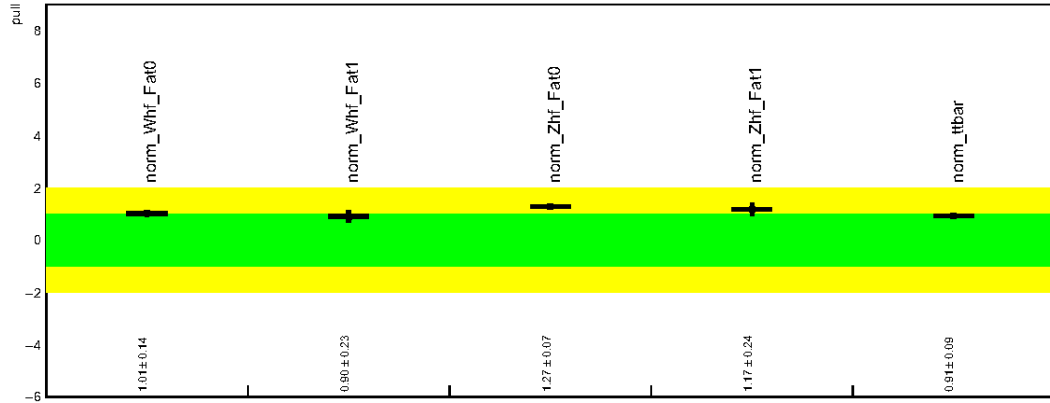


Figure 5.43 NP pulls for systematics related to floating normalization for W/Z+HF in resolved or merged regions and $t\bar{t}$. "Fat0" and "Fat1" represent the normalization in resolved or merged regions for W+jets and Z+jets, respectively. A value of 1 indicates that the fit aligns with the predicted normalization.

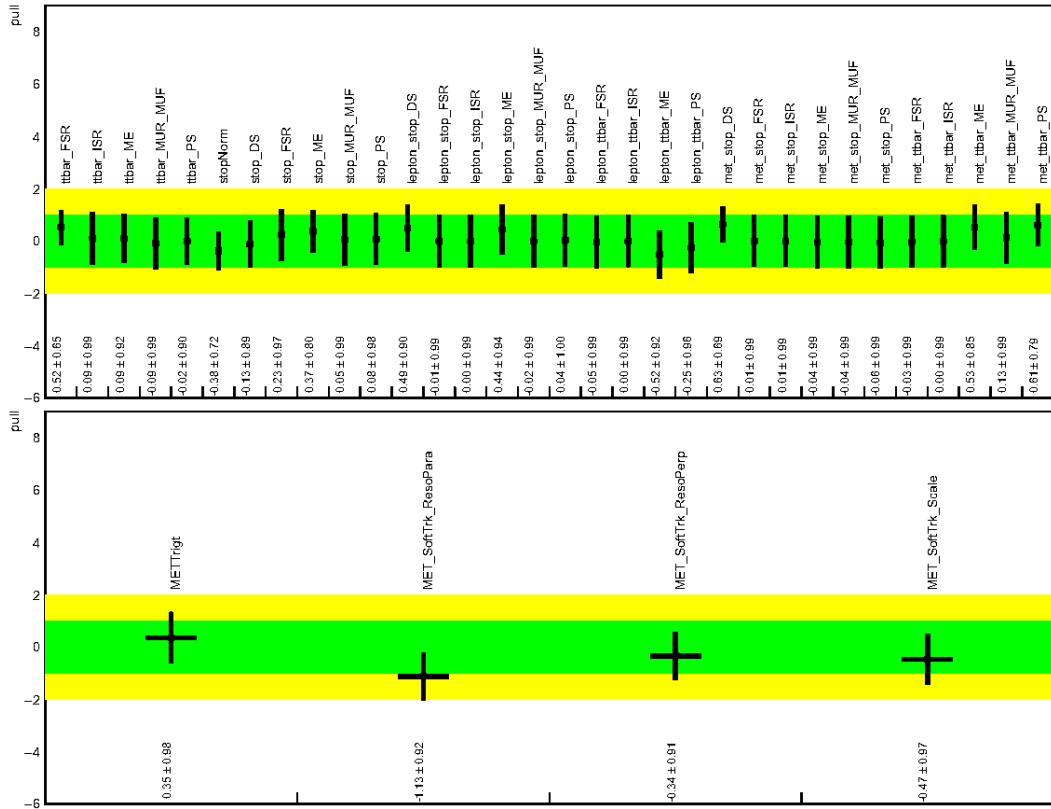


Figure 5.44 NP pulls for systematics related to $t\bar{t}$ and single top processes (top) and E_T^{miss} -related uncertainties (bottom).

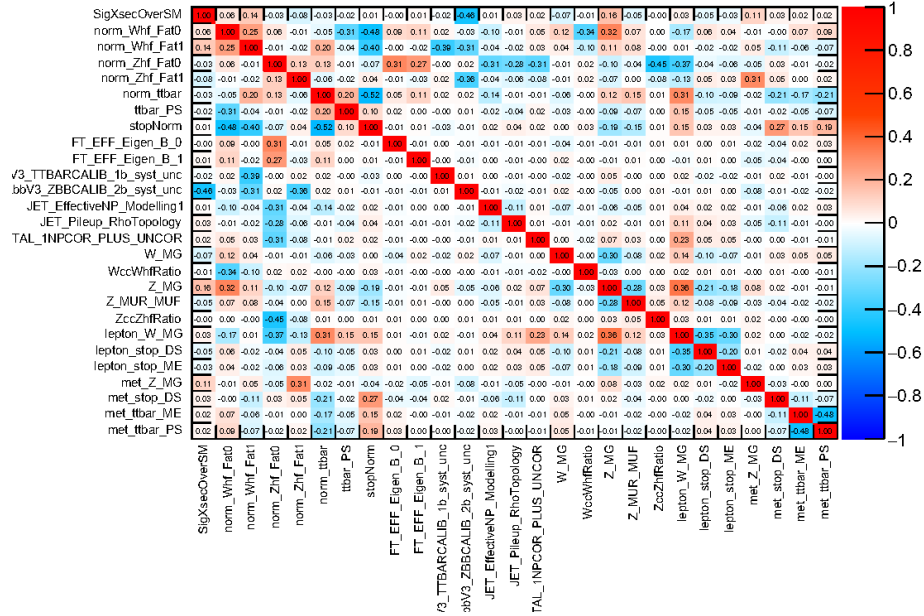


Figure 5.45 Correlation matrix for high-correlation NPs. High correlation refers to NPs with correlations above 0.25 with at least one other NP.

Table 5.11 Relative impact of the different sources of uncertainty on three selected signals in scenario 1: (a) $m_{Z'} = 3000$ GeV, $m_s = 50$ GeV, (b) $m_{Z'} = 3000$ GeV, $m_s = 130$ GeV and (c) $m_{Z'} = 2500$ GeV, $m_s = 150$ GeV.

Source of uncertainty	Fraction of total uncertainty [%]		
	(a)	(b)	(c)
Signal modeling	0	1	0
Z+jets normalization	41	11	11
W+jets normalization	8	13	13
$t\bar{t}$ normalization	1	7	8
Z+jets theory	16	24	25
W+jets theory	8	12	9
$t\bar{t}$ theory	3	8	11
Other background theory	10	16	22
MC statistics	15	17	18
Flavor tagging	18	47	37
Jet energy	3	7	11
Other experimental	2	4	3
Total systematic uncertainty	57	66	63
Data statistical uncertainty	82	75	77
Total uncertainty	100	100	100

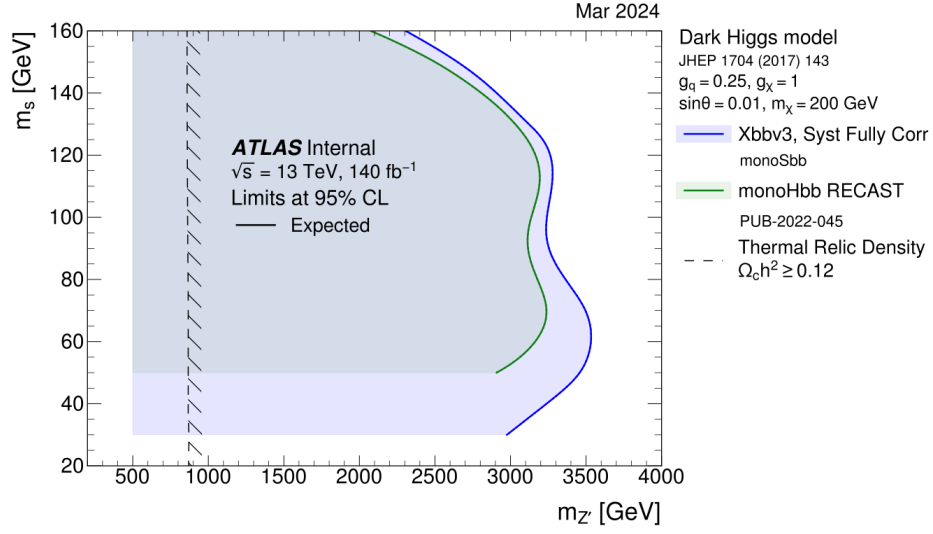


Figure 5.46 The exclusion curve on the dark Higgs model with 200 GeV DM particle compared to previous study. The improvement is mainly due to the optimized selection especially the b-tagging method, as well as the reclustering jet extend the mass range.

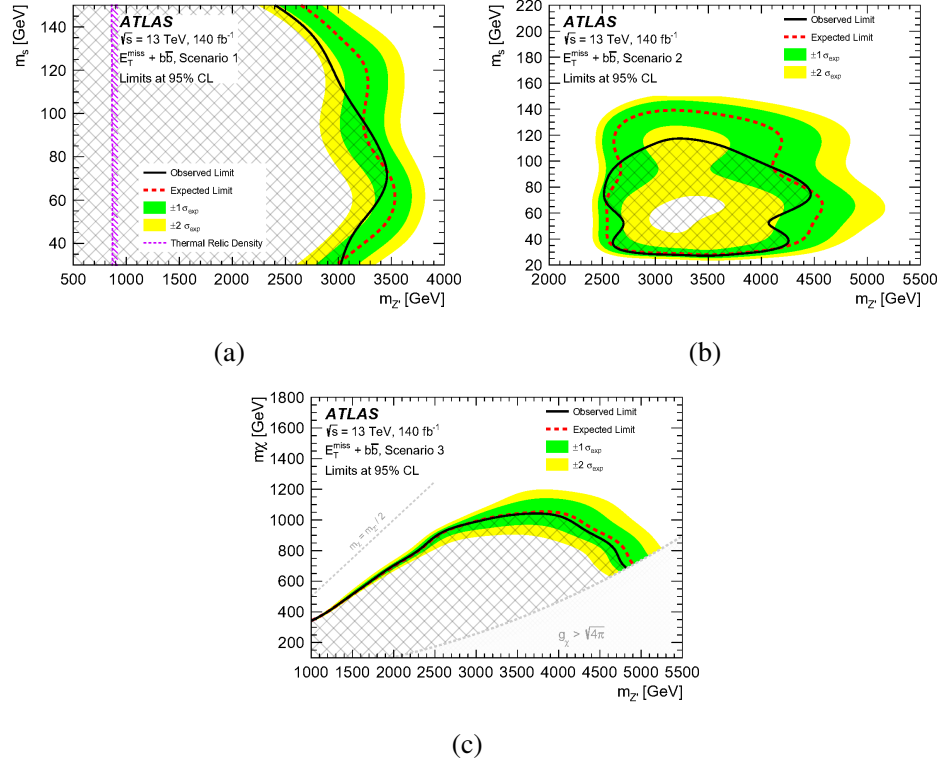


Figure 5.47 Observed (expected) exclusion regions at 95% CL for (a) scenario 1, (b) scenario 2 and (c) scenario 3. The $\pm 1\sigma$ ($\pm 2\sigma$) expected exclusion intervals are shown as the filled inner (outer) bands (a, b, c). The observed relic density is indicated with a dashed line for scenario 1 (a), with the diagonal lines indicating an overabundance of DM. The lower-right shaded area indicates the region beyond the Z' -DM coupling perturbative limit for scenario 3 (c).

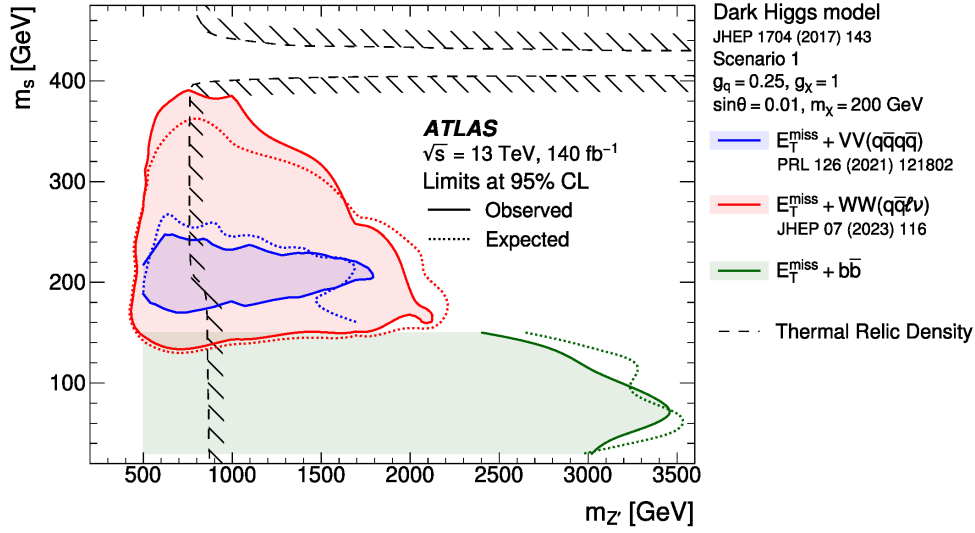


Figure 5.48 The completed exclusion curve on the dark Higgs model with 200 GeV DM particle and fixed coupling. The filled areas are excluded, with the open contours indicating regions not explored for a given signature. The black dashed line denotes the parameters which reproduce the relic density value from cosmology.

Chapter 6 Constrain the Dark Photon Model with Combination

6.1 Introduction

The dark matter could be completely neutral under the Standard Model (SM) fields, allowing it to evade all current intensive detection efforts. This has motivated the proposal of the dark photon, as discussed in detail in Section 2.2.4.

Several constraints on the dark photon have been provided using Run-2 data from pp collisions at a center-of-mass energy of 13 TeV by the CMS experiment. These include searches for Higgs boson events produced in association with a Z boson (ZH) with an integrated luminosity of 137 fb^{-1} ^[204], as well as via vector-boson fusion (VBF) production with 130 fb^{-1} ^[205]. A combination of these two searches has also been performed.

The ATLAS experiment has produced competitive results for both associated production with a Z boson (ZH)^[206] and vector-boson fusion (VBF)^[207]. Additionally, a reinterpretation of the ATLAS mono-photon results has been conducted in the context of searches for heavy Higgs bosons^[208].

A statistical combination of ATLAS results from different production channels—both Standard Model Higgs and heavy Higgs decaying into a photon and a massless dark photon—has been developed. This provides the most stringent constraints on the dark photon using collider experiment data.

6.2 Signal Model

The signal processes involved in this combination effort include the Standard Model (SM) Higgs boson and beyond the Standard Model (BSM) processes with a Higgs boson mass different from 125 GeV, decaying into a photon and an invisible dark photon (γ_d). Three production modes are considered: associated production with a Z boson (ZH), where both $q\bar{q} \rightarrow ZH$ and $gg \rightarrow ZH$ contribute to the total cross-section, gluon-gluon fusion (ggF), and vector boson fusion (VBF). The corresponding Feynman diagrams are shown in Figure 6.1 and Figure 6.2.

The signal samples are generated with a consistent setup for all model parameters except

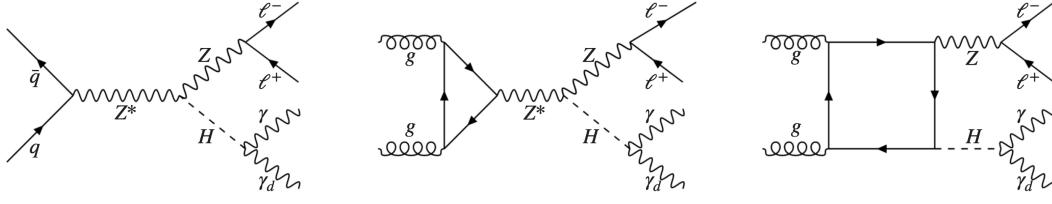


Figure 6.1 Feynman diagrams for $q\bar{q} \rightarrow ZH$ (left) and $gg \rightarrow ZH$ (middle and right) production modes.

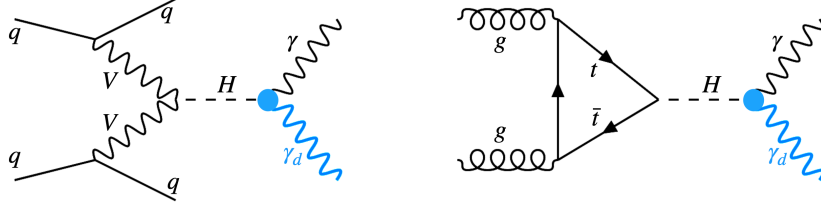


Figure 6.2 Feynman diagrams for $H \rightarrow \gamma\gamma_d$ for VBF (left) and ggF (right) production modes.

the mass of the Higgs boson. For the SM Higgs, the mass is set to 125 GeV, while for the BSM Higgs, it is allowed to vary and is coupled to the dark photon. The SM Higgs samples, along with their cross-section information, are detailed in Table 6.1, and the BSM samples are provided in Table 6.2 and Table 6.3.

Table 6.1 Configurations of the MC event generation for SM Higgs signal processes. The "ME Order" specifies the order of the perturbative calculation in the strong coupling constant. The tune denotes to the underlying-event tune applied to the parton shower.

Process	Generator	ME Order	Parton Shower	PDF	Tune	σ (pb)
$ggF, H \rightarrow \gamma\gamma_d$	POWHEG v2	NNLOPS	PYTHIA 8.244p3	PDF4LHC15	AZNLO	48.58
$VBF, H \rightarrow \gamma\gamma_d$	POWHEG v2	NLO	PYTHIA 8.244p3	CTEQ6L1	AZNLO	3.782
$ggZH \rightarrow \gamma\gamma_d$	POWHEG v2	NLO	PYTHIA 8.245	NNPDF3.0NNLO	AZNLO	0.761
$qqZH \rightarrow \gamma\gamma_d$	POWHEG v2	NLO	PYTHIA 8.245	NNPDF3.0NNLO	AZNLO.	0.123

6.3 Input Analyses And Orthogonality Check

The input analyses are briefly described in this section and detailed in previous work published in^[146,206-207] The selections for all three channels are summarized in Table 6.4.

The ZH analysis investigates Higgs production via associated production with a Z boson, where the Z decays leptonically. Selected events must have one photon with p_T larger than

Table 6.2 Configurations of the MC event generation for BSM Higgs signal processes. The "ME Order" specifies the order of the perturbative calculation in the strong coupling constant. The tune denotes to the underlying-event tune applied to the parton shower.

Process	Generator	ME Order	Parton Shower	PDF	Tune
$ggF, H \rightarrow \gamma\gamma_d$	POWHEG v2	NNLOPS	PYTHIA 8.306	CTEQ6L1	AZNLO
$VBF, H \rightarrow \gamma\gamma_d$ (used in Monophoton recast)	POWHEG v2	NLO	PYTHIA 8.306	CTEQ6L1	AZNLO
$VBF, H \rightarrow \gamma\gamma_d$ (used in VBF analysis)	POWHEG v2	NLO	PYTHIA 8.244p3	CTEQ6L1	AZNLO

Table 6.3 Signal grid and cross-section σ values of BSM Higgs boson for ggF and VBF processes.

m_H (GeV)	400	600	800	1000	1500	2000	2500	3000
σ_{ggF} (pb)	9.516	2.006	0.449	0.123	8.91×10^{-3}	1.08×10^{-3}	1.78×10^{-4}	3.50×10^{-5}
σ_{VBF} (pb)	0.758	0.327	0.162	0.087	2.28×10^{-2}	7.05×10^{-3}	2.36×10^{-3}	8.25×10^{-4}

25 GeV, two leptons with a reconstructed mass in the Z mass window (76-116 GeV), no more than two jets, and missing transverse energy (E_T^{miss}) greater than 600 GeV. The primary background originates from $VV\gamma$ processes (where V represents W or Z bosons) and fake E_T^{miss} , with the latter dominating. The fake E_T^{miss} background is estimated using a data-driven method, and its systematic uncertainty is a leading contributor to the overall uncertainty. The $VV\gamma$ background is estimated with Monte Carlo (MC) simulations and controlled using control regions (CRs).

To enhance the separation between real and fake E_T^{miss} , a multivariate technique based on a boosted decision tree (BDT)^[209] is employed, utilizing a combination of variables ranked by their importance. Among the key variables are E_T^{miss} significance (described in Section 3.4.5.3), the transverse mass $m_T(\gamma, E_T^{\text{miss}})$, which is defined as Eq. 6.1, and the invariant mass of leptons m_{ll} , the photon transverse momentum p_T^γ , and others.

$$m_T(\gamma, E_T^{\text{miss}}) = \sqrt{2E_T^\gamma E_T^{\text{miss}} \left[1 - \cos(\phi_\gamma - \phi_{E_T^{\text{miss}}}) \right]} \quad (6.1)$$

This method shows strong sensitivity in constraining the branching ratio of the SM Higgs

decaying into a photon and a dark photon, despite being statistically limited.

The *VBF* analysis targets events characterized by one photon, at least two VBF jets, zero leptons, and large E_T^{miss} . Events are triggered using E_T^{miss} triggers. The primary background sources are $W\gamma$, $Z\gamma$, and fake photons. The $V\gamma$ background is estimated and controlled using CRs, while fake photons, originating from jets or electrons, are estimated using data-driven methods. The systematic uncertainty from fake photons dominates the total uncertainty. This analysis is sensitive to a wide range of Higgs masses and dark photon couplings, covering both the SM Higgs and BSM Higgs scenarios.

The *mono- γ* recast uses results from a mono-photon analysis^[146] and reinterprets them in the context of the dark photon model, as the final states are similar. Events are triggered using a photon trigger with a high threshold of 140 GeV and are required to have no leptons, at most one jet with p_T larger than 30 GeV, and E_T^{miss} greater than 200 GeV. The main background contributions come from $V\gamma$, $\gamma + \text{jets}$, and fake photons. The dominant real photon background, $Z(\nu\nu)\gamma$, is estimated using MC simulations in conjunction with CRs, while the fake photon background is determined using data-driven methods, contributing a significant uncertainty. Due to the high photon energy threshold, this analysis is sensitive only to BSM Higgs bosons with masses up to 3 TeV.

Table 6.4 Summary of the event selections, discriminating variables and production channel considered in the input analyses.^[210]

Channels	VBF	ZH	mono- γ
Trigger	E_T^{miss}	Lepton(s)	Photon
Photons	$= 1, C_\gamma > 0.4$	$= 1$	≥ 1
E_T^γ [GeV]	$\in (15, \max(110, 0.733 \times m_T))$	> 25	> 150
E_T^{miss} [GeV]	> 150	> 60	> 200
Jets	2 or 3, $m_{j_1 j_2} > 250$ GeV, $ \Delta\eta_{j_1 j_2} > 3$ $\eta_{j_1} \cdot \eta_{j_2} < 0, \Delta\phi_{j_1 j_2} < 2, C_{j_3} < 0.7$	≤ 2	≤ 1
Leptons	$= 0 (e, \mu)$	$= 2$, SFOC $m_{ll} \in (76, 116)$ GeV	$= 0 (e, \mu, \tau)$
Disc. variables	m_{jj} and m_T in SR and 4 CRs	BDT score and 1 CR	E_T^{miss}
Reference	^[207]	^[206]	^[146]
Processes considered in the combination	VBF, ggF	ZH	ggF, VBF
Combination scenario	SM, BSM	SM	BSM

The orthogonality of events across the three analyses was verified under different combination scenarios, as described in Table 6.6. For the combination of the SM Higgs decaying into a dark photon, the ZH and VBF analyses are involved. The lepton selection is orthogonal in the ideal case: the ZH analysis selects events with two leptons, while the VBF analysis vetoes events containing any electrons or muons. A check performed on the data confirmed this conclusion, with zero events found to overlap in any regions across the analyses.

For the combination of the BSM Higgs analyses, the jet selection criteria for the VBF and $mono-\gamma$ analyses are, by definition, orthogonal. The VBF analysis requires at least two VBF jets, while the $mono-\gamma$ analysis allows at most one jet, accounting for initial-state radiation (ISR). In real data, a small overlap was observed due to differences in jet definitions and potential fake or missing jet reconstruction. This is illustrated in Figure 6.5.

Table 6.5 Information regarding jet reconstruction and JVT cuts in VBF and MonoPhoton analyses.

	VBF analysis	mono- γ
<i>Jet</i>	AntiKt4PFlow, $p_T > 25$ GeV, $ \eta < 4.5$, JVT > 0.20 (95% eff. wp) if $p_T < 60$ GeV and $ \eta < 2.4$. Leading two jets must pass $f_{JVT} < 0.4$, $ \text{JetTiming} < 11$ ns.	AntiKt4EMTopo jets, $p_T > 30$ GeV, $ \eta < 4.5$
<i>JVT</i>	JVT > 0.20 (95% eff. wp) if $p_T < 60$ GeV and $ \eta < 2.4$	JVT WP = Medium, JVT > 0.59 for $p_T < 60$ GeV and $ \eta < 2.4$

Both the VBF and $mono-\gamma$ analyses have sensitivity to both the VBF and ggF production channels. This arises because VBF events with missing jet reconstruction or ggF events with an ISR jet result in a mixture of event definitions. However, the observed overlap was found to be negligible and does not impact the combined results.

The good orthogonality of the input analyses ensures maximal improvement in sensitivity through the statistical combination.

6.4 Combination Technique

The combination is centered on the likelihood function, which is detailed in Section 5.7.1. Parameters with the same physical meaning are merged in the combined likelihood, and the function is extended to include all bins and regions from the input analyses, as illustrated in

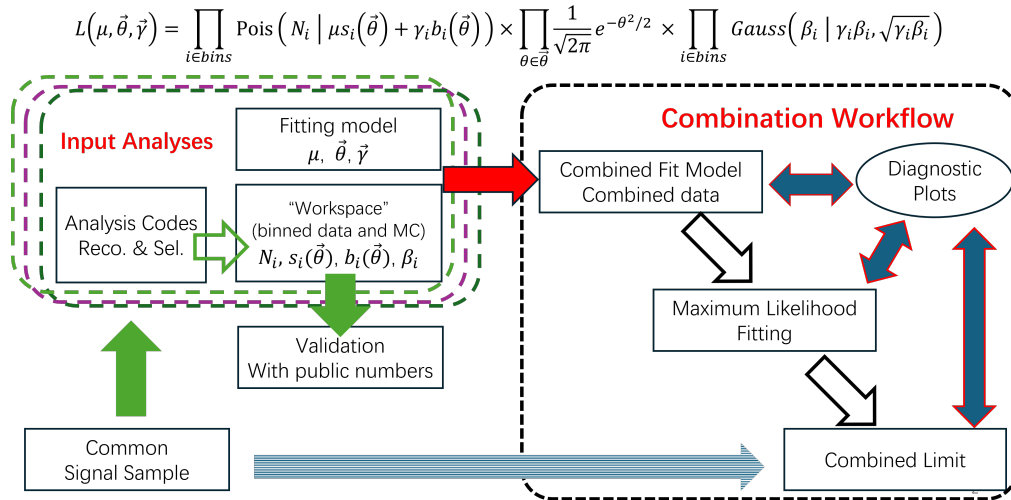
Table 6.6 Combination Scenario

Analysis	Main production channel	SM Higgs Comb.	BSM Higgs Comb.
ZH	ZH	✓	
VBF	VBF	✓	✓
mono- γ	ggF		✓

Figure 6.3.

A specific procedure is required to correlate the parameters, particularly the parameter of interest (POI) and nuisance parameters (NPs) arising from systematic uncertainty sources that are not exactly the same but are related. Technically, the POI definitions in the fitting frameworks of each input analysis vary, as shown in Table 6.7. To unify the analyses under a single POI—defined as the signal strength under a single dark photon hypothesis—the likelihood must be reformulated.

For the treatment of NPs, which are based on different physics considerations, a discussion is presented in the following section.

**Figure 6.3 Workflow of the combination analysis with the likelihood formalism defined in Equation 5.7.1.**

6.5 Correlation of Systematic NPs

The pulls and constrained nuisance parameters (NPs) observed in the input analyses during data fitting are well understood by each analysis group. However, in the combination,

Table 6.7 POI definitions in each channel and rescaling factors for two combination scenarios.

	Original POI	ZH+VBF Rescaling	VBF+Monophoton-recast Rescaling
VBF search	$BR(H \rightarrow \gamma\gamma_D)$	1.0	$\sigma^{\text{VBF+ggF}}(m_H)$
ZH search	μ_{SIG} assuming $BR = 5\%$	0.05	-
Monophoton recast	$\sigma^{\text{VBF+ggF}}(m_H) \times BR(H \rightarrow \gamma\gamma_D)$	-	1.0

the correlations between these NPs must be carefully examined to determine whether the impact of a given systematic uncertainty in one phase space or process has a direct or indirect influence on another.

Incorrectly correlating two systematic NPs, even if they share the same name and definition, could introduce biases in the combination. For instance, data in one channel might overly constrain the estimation of an uncertainty in an unrelated phase space, leading to inaccurate results.

The final determined correlations of experimental uncertainties are summarized in Table 6.8.

Table 6.8 Simplified Overview of uncertainty correlations. ● means correlated, ◐ means partially correlated.

	VBF	ZH	ggF(monophoton)
LUMI	●	●	●
PRW	●	●	●
JES	◐	◐	◐
JER	○	○	○
JVT	◐	◐	◐
EG Resolution and scale	◐	◐	◐
EL ISO/RECO efficiency	●	●	●
EL ID efficiency	●	●	●
MET	◐	◐	◐
MUON ISO/RECO efficiency	●	●	●
MUON ID/MS/SAGITTA/SCALE	●	●	●
Flavor tagging	●	●	●
MC Stat	○	○	○

The correlation scheme for theoretical uncertainties, particularly in signal and background modeling, is based on the principle that the signatures considered in different channels are diverse, and the modeling shares minimal information between the phase spaces of the

Furthermore, nuisance parameters (NPs) that are significantly over-constrained (less than 70%) or strongly pulled (greater than 50%) are decorrelated to avoid biases, as previously discussed.

No significant bias is observed with this correlation scheme. An example check of jet-related systematic NPs is shown in Figure 6.4. The suffixes "VBF" or "ggF" denote the uncorrelated jet systematic NPs, and consistent behavior is observed before and after the combination, confirming that no additional bias is introduced. For instance, the `JET_Pileup_PtTerm` uncertainty in the VBF analysis, which appears pulled, does not bias the NP of the same name in the mono- γ analysis, as the selected jets originate from substantially different sources in the two analyses.

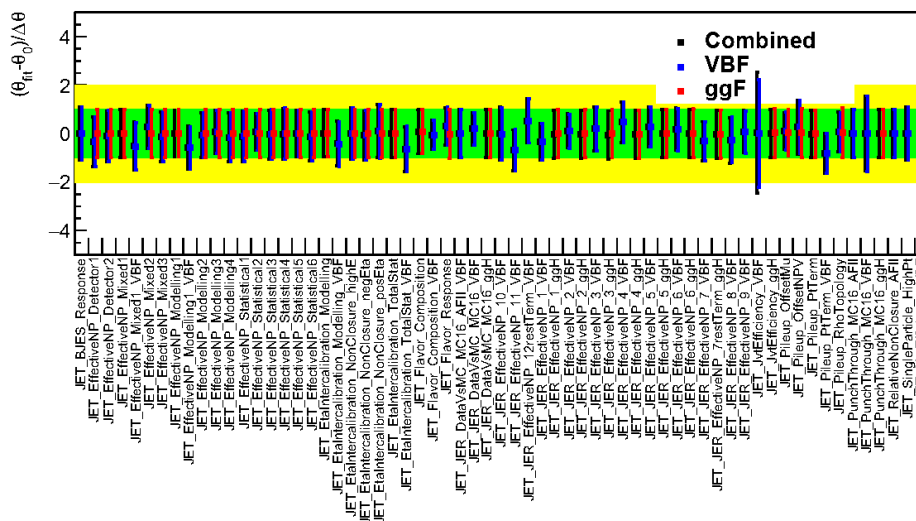


Figure 6.4 NP pull check for VBF+mono-photon combination. The `JET_Pileup_PtTerm` NP is highly pulled in VBF channel but not others. The combined NPs get decorrelated in each channel.

6.6 Combined Results

The combined profiling likelihood analysis is performed, and the CLs method^[200] is used to set the 95% confidence level (CL) limit on the dark photon model. One of my major contributions to this combination effort was the development of a visualization tool, which greatly facilitated the interpretation of the results. The combined fitting process is illustrated in Figure 6.5 for the SM Higgs and 6.6, 6.7 for BSM Higgs, where the coverage of the fit is thoroughly validated.

At the 95% confidence level, the branching ratio of the Standard Model (SM) Higgs boson decaying into a photon and a dark photon is constrained to be less than 1.3%, as shown in Figure 6.8. This result represents the current best collider constraint on the dark photon model with Higgs coupling. It benefits from the strong sensitivity of the input analyses—most notably from the VBF analysis—and the statistical combination, which provides a 29% improvement compared to using the VBF analysis alone.

The systematic impacts are summarized in Table 6.9. The dominant systematic uncertainties arise from background modeling, jet and E_T^{miss} reconstruction, fake estimation, and MC statistical uncertainties. Nevertheless, the analysis remains statistically limited, and the additional data expected from the ongoing Run-3 data-taking period will likely enhance the sensitivity of the dark photon search, enabling even stronger constraints.

For the BSM Higgs, the limits on individual channels are shown in Fig. 6.9, validated against the results of the input analyses for commonly available points. New signal points are incorporated into the input analyses using the RECAST^[211] technique, a portable method to rerun the original analysis and background estimation with the new signal injected.

To further check the impact of the systematic uncertainty correlation scheme, the combination is tested with and without NP correlations, as shown in Fig. 6.10. The combined results without correlation represent the most conservative estimation, meaning the combination does not benefit from the shared detector response across different channels, and each channel constrains the NPs independently. Negligible impact on the final combined limit is observed, as the correlation scheme mainly involves jet uncertainties, which are not the dominant source of systematic uncertainty.

The combined results exclude Higgs masses up to 1.5 TeV, with the strongest sensitivity achieved by the mono- γ analysis, as shown in Figure 6.11. The search extends the mass

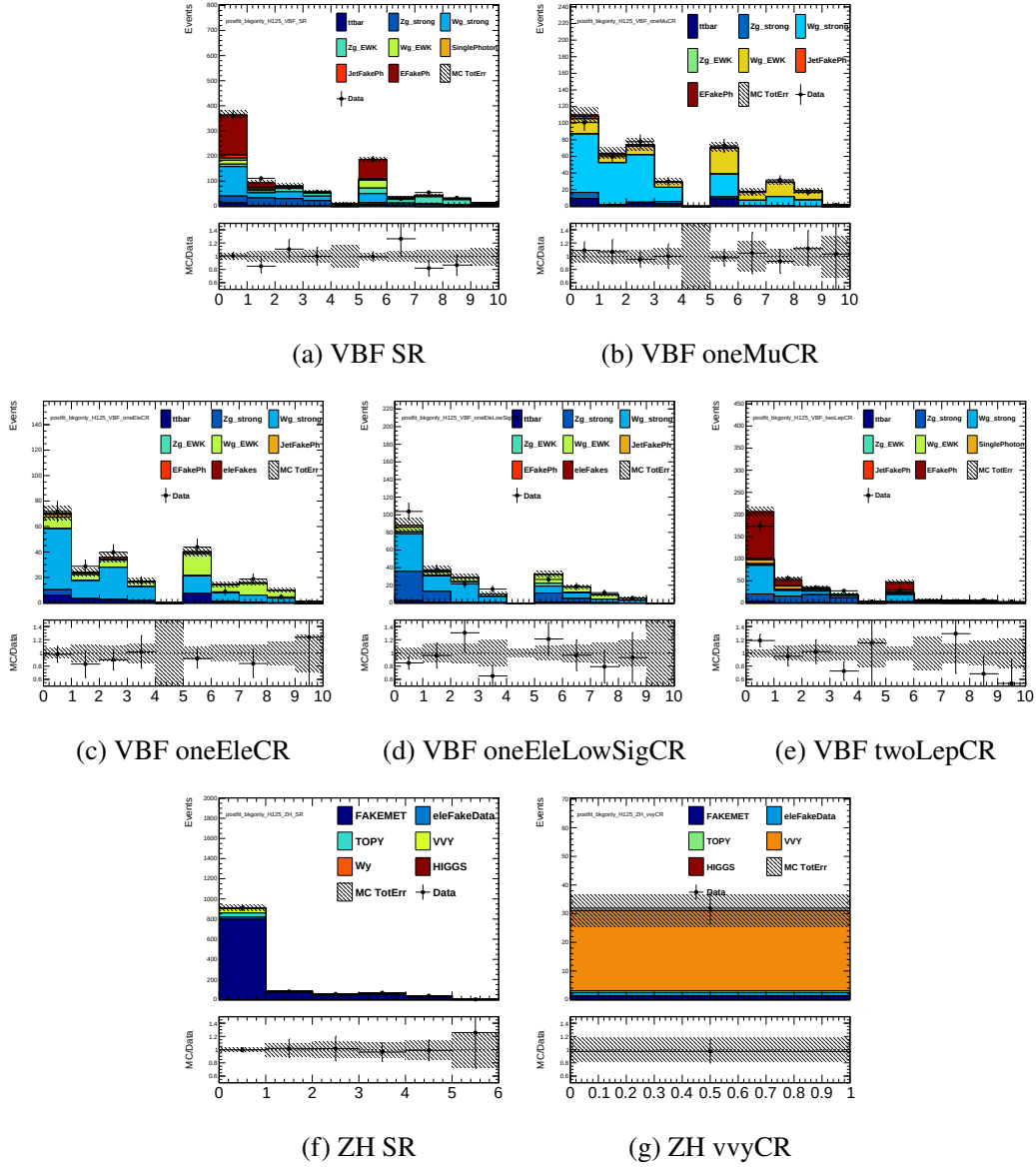


Figure 6.5 Post-fit plots of VBF+ZH combination (SM Higgs). The error band on MC is derived with "VisualizeError" funtion in RooFit package. Error on data point is calculated assuming Poisson fluctuation.

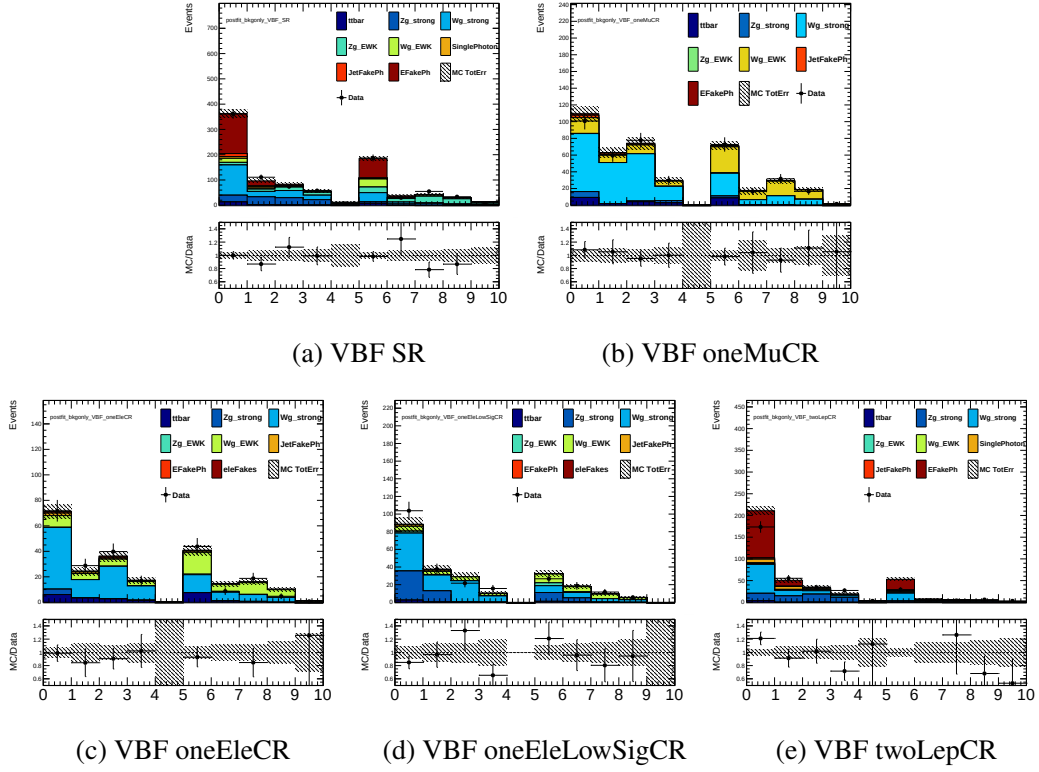


Figure 6.6 Post-fit plots of VBF channel in VBF+MonophotonRecast combination (Heavy Higgs). The error band on MC is derived with "VisualizeError" funtion in RooFit package. Error on data point is calculated assuming Poisson fluctuation.

region up to 3 TeV, which has not been explored in previous studies.

The systematic impacts are summarized in Table 6.10, showing a similar ranking to the SM Higgs to dark photon search. However, the data statistical uncertainty increases significantly, reaching up to 85% for the highest mass point at 3 TeV for the BSM Higgs. This highlights the potential for further improvements with additional data from future Run3 data-taking periods. The *ad-hoc* norm. uncertainty, representing the difference observed between the RECAST results and the original analysis, has a minor impact compared to data fluctuations.

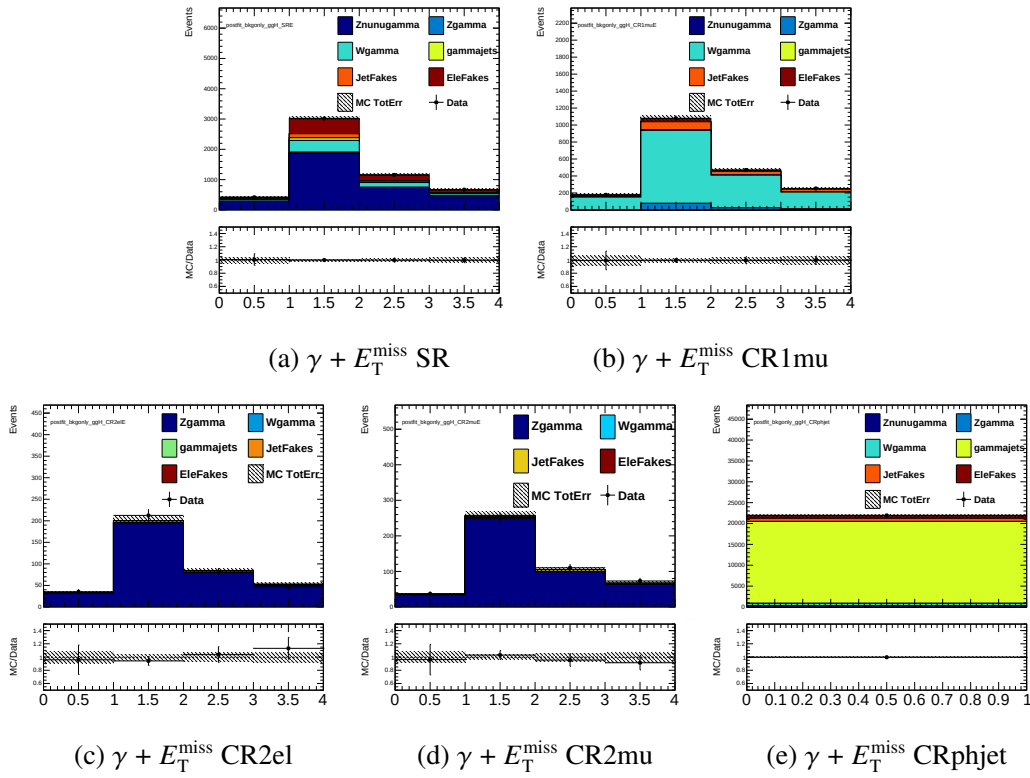


Figure 6.7 Post-fit plots of $\gamma + E_T^{\text{miss}}$ channel in VBF+MonophotonRecast combination (Heavy Higgs). The error band on MC is derived with "VisualizeError" function in RooFit package. Error on data point is calculated assuming Poisson fluctuation.

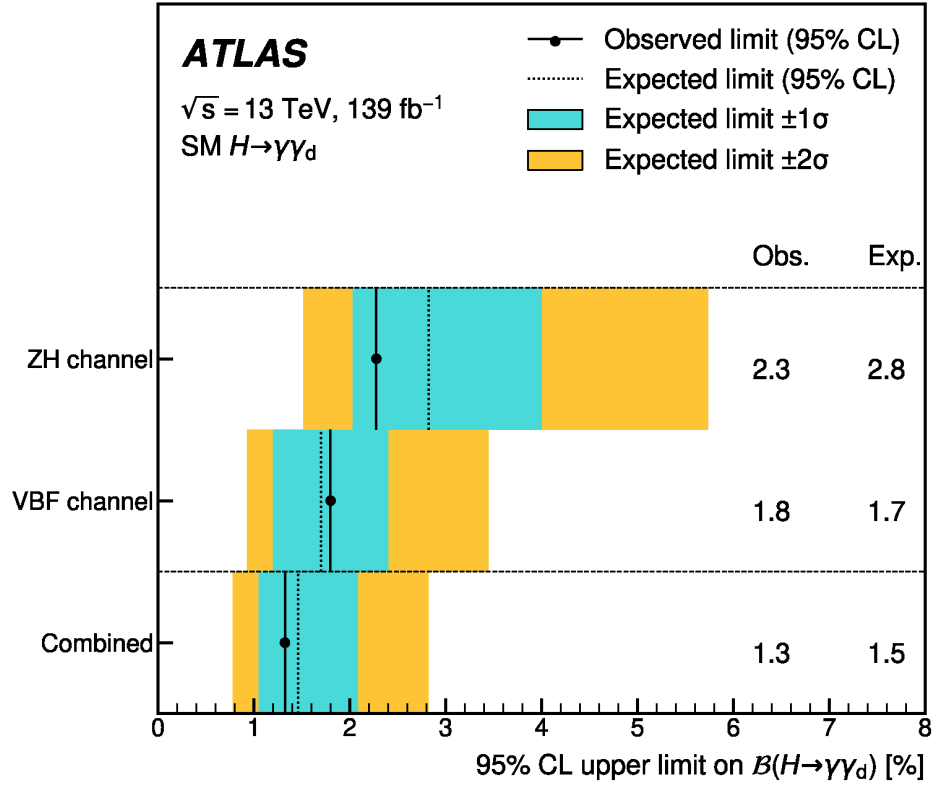


Figure 6.8 Observed and expected upper limits at 95% CL on the branching ratio $BR(H \rightarrow \gamma\gamma_D)$ [210]

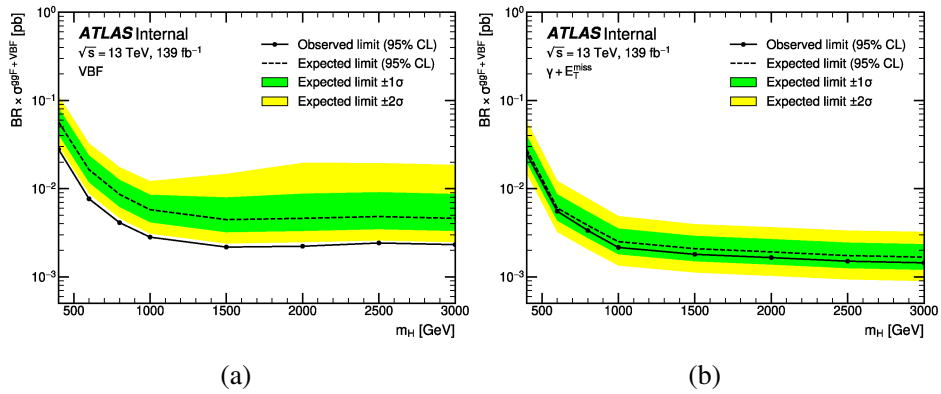


Figure 6.9 Observed and expected exclusion limits at 95% CL on $\sigma \times BR(\gamma\gamma_D)$ for m_H from 400 to 3000 GeV of VBF(a) and $\gamma + E_T^{\text{miss}}$ (b) channel. Expected limit is shown in dashed line with 1σ and 2σ band. Observed limit is shown in solid line.

Table 6.9 Uncertainties $\Delta\mu$ on the best-fit μ in the VBF-ZH combination search for massless γ_D with SM H coupling. The uncertainty from a group of sources is evaluated by fixing the relevant nuisance parameters to their best-fit values and subtracting in square the resulting total uncertainty from the original one. The contribution of the statistical uncertainty is assessed by fixing all nuisance parameters using this procedure. Due to correlations among systematic uncertainties, the total uncertainty does not equal the quadrature sum of the individual terms in the table.

Uncertainty source	$\Delta\mu$ [%]
Statistical unc.	66.3
Systematic unc.	74.9
Theory unc.	48.8
Modelling of signal	2.2
Modelling of background	46.5
Experimental unc.	62.7
Luminosity, pile-up	0.0
Jets, E_{miss}^T	40.4
Electrons, muons	10.9
Fake Estimation	35.1
MC statistical unc.	35.6
Total unc.	100.0

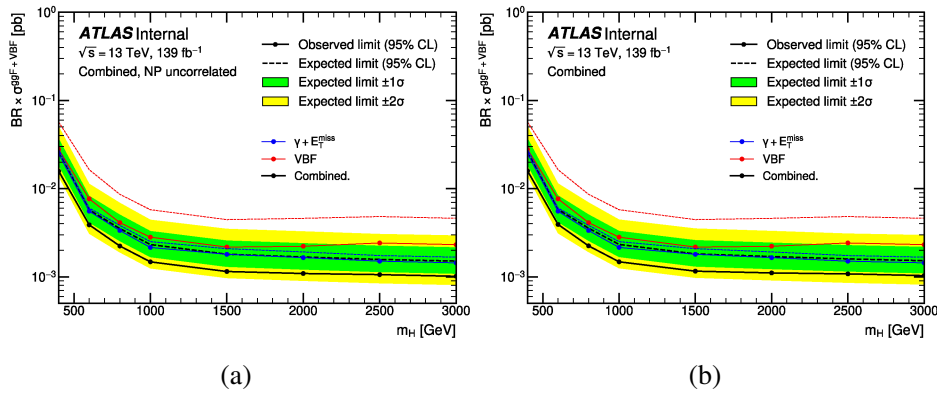


Figure 6.10 Observed and expected exclusion limits at 95% CL on $\sigma \times BR(\gamma\gamma_D)$ for m_H from 400 to 3000 GeV without (a) or with (b) correlation of systematic uncertainty NP. Expected limit is shown in dashed line with 1σ and 2σ band. Observed limit is shown in solid line. Combined limit is colored in black, VBF channel in red and $\gamma + E_T^{\text{miss}}$ channel in blue.

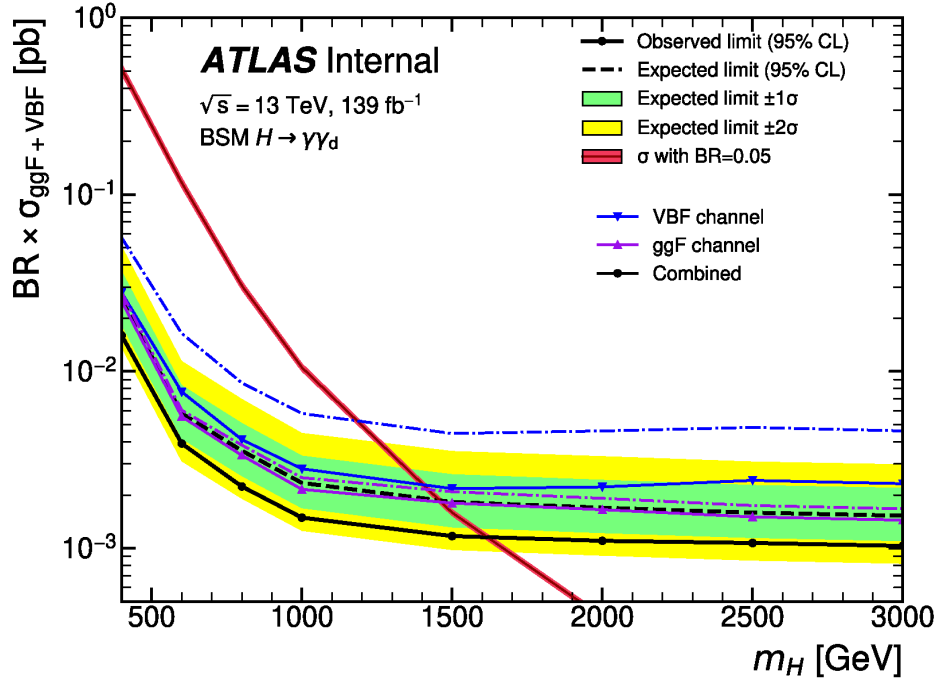


Figure 6.11 Observed and expected exclusion limits at 95% CL on $\sigma \times BR(\gamma\gamma_D)$ for m_H from 400 to 3000 GeV. Combined limit is obtained with correlation scheme of systematics uncertainty NPs as described in Section 6.5. Observed limit is shown in solid line while expected one in dashed line. Combined limit is colored in black, VBF channel in blue and $\gamma + E_T^{\text{miss}}$ channel in violet. The theoretically predicted cross-section of a heavy Higgs boson produced via ggF and VBF is superimposed assuming a $\text{BR} = 0.05$.

Table 6.10 Uncertainties $\Delta\mu$ on the best-fit μ in the VBF-Monophoton recast combination for heavy Higgs decaying to $\gamma\gamma_D$. The uncertainty from a group of sources is evaluated by fixing the relevant nuisance parameters to their best-fit values and subtracting in square the resulting total uncertainty from the original one. The contribution of the statistical uncertainty is assessed by fixing all nuisance parameters using this procedure. Due to correlations among systematic uncertainties, the total uncertainty does not equal the quadrature sum of the individual terms in the table.

$m_H(\text{GeV})$	400	800	1000	2000	3000
Statistical unc.	74.6	83.5	87.0	84.8	85.6
Systematic unc.	66.6	55.0	48.7	53.0	51.6
Theory unc.	30.0	26.7	27.6	40.0	34.6
Signal modelling	2.2	4.6	5.2	6.9	2.0
Background modelling	29.6	26.5	27.4	38.2	34.2
Experimental unc.	63.6	51.2	44.6	37.4	41.2
Luminosity, pile-up	4.6	2.6	2.9	2.8	2.3
Jets, E_{miss}^T	22.2	11.5	10.7	13.4	14.1
Electrons, muons	20.0	22.7	18.1	13.4	14.1
Fake Estimation	52.4	40.6	34.6	25.3	28.5
MC statistical unc.	19.9	17.1	19.1	19.3	23.4
Ad-hoc norm. unc.	–	–	–	4.6	0.0
Total unc.	100.0	100.0	100.0	100.0	100.0

What is the next chapter of dark matter searches at colliders?

Chapter 7 Hunting the Dark Matter Beyond Model

Most of the studies in this thesis focus on searching for dark matter at colliders within the framework of specific models. However, like the outcomes of many current searches, no significant deviations from the Standard Model have been observed. This outcome has led me to question whether all possible avenues have been explored and whether it is feasible to search for dark matter without relying on model-dependent assumptions. This section presents the preliminary results of ongoing studies conducted during the final phase of my PhD. I believe these efforts will open a new avenue for discovering dark matter, moving beyond traditional model-dependent approaches.

7.1 Model independent Dark Matter search

Typical dark matter searches in collider experiments begin by identifying a signature indicative of a specific set of exotic decays or an excess in certain physics variables. The data are then compared to Monte Carlo (MC) simulations under a specific hypothesis, with any observed disagreement attributed to either statistical fluctuations, systematic uncertainties, or the existence of a new signal. Effective field theory (EFT)-based studies^[212], which search for general phenomena arising from high-order EFT operators, are not discussed here. This is primarily because EFT studies are typically designed to probe new physics phenomena distinct from the Standard Model (SM), where dark matter is not necessarily the focus. Additionally, they are constrained by the limited energy scales currently accessible at colliders.

These searches face intrinsic limitations due to pre-selection criteria, often tied to specific triggers or phase space assumptions. Individual analyses are generally optimized for narrow phase spaces and specific dark matter models. However, the number of potential models far exceeds the data, and while recasting techniques allow existing analyses to constrain new models, they remain inherently limited by the original analysis setup. A truly model-independent dark matter search aims to overcome these constraints by exploring the entire phase space, scanning a broad spectrum of dark matter possibilities, and fully utilizing the vast datasets already collected during the LHC's Run-3 and beyond.

One promising approach to model-independent searches is anomaly detection (AD), a technique adapted from computer science^[213]. In high-energy physics (HEP), AD seeks unusual events—defined as outliers or overdensities in expected distributions—that may indicate new phenomena. This method has been successfully demonstrated in several studies^[214-219]. Similar to its applications in industry, where AD identifies faults or fraud, it holds promise for identifying new physics in HEP.

Traditional physics analyses often use discriminants, such as invariant mass or multivariate classifiers, to detect anomalies. These methods can be considered specialized AD approaches, relying on high-level variables and statistical techniques to quantify deviations. However, they are typically limited by the choice of one-dimensional physics variables or multivariate variables designed with specific signal models in mind.

Machine learning (ML) offers a powerful alternative for performing AD-based model-independent searches. As discussed in Section 4, deep neural networks can effectively combine multiple physics inputs, such as jet transverse momentum (p_T) and constituent particle information, into a single variable for classification tasks. Similarly, ML-based methods can create variables sensitive to unknown phenomena. Moreover, the output of ML models can exist in high-dimensional representation spaces^[220], where anomalies may be more easily identified compared to traditional variables like p_T or mass.

This concept has been explored using various methods, though most rely on supervised learning approaches that depend heavily on MC-generated datasets. Such methods are inherently constrained by the accuracy and scope of the simulations. Recently, self-supervised approaches have emerged as a promising alternative, enabling models to learn directly from data without relying on predefined labels or MC-based training. However, these methods often focus solely on kinematic features and are challenging to extend to include other important inputs, such as tracking and particle identification (PID) information.

This chapter introduces a proof-of-concept development of a self-supervised method capable of utilizing the full feature set of particles. Preliminary results are presented for an anomaly detection model designed to operate independently of MC simulations, demonstrating the potential for advancing model-independent dark matter searches.

7.2 Learning of Jet Representation

The architecture of the model, named P-JEPA (Particle Jet Encoder-Predictor Architecture), is illustrated in Figure 7.1. The model consists of three main components: the context encoder, the target encoder, and the predictor, inspired by the study in computer vision field^[221]. All components are based on the transformer architecture^[222], inspired by the Particle Transformer framework^[223], as demonstrated in Figure 7.1.

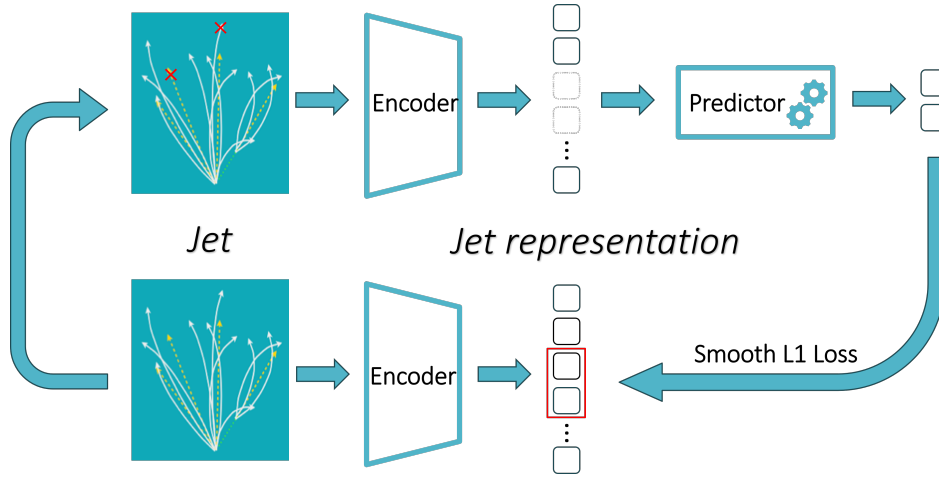


Figure 7.1 Architecture of the P-JEPA Model.

The dataset used in this study is JetClass, a widely recognized benchmark in high-energy physics. It contains 10 classes of large- R jets, originating from processes such as $H \rightarrow b\bar{b}$, $H \rightarrow c\bar{c}$, QCD multijets, hadronic top decays, and W/Z boson decays. Each entry in the dataset represents a single jet, including all its constituent particles with detailed kinematic, tracking, and particle identification (PID) information, all of which are utilized in the study. The jets are simulated using standard high-energy physics toolsets: MadGraph^[224] for matrix element calculations, Pythia^[225] for parton showering, and Delphes^[226] for detector simulation. With 100 million jets per class, this dataset is both large and highly realistic.

The self-supervised learning process operates as follows: each jet, represented by its constituent particles, undergoes a masking procedure where approximately 30% of the particles are randomly removed. The remaining particles are passed through a context encoder, which maps them into a high-dimensional representation called "context." Simultaneously, the target encoder processes the complete, unmasked jet to produce "target" representations for the masked particles. The context and target encoders are synchronized using an expo-

nential moving average^[227], ensuring that the "context" and "target" representations remain consistent while representing different partitions of the same jet. A smaller network, the predictor, takes the "context" representation and attempts to predict the "target," effectively reconstructing the masked jet in representation space. This approach requires no labels or supervised training, allowing the model to learn in a fully self-supervised manner.

The representation learned by this model is believed to encapsulate the complete physics information of the jet, transforming it into a format that is easily interpretable and usable by other machine learning models. This representation benefits a range of downstream tasks, a process known as transfer learning or fine-tuning^[228]. Potential applications include jet flavor tagging, particle mass regression, jet variable reconstruction, and more. Anomaly detection (AD) is one particularly important application built on this foundation and is described in the following section.

7.3 Anomaly Detection using Classification-Without-Labels (CWoLa)

The trained model is fine-tuned to perform anomaly detection (AD). This study employs a widely-used AD method called Simulation Assisted Likelihood-free Anomaly Detection (SALAD)^[215], along with a state-of-the-art supervised approach from Ref.^[229]. These methods provide a benchmark for performance comparison across a variety of existing studies. The evaluation follows the methodology outlined in Ref.^[229].

The JetClassII-SM dataset^[229], which was not seen by the self-supervised model during training, is used to evaluate AD performance. The goal is to determine whether the model can detect unknown signals. The target encoder component of the machine learning model generates representations for the two leading jets in each event. These representations are then combined using two fully connected layers to form an event-level representation.

The dataset is evenly divided into two regions, with a specific amount of signal injected into one to simulate the signal-enriched region. This setup is achievable under minimal assumptions in the real physics analysis, such as applying a rough mass cut, with the only requirement being that the signal density in one region is higher than in the other. Ideal background estimation for the two regions is applied in current study, where events are directly taken from the simulated dataset. Future developments aim to model the background using the generative mode of P-JEPA, which will further expand its applicability with the

goal of fully eliminating reliance on Monte Carlo simulations.

An AD classifier is subsequently trained to distinguish between events in these two regions. The classifier is then tested on pure signal events to evaluate its discovery potential. The entire process is illustrated in Figure 7.2.

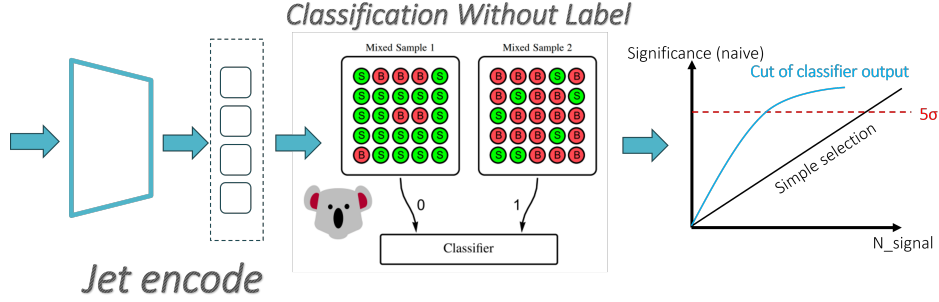


Figure 7.2 Application of Jet Representation in Anomaly Detection for High-Energy Physics Discovery. From left to right, the jet representation output from the model is utilized for label-free anomaly detection (AD) classification^[230]. The resulting scores are then employed for event selection, enhancing the signal-to-background ratio. This improvement enables discoveries with fewer signal events, increasing sensitivity to discover dark matter with lower production cross-sections.

The BSM triboson process is selected as the unknown signal for testing, as it was not included during the anomaly detection (AD) model training. The specific signal tested is $W' \rightarrow W\Phi \rightarrow WWW$, with a W' mass of 3 TeV and a Φ mass of 400 GeV, where all W bosons decay hadronically^{[231][232]}.

7.4 Preliminary Results

The performance of the anomaly detection (AD) model is characterized by the significance improvement (SIC), which quantifies the enhancement in signal significance after applying a cut on the model output score. The significance, approximately given by $S/\sqrt{B}$ (where S and B represent the signal and background yields, respectively), is used as the primary metric for evaluation.

The model is compared against other methods, including: "From-scratch" models: These have the same architecture and number of parameters as the self-supervised model but lack pretraining. "High-level" models: These rely solely on high-level variables such as jet kinematics and are benchmarked against results from^[229], representing optimal performance based on traditional physics features.

The self-supervised model demonstrates a clear improvement over both alternatives. For the specific signal tested, even with a low signal fraction of approximately 0.7% in the signal-enriched region, the self-supervised method significantly boosts the discovery potential. It effectively reduces background contamination, achieving a sensitivity enhancement close to a 5σ discovery threshold under these conditions.

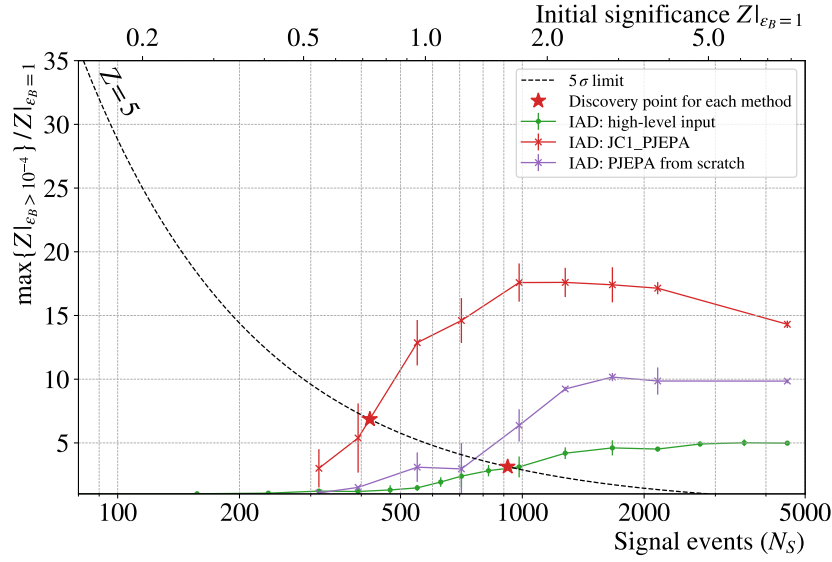


Figure 7.3 Performance of Anomaly Detection using the P-JEPA Algorithm. The X-axis represents the number of signal events in the signal region, with the corresponding trivial significance shown on the upper X-axis. The Y-axis indicates the maximum significance improvement achieved after applying a specific method to isolate the signal. For a given algorithm that assigns a score to events, the cut point on the score distribution is scanned to optimize the signal-to-background separation. This process can be performed in a real analysis without prior knowledge of the signal model. The dashed black line represents the 5σ significance threshold, indicating discovery potential if a method reaches this level, as the signal-to-background ratio after applying the cut is sufficient for a discovery claim. The red, purple, and green lines correspond to the full P-JEPA model for anomaly detection, the P-JEPA model without training on the large unlabeled dataset, and a supervised model using commonly employed physics variables such as mass and τ_2 ^[233], respectively.

This work is still under active development, and I firmly believe that, in the near future, it or similar inspired methods will be implemented at the LHC. With continued advancements, these approaches hold great promise for uncovering something akin to dark matter and addressing one of the largest missing pieces in our understanding of the standard model of the universe.

Chapter 8 Conclusion and Outlook

The searches for dark matter using novel techniques at the Large Hadron Collider (LHC) are described in this thesis. These include the search for the dark Higgs model with novel boosted double-tagging, the search for the dark photon through statistical combination techniques, and the preliminary research and development of self-supervised anomaly detection for model-independent dark matter searches.

The utilization of deep learning-based boosted Xbb tagging has significantly enhanced sensitivity in the search for the dark Higgs decaying into two b quarks at ATLAS. In the absence of a significant excess, the analysis excludes mediator masses up to 3.5 TeV. This work also completes the search for high-mass dark Higgs bosons, excluding benchmark parameters for dark Higgs masses ranging from 30 GeV to 400 GeV. Furthermore, this analysis is the first to test relic-density-compatible parameter settings in collider dark matter searches, probing a larger parameter space, including dark matter masses up to 900 GeV and $m_{Z'}$ up to the perturbative theory limit.

A statistical combination of searches for massless dark photons with Higgs coupling was performed at ATLAS. This combination sets the best collider limits on the Standard Model (SM) Higgs boson and beyond-the-Standard-Model (BSM) Higgs bosons decaying into a photon and a dark photon. The analysis involved extensive checks, validations, and technical developments.

Additionally, a novel self-supervised anomaly detection technique demonstrates its potential for model-independent dark matter searches using small-scale simulated datasets. Active development is ongoing to implement this approach in a future model-independent search at the LHC.

I strongly believe that, with the innovative techniques developed and those currently under development, the detection of dark matter at the world's largest particle collider will become a reality one day.

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Appendix A Technical Information for DXbb Tagging and MonoS(bb) Search

A.1 Samples for ttbar calibration of DXbb tagger

Table A.1 Summary of the nominal and alternative simulated event samples.

Category	Generator+Showering	XS precision	PDF
$t\bar{t}$ semi-lep	PowhegBox v2 + Pythia8.230	NNLO+NNLL	NNPDF3.0NLO
	MadGraph5_aMC@NLO v2.6.0 + Pythia8.230	NNLO+NNLL	NNPDF3.0NLO
	PowhegBox v2 + Herwig7.04	NNLO+NNLL	MMHT2014LO
	PowhegBox v2 + Pythia8.230 (hdamp=3.0 m_{top})	NNLO+NNLL	NNPDF2.3LO
Single-top t -chan	PowhegBox v2 + Pythia8.230	NLO	NNPDF3.0NLOf4
	MadGraph5_aMC@NLO v2.6.0 + Pythia8.230	NLO	NNPDF3.0NLO
	PowhegBox v2 + Herwig7.04	NLO	MMHT2014LO
Single-top s -chan	PowhegBox v2 + Pythia8.230	NLO	NNPDF3.0NLO
	MadGraph5_aMC@NLO v2.6.0 + Pythia8.230	NLO	NNPDF3.0NLO
	PowhegBox v2 + Herwig7.04	NLO	MMHT2014LO
Single-top tW	PowhegBox v2 + Pythia8.230	NLO	NNPDF3.0NLO
	PowhegBox v2 + Pythia8.230	NLO	NNPDF3.0NLO
	MadGraph5_aMC@NLO v2.6.0 + Pythia8.230	NLO	NNPDF3.0NLO
	PowhegBox v2 + Herwig7.04	NLO	MMHT2014LO
W + jets	Sherpa 2.2.1	NNLO	NNPDF3.0NNLO
Z + jets	Sherpa 2.2.1	NNLO	NNPDF3.0NNLO
Diboson	Sherpa 2.2.2/2.2.1(4nu)	NLO	NNPDF3.0NNLO
$t\bar{t}V$	aMC@NLO 2.3.3 + Pythia8.210	NLO	NNPDF2.3

A.2 Good-Run-List(GRL)

Table A.2 GRL data lists for each year and their corresponding luminosity.

Period	GRL	Luminosity/ fb^{-1}
2015	data15_13TeV.periodAllYear_DetStatus-v89-pro21-02_Unknown_ PHYS_StandardGRL_All_Good_25ns	3.2
2016	data16_13TeV.periodAllYear_DetStatus-v89-pro21-01_DQDefects-00-02-04_ PHYS_StandardGRL_All_Good_25ns	33
2017	data17_13TeV.periodAllYear_DetStatus-v99-pro22-01_Unknown_ PHYS_StandardGRL_All_Good_25ns_TriggerNo17e33prim	44.3
2018	data18_13TeV.periodAllYear_DetStatus-v102-pro22-04_Unknown_ PHYS_StandardGRL_All_Good_25ns_TriggerNo17e33prim	58.5

A.3 List of Triggers

Table A.3 MET Trigger used in the analysis.

Period	E_T^{miss}
2015	HLT_xe70_mht
2016(A-D3)	HLT_xe90_mht_L1XE50
2016(D4-end)	HLT_xe110_mht_L1XE50
2017(B-D5)	HLT_xe110_pufit_L1XE55
2017(D6-end)	HLT_xe110_pufit_L1XE50
2018	HLT_xe110_pufit_xe70_L1XE50

Table A.4 Un-prescaled electron triggers used in the analysis.

Period	Lowest un-prescaled Electron
2015(D3-end)	HLT_e24_lhmedium_L1EM20VH_OR_HLT_e60_lhmedium_OR_HLT_e120_lhloose
2016(A)	HLT_e60_lhmedium_nod0_OR_HLT_e140_lhloose_nod0
2016(B-D3)	HLT_e60_lhmedium_nod0_OR_HLT_e140_lhloose_nod0
2016(D4-end)	HLT_e26_lhtight_nod0_ivarloose_OR_HLT_e60_lhmedium_nod0_OR_HLT_e140_lhloose_nod0
2017	HLT_e26_lhtight_nod0_ivarloose_OR_HLT_e60_lhmedium_nod0_OR_HLT_e140_lhloose_nod0
2018	HLT_e26_lhtight_nod0_ivarloose_OR_HLT_e60_lhmedium_nod0_OR_HLT_e140_lhloose_nod0

Table A.5 Un-prescaled muon trigger used in the analysis.

Period	Lowest un-prescaled Muon
2015(D3-end)	HLT_mu20_iloose_L1MU15_OR_HLT_mu40
2016(A)	HLT_mu24_ivarmedium_OR_HLT_mu40
2016(B-D3)	HLT_mu24_ivarmedium_OR_HLT_mu50
2016(D4-end)	HLT_mu26_ivarmedium_OR_HLT_mu50
2017	HLT_mu26_ivarmedium_OR_HLT_mu50
2018	HLT_mu26_ivarmedium_OR_HLT_mu50

A.4 Cutflow and Selection Efficiency for Signal

A.5 List of NPs

The nuisance parameters are listed in Table A.8, A.9 and A.10.

A.6 Check and study of NP correlation

Correlation with notable value or suspicious behaviour shown in Figure 5.31 is studied and the details are documented in Table A.11 in this section.

Table A.6 Cutflow of benchmark signal (zp2000_dm200_dh90) in the resolved region

Initial	30000
PassGRL	30000
passLArTile	30000
Trigger	20814
HasVtx	20814
BadJet	20814
CosmicMuon	20813
BadMuon	20813
PFlow Electron veto	20813
IsMETTrigPassed	20674
0 baseline electrons	20570
0 baseline muons	20519
Tau Veto	20402
Extended Tau Veto (resolved)	19860
(MetTST>150 && MetTST<500)	14366
>=2 jets	12956
<=4 jets	11638
==2 b-tags	5280
mjj_corr >20	5280
mjj_corr <270	5247
DeltaPhiMin3 >20deg	5060
METSig>12	4873
pt_jj_corr >100000	4690
mT_METclosestBJet >170000	4033
mT_METfurthestBJet >200000	3865
(metptjj <1.30 && metptjj >0.70)	3394

Table A.7 Cutflow of benchmark signal (zp2000_dm200_dh90) in the merged region

Initial	30000
PassGRL	30000
passLArTile	30000
Trigger	20814
HasVtx	20814
BadJet	20814
CosmicMuon	20813
BadMuon	20813
PFlow Electron veto	20813
IsMETTrigPassed	20674
0 baseline electrons	20570
0 baseline muons	20519
Tau Veto	20402
Extended Tau Veto (merged)	19984
MetTST>500	2705
>=1 fat-jets	2687
mJ_corr >20	2649
mJ_corr <270	2550
DeltaPhiMin3 >20deg	2404
passed_0L_SR_Merged == 1.00	2396
N_associated_Jets02 >= 2.00	2235
Trkjet pass OR	2105
2massoverpt <0.60	1921
(metptJ <1.30 && metptJ >0.70)	1761
BTagging in Merged Region	810

Table A.8 Nuisance parameters related to experimental/detector systematic uncertainty (affecting both shape and normalization) and their treatment (S=smoothed, Sym1=symmetrised (one-sided systematic), Sym2=symmetrised (two-sided systematic)). The normalization and shape effects are decorrelated and are denoted by keywords, as described in Sec. 5.7.5.

NP Name	Treatment
EL_EFF_*	-
EG_RESOLUTION_*	S
EG_SCALE_*	S
MUON_EFF_*	S, Sym2
MUON_EFF_Trig*	-
MUON_SAGITTA_*	S, Sym2
MUON_SCALE_*	S
MUON_MS_*	S
MUON_ID_*	S
TAUS_TRUEHADTAU_SME_*	S, Sym2
JET_EffectiveNP_*	S, Sym2
JET_Eta*	S, Sym2
JET_JET_Flavor_*	S, Sym2
JET_CombMass_*	S, Sym2
JET_JET_LargeR_*	S, Sym2
JET_JET_MassRes_*	S, Sym2
JET_Pileup_*	S, Sym2
JET_PunchThrough	S, Sym2
JET_RelativeNonClosure	S, Sym2
JET_BJES_Response	S, Sym2
JET_JVT_*	S, Sym2
JET_fJVT_*	S, Sym2
JET_SingleParticle	S, Sym2
JET_JER_*	S, Sym1
FT_EFF_*	S, Sym2
METTrig_*	S
MET_SoftTrk_Scale_*	S, Sym1
MET_SoftTrk_Reso_*	S, Sym1
PRW_DATASF	S, Sym2

Table A.9 Nuisance parameters related to uncertainties that affect the overall normalisation (event yield) of the physics process (flat or the 1σ prefit unc. of Gaussian prior). Affected samples and regions are listed and "all" denotes the NP is correlated for all relevant.

NP Name	Prior	Sample	Region
norm_Zhf	flat	Zhf	Resolved/Merged decorr.
norm_Whf	flat	Whf	Resolved/Merged decorr.
norm_ttbar	flat	$t\bar{t}$	all
stopNorm	40%	Wt , s and t -channel top	all
VVNorm	15%	WW, WZ, ZZ	all
VHbbNorm	5%	VHbb	all
WclNorm	55%	Wcl	all
ATLAS_LUMI	0.83%	all	all

The systematic uncertainty impact of XbbV3_ZBBCALIB_2b ($DXbb$ tagger calibration of bb flavor) is shown in Figure A.1

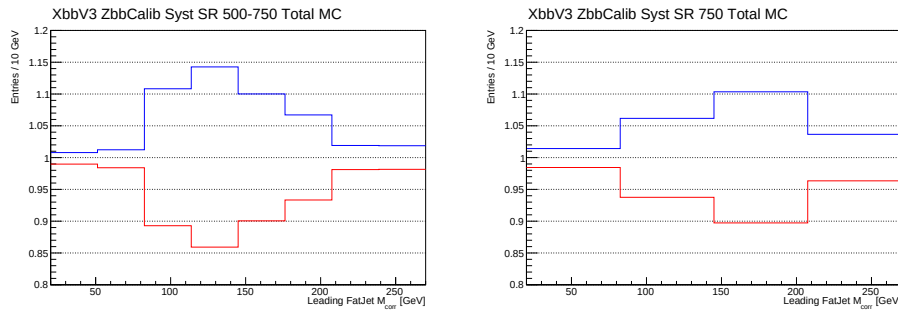


Figure A.1 Impact of Xbb Zbb calibration systematic. Total MC is used since the systematic is applied on all the process with 2b flavor decay from Higgs or Z boson (VHbb and ZZbb). Blue line indicates the "up" variation where NP=+1 and red for "down".

The systematic uncertainty impact of XbbV3_TTBARCALIB_1b ($DXbb$ tagger calibration of bx flavor) is shown in Figure A.2

The systematic uncertainty impact of lepton_W_MG (transition systematic from generator of MG) is shown in Figure A.3

The systematic uncertainty impact of Z_MG (generator shape variation of Z+jets) in resolved region is shown in Figure A.4

Table A.10 Nuisance parameters related to theory uncertainty (affecting both shape and normalization) and their treatment (S=smoothed, Sym1=symmetrised (one-sided systematic), Sym2=symmetrised (two-sided systematic)). The normalization and shape effects are decorrelated and are denoted by keywords, as described in Sec. 5.7.5. Affected samples are listed and "all" denotes the NP is correlated for all relevant.

NP Name	Treatment	Sample
Z_MUR_MUF	S, Sym2	Zhf, Zcl, Zl
Z_ckkw	S, Sym2	Zhf, Zcl, Zl
Z_qsf	S, Sym2	Zhf, Zcl, Zl
Z_PDF	S, Sym2	Zhf, Zcl, Zl
Z_PDFalphaS	S, Sym2	Zhf, Zcl, Zl
Z_MG	S, Sym1	Zhf, Zcl, Zl
W_MUR_MUF	S, Sym2	Whf, Wcl, Wl
W_ckkw	S, Sym2	Whf, Wcl, Wl
W_qsf	S, Sym2	Whf, Wcl, Wl
W_PDF	S, Sym2	Whf, Wcl, Wl
W_PDFalphaS	S, Sym2	Whf, Wcl, Wl
W_MG	S, Sym1	Whf, Wcl, Wl
ttbar_MUR_MUF	S, Sym2	$t\bar{t}$
ttbar_PDFalphaS	S, Sym2	$t\bar{t}$
ttbar_PDF	S, Sym2	$t\bar{t}$
ttbar_ISR	S, Sym2	$t\bar{t}$
ttbar_FSR	S, Sym2	$t\bar{t}$
ttbar_ME	S, Sym1	$t\bar{t}$
ttbar_PS	S, Sym1	$t\bar{t}$
stop_MUR_MUF	S, Sym2	$Wt/s/t$ -channel top
stop_PDF	S, Sym2	$Wt/s/t$ -channel top
stop_ISR	S, Sym2	$Wt/s/t$ -channel top
stop_FSR	S, Sym2	$Wt/s/t$ -channel top
stop_ME	S, Sym1	$Wt/s/t$ -channel top
stop_PS	S, Sym1	$Wt/s/t$ -channel top
stop_DS	S, Sym1	Wt -channel top
VV_MUR_MUF	S, Sym2	WW, WZ, ZZ
VV_PDFalphaS	S, Sym2	WW, WZ, ZZ
VV_PDF	S, Sym2	WW, WZ, ZZ
VV_PS	S, Sym2	WW, WZ, ZZ
VV_PowPy	S, Sym2	WW, WZ, ZZ
VHbb_MUR_MUF	S, Sym2	VHbb
VHbb_PDF	S, Sym2	VHbb
VHbb_PS	S, Sym1	VHbb

Table A.11 List of notable or suspicious correlations Asimov fit. "Fat0" denotes resolved region and "Fat1" for merged region. "lepton_W_MG" denotes the transition effect of W+jets generator systematic uncertainty between different lepton regions.

term	term	corr	reason
XbbV3_ZBBCALIB_2b	POI	-0.36	Syst increase signal yield
XbbV3_ZBBCALIB_2b	norm_Zhf_Fat1	-0.36	Syst increase VHbb and ZZbb yield in SR
XbbV3_ZBBCALIB_2b	norm_Whf_Fat1	-0.30	Syst increase VHbb and ZZbb yield in SR
XbbV3_ZBBCALIB_2b	Diboson_PowPy	0.17	Opposite impact to ZZbb
XbbV3_TTBARCALIB_1b	norm_ttbar	0.02	Dominated by resolved region
XbbV3_TTBARCALIB_1b	norm_Whf_Fat1	-0.40	Syst increase ttbar/top yield in SR&CR1
lepton_W_MG	norm_Zhf_Fat0	-0.62	Syst increase W+jets yield in SR
lepton_W_MG	norm_Whf_Fat0	0.25	Syst decrease W+jets in CR1
Z_MG	norm_Zhf_Fat0	-0.24	Syst increase high mass Z+jets in resolved regions
Z_MG	norm_Whf_Fat0	0.44	Negatively correlated with Zhf

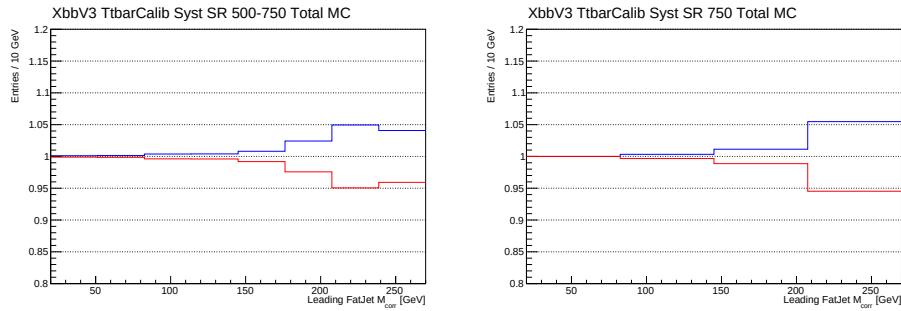


Figure A.2 Impact of Xbb Ttbar calibration systematic. Total MC is used since the systematic is applied on all the process with 1b flavor decay from top (ttbar and single top). Blue line indicates the "up" variation where NP=+1 and red for "down".

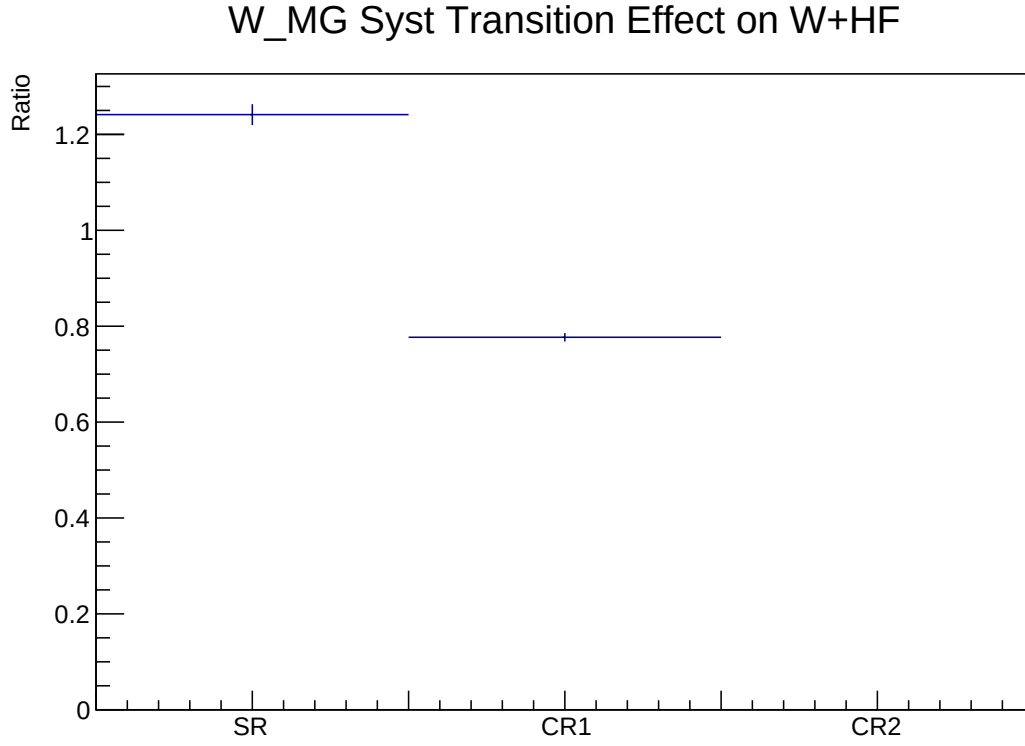


Figure A.3 Transition effect to the yield in different lepton region (SR v.s. CR1) for the W+jets generator systematic uncertainty

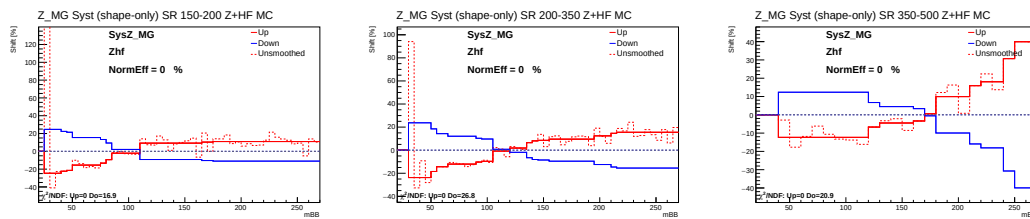


Figure A.4 Shape effect of the Z+jets generator systematic uncertainty

Appendix B Summary of ATLAS DM searches in the context of 2HDM+a

A significant number of dark matter (DM) searches have been conducted in ATLAS, targeting various final states and signatures. A comprehensive summary and combination^[234] were performed within the framework of the 2HDM+a (Two Higgs Doublet Model plus pseudo-scalar mediator a)^[235] theoretical model to evaluate the sensitivity and complementarity of these analyses, as well as to establish the most stringent collider constraints on the parameter space. This section provides a brief overview of Ref.^[234] and focuses on the statistical study to which I contributed. Additionally, it presents the latest combined results with the aim of guiding future DM searches and emphasizing the importance of pursuing DM detection in collider experiments by integrating all possible signatures.

B.1 2HDM+a Model

The 2HDM+a model connects the extended Higgs sector to the dark sector through the inclusion of an additional pseudoscalar particle, a . The Two Higgs Doublet Model (2HDM) extends the Standard Model (SM) by introducing a second complex Higgs doublet. It assumes a CP-conserving potential and a softly broken Z_2 symmetry^[236]. After electroweak (EWK) spontaneous symmetry breaking, the model predicts the existence of five Higgs bosons, as summarized in Table B.1. The framework follows the Type-II setup^[236] of the 2HDM, assuming the alignment and decoupling limits, where the lighter CP-even Higgs boson is identified as the SM Higgs boson.

Higgs Boson	Description
h	Light CP-even Higgs boson (identified as the SM Higgs)
H	Heavy CP-even Higgs boson
A	CP-odd Higgs boson
H^+	Charged Higgs boson
H^-	Charged Higgs boson (conjugate of H^+)

Table B.1 The five Higgs bosons predicted in the 2HDM+a model after electroweak symmetry breaking.

The additional pseudoscalar (CP-odd) mediator (a) connects the dark sector through

Yukawa-like couplings to both Standard Model (SM) fermions and dark matter (DM) fermions χ . The mediator mixes with the CP-odd Higgs boson A in the 2HDM sector via a mixing angle θ , forming a theoretical framework that naturally predicts dark matter in a UV-complete, gauge-invariant, and renormalizable manner.

The 2HDM+a model exhibits a rich phenomenology and predicts a wide range of signatures, including both invisible decays (such as $E_T^{\text{miss}} + X$ signatures) and visible mediator decays (e.g., four-fermion final states). The dominant production channel at the LHC arises from gg -initiated, with the relevant diagrams illustrated in Figure B.1. Additional contributions from $b\bar{b}$ -initiated and tW processes are also considered, with their diagrams summarized in Figures B.2.

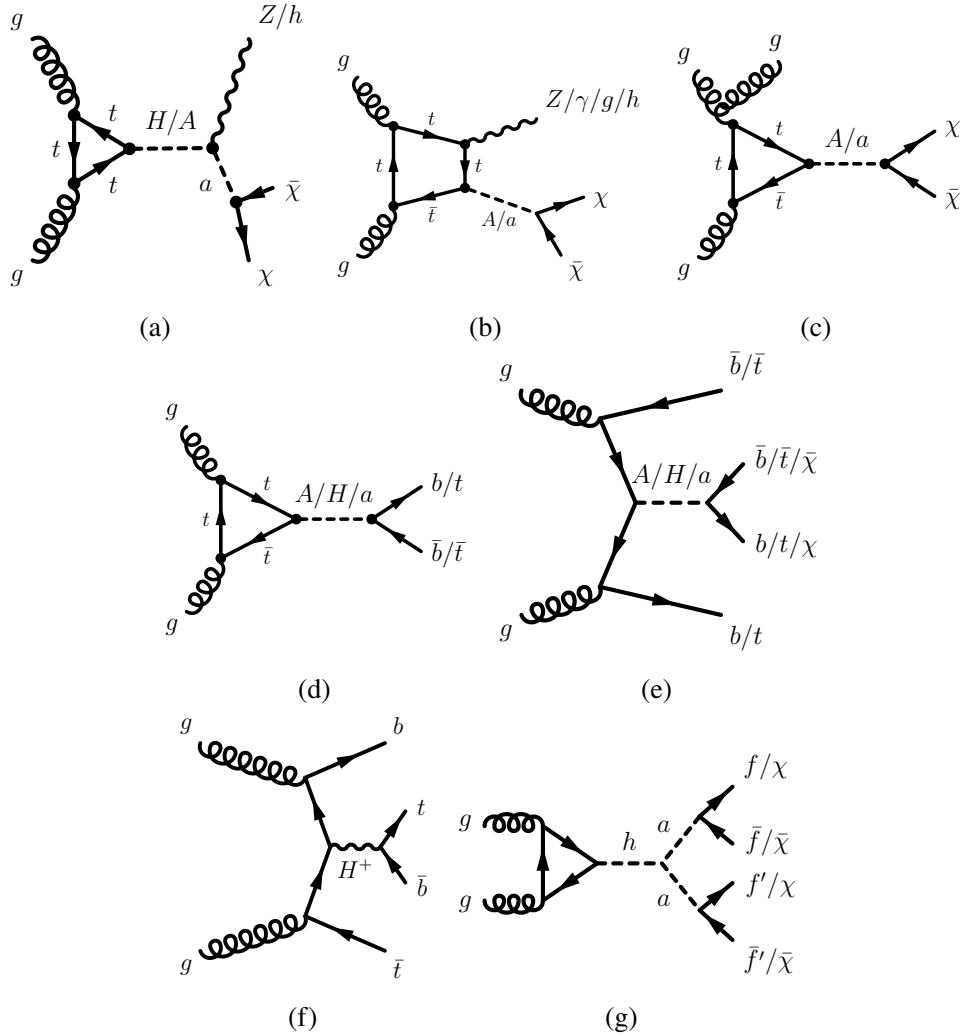


Figure B.1 Feynman diagrams for the 2HDM+a model (gg -initiated).

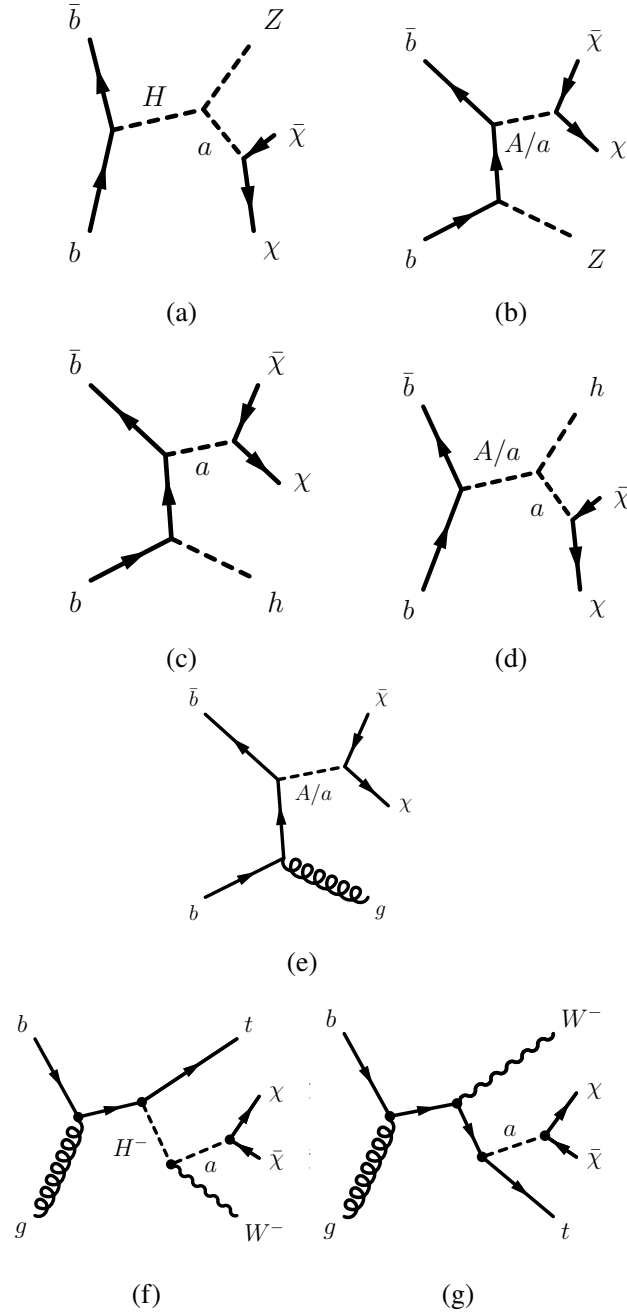


Figure B.2 Feynman diagrams for the 2HDM+a model ($b\bar{b}$ -initiated and tW).

The model is characterized by 14 parameters that fully define its phenomenology. To facilitate experimental studies and ensure compatibility with current constraints from measurements and theoretical considerations, a simplified setup with five parameters^[235,237] is adopted. This reduced parameter space serves as the LHC Dark Matter Benchmark Model^[237] and is employed consistently across multiple experiments. A detailed summary of the full parameter set and the fixed values used in this context is provided in Table B.2.

Table B.2 Parameters and simplified setup of 2HDM+a model.

Parameter	Description
m_A	Mass of the CP-odd Higgs boson (A)
m_a	Mass of the mediator (a)
m_χ	Mass of the dark matter particle (χ)
$\tan\beta$	Ratio of the VEVs of the two Higgs doublets
θ	Mixing angle of the CP-odd weak eigenstates (a - A)
m_h	Mass of the light CP-even Higgs boson (h), fixed to SM
v	Electroweak vacuum expectation value (VEV), fixed to SM
m_H	Mass of the heavy CP-even Higgs boson (H), fixed to m_A
$m_{H^\pm}$	Mass of the charged Higgs bosons ($H^\pm$), fixed to m_A
λ_3	Quartic coupling of the pure 2HDM potential term, fixed to 3
$\lambda_{P1}, \lambda_{P2}$	Quartic couplings of the potential term connecting the doublet and singlet fields, fixed to 3
α	Mixing angle of the CP-even weak eigenstates, fixed with $\cos(\beta - \alpha) = 0$
g_χ	Yukawa coupling strength between the mediator and the DM particle, fixed to 1

B.2 Study of Combination Scenarios and Results

Several scenarios are explored in this summary, focusing on different representative parameter setups, as shown in Table B.3. Relevant analyses are studied in each scenario to benchmark sensitivity and establish the latest exclusion limits, which are summarized in Table B.4 along with references to each analysis.

B.2.1 m_a - m_A Scan

The two-dimensional plane of the two pseudoscalar masses, m_a - m_A , is studied to explore the rich decay and production channels kinematically. The parameter $\tan\beta$ is fixed to 1 to favor the top quark coupling, while the mixing angle is set to either 0.35 or 0.7 ($\approx \frac{1}{\sqrt{2}}$) to investigate low or maximal mixing between A and the DM mediator a .

The summary of all relevant analyses is shown in Figure B.3. The $E_T^{\text{miss}} + h$ and $E_T^{\text{miss}} + Z$

Table B.3 Summary of the parameter settings for 2HDM+a benchmark scenarios.^[234]

Scenario		Fixed parameter values				Varied parameters	
		$\sin \theta$	m_A [GeV]	m_a [GeV]	m_χ [GeV]	$\tan \beta$	
1	a	0.35	—	—	10	1.0	(m_a, m_A)
	b	0.70	—	—	10	1.0	
2	a	0.35	—	250	10	—	$(m_A, \tan \beta)$
	b	0.70	—	250	10	—	
3	a	0.35	600	—	10	—	$(m_a, \tan \beta)$
	b	0.70	600	—	10	—	
4	a	—	600	200	10	1.0	$\sin \theta$
	b	—	1000	350	10	1.0	
5		0.35	1000	400	—	1.0	m_χ
6		0.35	1200	—	—	1.0	(m_a, m_χ)

Table B.4 Input analyses used in 2HDM+a summary and combination.^[234]

Analysis/Scenario	1a	1b	2a	2b	3a	3b	4a	4b	5	6
$E_T^{\text{miss}} + Z(\ell\ell)$ ^[238]	x	x	x	x	x	x	x	x	x	
$E_T^{\text{miss}} + h(b\bar{b})$ ^[239]	x	x	x	x	x	x	x	x	x	x
$E_T^{\text{miss}} + h(\gamma\gamma)$ ^[240]	x	x			x	x	x	x		
$E_T^{\text{miss}} + h(\tau\tau)$ ^[241]	x			x						
$E_T^{\text{miss}} + tW$ ^[242]	x	x	x	x	x	x	x	x		
$E_T^{\text{miss}} + j$ ^[140]	x	x			x	x	x	x		
$h \rightarrow \text{invisible}$ ^[243]	x	x			x					x
$E_T^{\text{miss}} + Z(q\bar{q})$ ^[143]	x						x	x		
$E_T^{\text{miss}} + b\bar{b}$ ^[244]							x	x		
$E_T^{\text{miss}} + t\bar{t}$ ^[244-245]							x	x		
$t\bar{t}t\bar{t}$ ^[246]	x	x	x	x	x	x	x	x	x	
$tbH^\pm(tb)$ ^[247]	x	x	x	x	x	x	x	x	x	
$h \rightarrow aa \rightarrow f\bar{f}f'\bar{f}'$ ^[248-252]										x

signatures exhibit similar exclusion patterns on the m_a - m_A plane due to analogous production diagrams. With the lepton trigger and the lower mass of the Z boson, the $E_T^{\text{miss}} + Z(\ell\ell)$ channel demonstrates better sensitivity for lower m_A (lower E_T^{miss}). Conversely, the $E_T^{\text{miss}} + h(b\bar{b})$ channel achieves the best sensitivity among all $E_T^{\text{miss}} + h$ channels, excluding m_a values up to 500 GeV. The $E_T^{\text{miss}} + \text{jet}$, charged Higgs ($tbH^\pm$), and four-top signatures present distinctly different exclusion patterns compared to the $E_T^{\text{miss}} + Z$ and $E_T^{\text{miss}} + h$ channels, as they do not directly probe the mediator a . Notably, the charged Higgs channel provides the strongest exclusion limits across nearly the entire m_a range, offering valuable complementarity to earlier combinations that considered only the $E_T^{\text{miss}} + Z$ and $E_T^{\text{miss}} + h$ channels^[253].

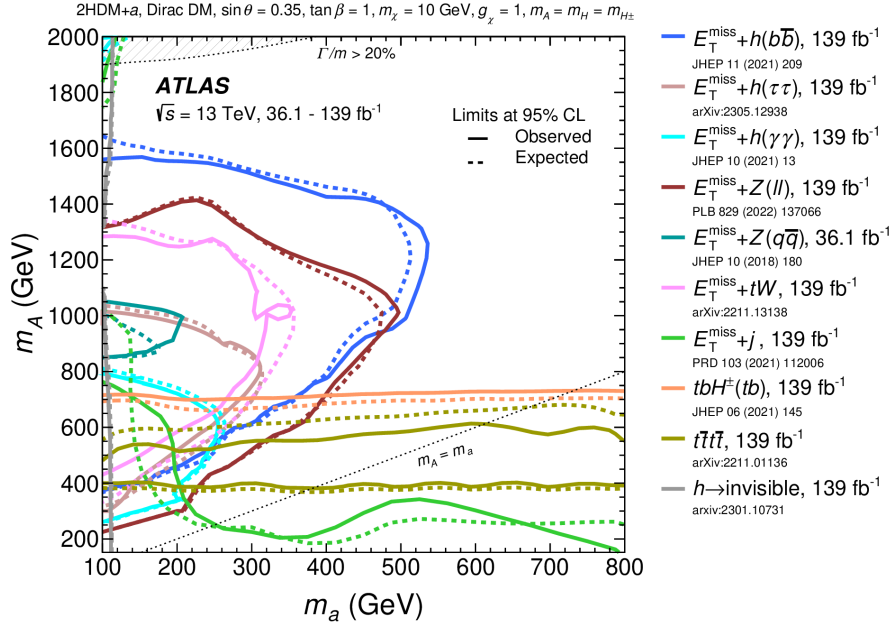


Figure B.3 Exclusion limits of individual analyses on the m_a - m_A scan of 2HDM+a model.

The three most sensitive channels— $E_T^{\text{miss}} + Z(\ell\ell)$, $E_T^{\text{miss}} + h(b\bar{b})$, and $tbH^\pm$ —are selected for statistical combination to achieve the strongest exclusion limits. Other analyses are excluded due to their significantly lower sensitivity and limited contributions to the overall results. However, combining all three analyses across the entire parameter space poses computational challenges, necessitating an optimized combination strategy.

B.2.1.1 Study of the Hybrid Combination Method

The Hybrid Combination strategy is proposed to enhance efficiency by selecting only the most sensitive channels for specific regions of the parameter space. In the area $m_A >$

1500GeV, $tbH^\pm$ channel is not relevant and only $E_T^{\text{miss}} + Z(\ell\ell)$ and $E_T^{\text{miss}} + h(b\bar{b})$ analyses are combined. When $m_A < m_a$ where $E_T^{\text{miss}} + X$ signature becomes off-shell, only $tbH^\pm$ limit is considered. In the region between all the three channels are combined.

The combined results are shown in Figure B.6. Compared to the individual analyses as Figure B.3, the inclusion of $tbH^\pm$ channel excludes additional parameter space, particularly in the overlap region around $(m_A, m_a) = (800, 400)$. To validate this strategy, an alternative scheme, as shown in Figure B.4—is tested. The results, with $\sin\theta=0.35$ for example shown in Figure B.5, demonstrate no major bias introduced by different schemes. The Hybrid Combination method achieves robust outcomes with significant computational savings.

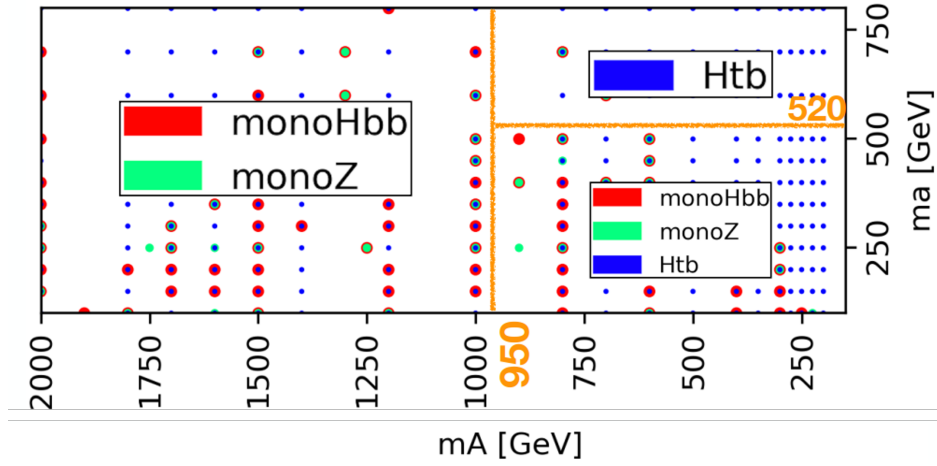


Figure B.4 Alternative combination scheme for the exclusion limits setting on the m_a - m_A scan of 2HDM+a model.

B.2.1.2 Study of Fine-Grained Signal Grids

During the statistical study in the early stage, it was observed that interpolation of the exclusion limit curves introduced significant biases, such as the one with $\sin\theta=0.7$ shown in Figure B.7. For instance, the combined limit excluded signals around $(m_A, m_a) = (800, 500)$, despite individual channels exhibiting limited sensitivity in this region. Further investigation revealed that these artifacts were caused by interpolation methods, particularly in regions where the exclusion limits vary significantly.

An intensive study was conducted to evaluate various interpolation methods, including different spline function setups. It was ultimately determined that interpolation alone could not reliably provide robust physical limits without directly evaluating the sensitivity at the

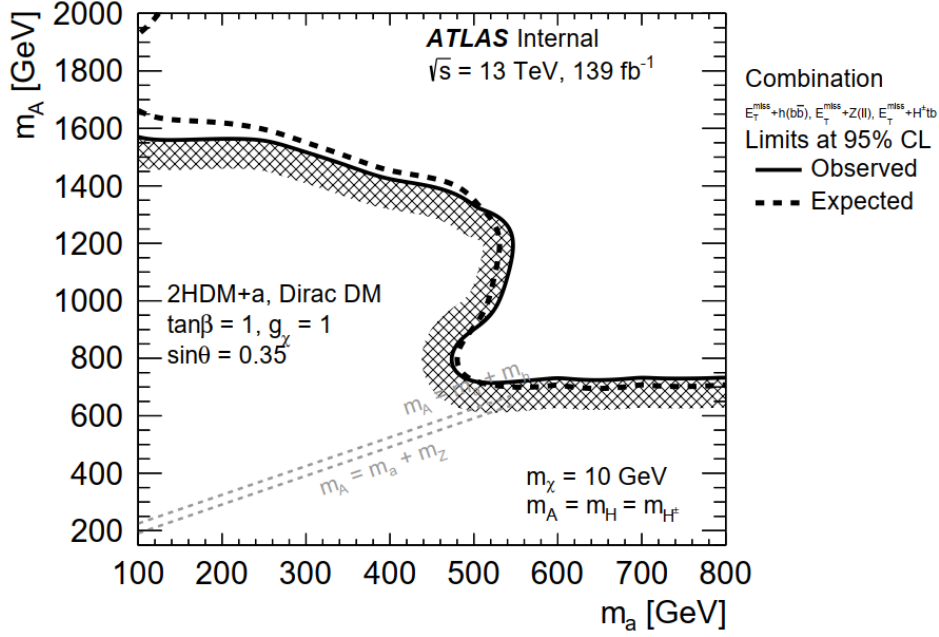


Figure B.5 Combined exclusion limits with alternative scheme on the m_a - m_A scan of 2HDM+a model.

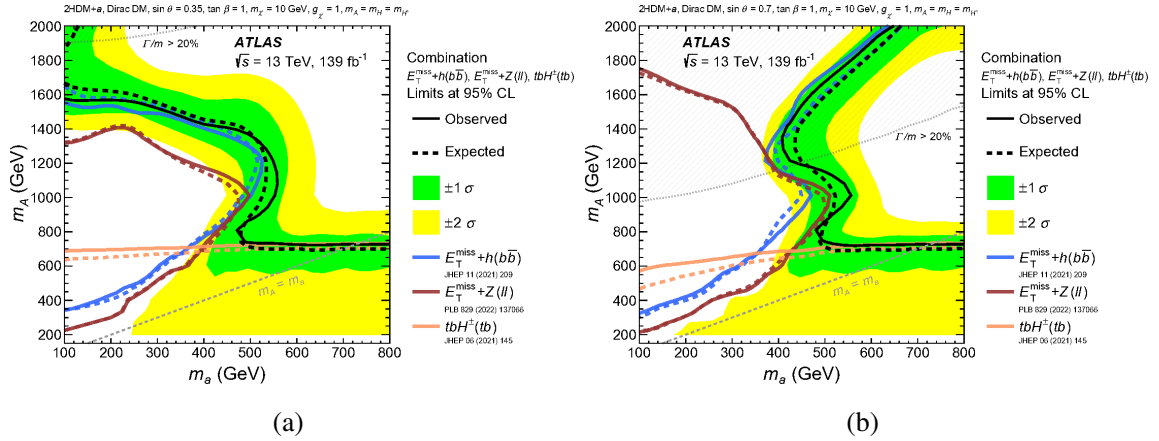


Figure B.6 Combined exclusion limits with Hybrid scheme on the m_a - m_A scan of 2HDM+a model. Observed (solid lines) and expected (dashed lines) exclusion regions at 95% CL in the (m_a, m_A) plane are shown assuming (left) $\sin \theta = 0.35$ (Scenario 1a) and (right) $\sin \theta = 0.7$ (Scenario 1b).^[234]

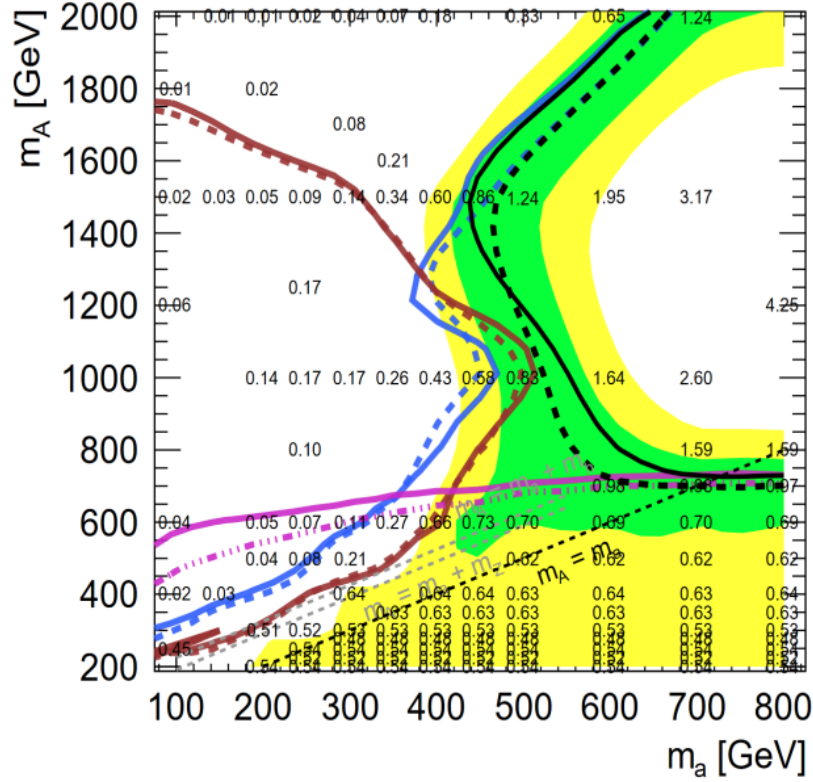


Figure B.7 Combined exclusion limits on the m_a - m_A scan of 2HDM+a model with few signal points.

signal points, especially in regions where the exclusion limits exhibit highly non-linear behavior with respect to the signal parameters.

To address this issue, a finer signal grid was implemented. By leveraging the efficiency of the Hybrid Combination strategy, the computational overhead was minimized, as not all signal points required evaluation by all channels. The refined ones, shown in the final results Figure B.6, present a smoother and more accurate combined exclusion curve, with interpolation artifacts effectively eliminated.

B.2.2 2HDM m_a/m_A - $\tan\beta$ Scan

This benchmark scenario is inspired by the mass- $\tan\beta$ parameterization used to summarize constraints on type-II 2HDM models, such as the hMSSM—a Minimal Supersymmetric extension of the SM with a lighter scalar state at a mass of 125 GeV^[254]. Similar $\sin\theta$ values are chosen at 0.35 and 0.7. The fixed mass parameter values are motivated by the exploration of fully invisible decays and constraints from existing measurements, such as B -meson decays^[235,255]. The summary is shown in Figure B.8.

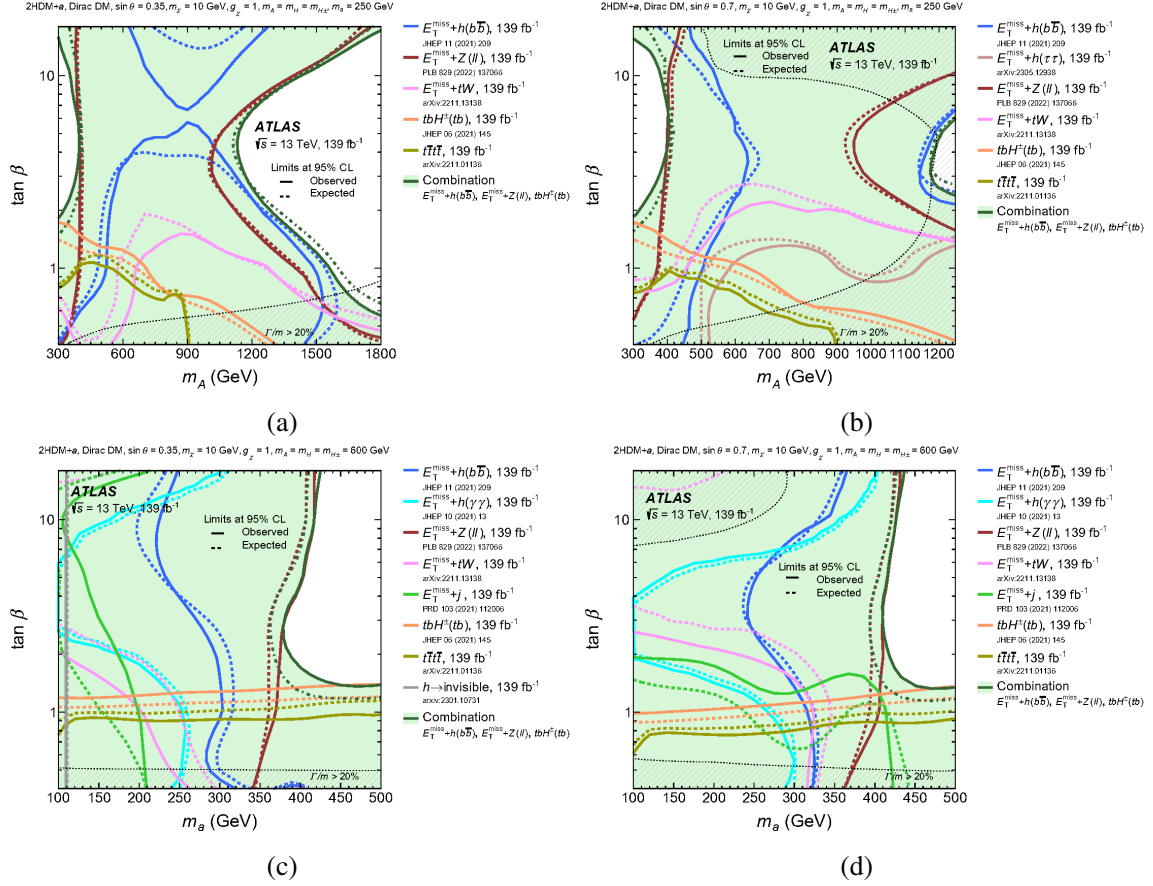


Figure B.8 Combined and individual exclusion limits on the m_a/m_A - $\tan\beta$ scan of 2HDM+a model. Observed (solid lines) and expected (dashed lines) exclusion regions at 95% CL in the upper (m_A , $\tan\beta$) and lower (m_a , $\tan\beta$) plane are shown assuming (left) $\sin\theta = 0.35$ (Scenario 2a/3a) and (right) $\sin\theta = 0.7$ (Scenario 2b/3b).^[234]

The $E_T^{\text{miss}} + Z(\ell\ell)$, $E_T^{\text{miss}} + h(b\bar{b})$, and $tbH^\pm$ channels provide the strongest sensitivity and are combined to establish the latest limits. The sensitivity of $E_T^{\text{miss}} + Z(\ell\ell)$ and $E_T^{\text{miss}} + h(b\bar{b})$ varies with $\tan\beta$: at high $\tan\beta$, $b\bar{b}$ -initiated production becomes dominant, while at low $\tan\beta$, the $tbH^\pm$ and four-top signatures show good sensitivity due to the preference for third-generation couplings.

B.2.3 Mixing $\sin\theta$ Scan

The scan of the mixing parameter highlights the interplay between invisible signatures ($E_T^{\text{miss}} + X$) and visible signatures (e.g., four tops). When $\sin\theta$ approaches zero, the Aha , HZa , and att couplings vanish, rendering the $E_T^{\text{miss}} + X$ diagrams irrelevant and the sensitivity of invisible signatures negligible. The summary results are shown in Figure B.9.

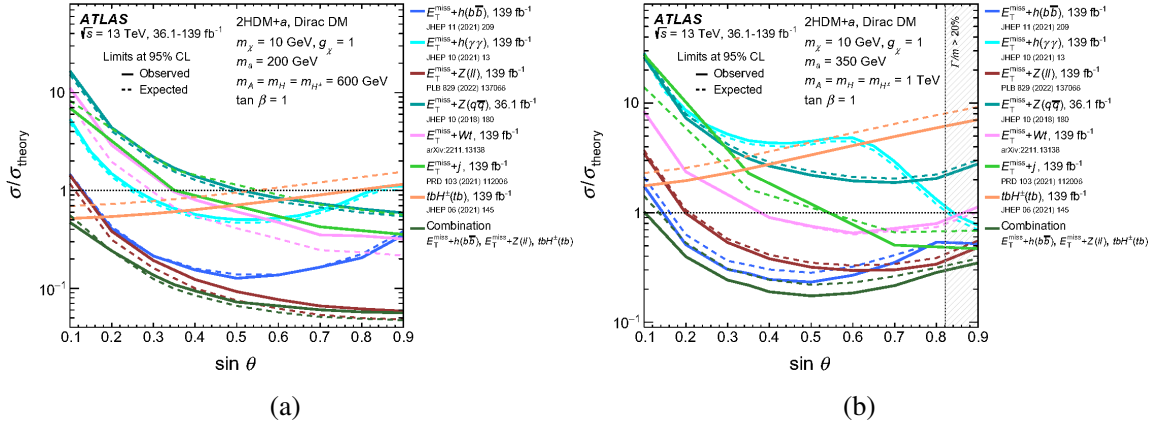


Figure B.9 Combined and individual exclusion limits on the cross-section as a function of $\sin\theta$ for 2HDM+a model. Observed (solid lines) and expected (dashed lines) exclusion regions at 95% CL with (upper) $m_A = 0.6$ TeV and (lower) $m_A = 1$ TeV are shown assuming $\tan\beta = 1$ (Scenario 4).^[234]

B.2.4 DM Mass m_χ Scan

Probing the DM mass enables cross-talk between collider experiments, cosmology, and direct/indirect detection experiments. The DM mass significantly affects non-collider constraints, especially the relic density as described in Sec. 2.2.2, which is observed in cosmology and constrains DM models if they overpredict it.

The summary results are shown in Figure B.10. The predicted relic density decreases when $m_\chi = \frac{1}{2}m_a$ or $\frac{1}{2}m_A$, as DM annihilation into a or A and subsequently into SM particles depletes the relic density. Low DM masses are disfavored due to overproduction of the

cosmological relic density. For high DM masses, the $tbH^\pm$ channel exhibits good sensitivity, excluding models at cross-sections 2-3 times the theoretical prediction. The sensitivity remains almost flat for all DM masses, as χ does not directly participate in the leading-order diagrams.

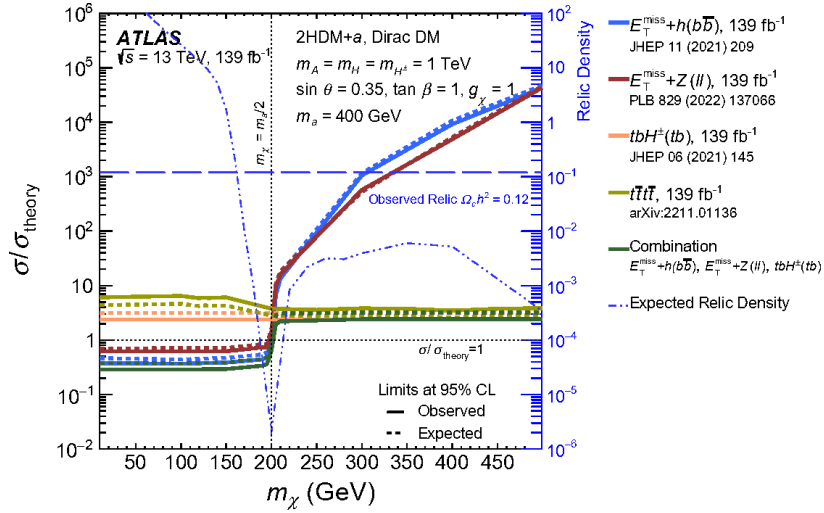


Figure B.10 Combined and individual exclusion limits on the cross-section as a function of m_χ for 2HDM+a model. Observed (solid lines) and expected (dashed lines) exclusion regions at 95% CL are shown assuming $m_A = 1.0$ TeV, $m_a = 400$ GeV, $\tan\beta = 1.0$, and $\sin\theta = 0.35$ (Scenario 5). The relic density for each m_χ assumption is superimposed in the plot (dashed line) and described by the right vertical axis.^[234]

B.2.5 m_a - m_χ Scan

Exotic decays of the light Higgs boson play a significant role in constraining the 2HDM+a model, particularly in the m_a - m_χ plane where the a mass is smaller than $\frac{1}{2}$ of the SM Higgs mass and twice the DM mass. As shown in Figure B.11, $H \rightarrow aa \rightarrow 4f$ searches exhibit strong sensitivity in regions where visible decays of a are favored and the SM Higgs channel is kinematically open. Sensitivity decreases at the J/ψ and Υ resonances due to mediator mass effects, but other regions are almost entirely excluded by these analyses. For $m_a > 2m_\chi$, invisible channels dominate, such as invisible Higgs decays or $E_T^{\text{miss}} + h(bb)$. However, these regions are disfavored by relic density constraints because DM annihilation into SM particles is kinematically forbidden at low DM masses.

In summary, the broad variety of searches in ATLAS, combined with cosmological constraints, excludes large areas of the parameter space in the 2HDM+a context. The

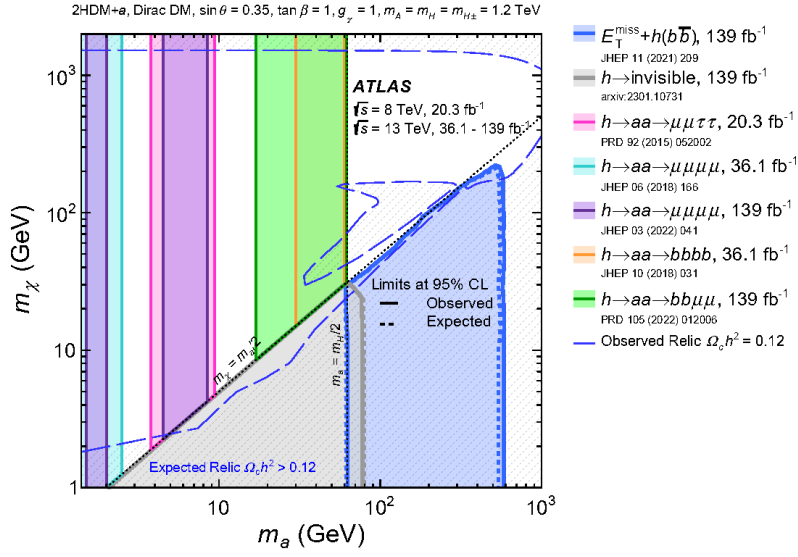


Figure B.11 Combined and individual exclusion limits on the m_a - m_χ scan of 2HDM+a model. Observed (solid lines) and expected (dashed lines) exclusion regions at 95% CL are shown assuming $m_A = 1.2$ TeV, $\tan \beta = 1.0$, and $\sin \theta = 0.35$ (Scenario 6). The relic density contour for the case $\Omega_c h^2 = 0.12$ is superimposed in the plot (long-dashed line). The shaded regions mark parameter values for which the model predicts a relic density greater than the cosmological observation.^[234]

benchmark performance of each channel and their complementarity provide critical insights for future collider DM searches, emphasizing the importance of combining all possible signatures and utilizing a wide spectrum of sensitive channels. These results demonstrate promising potential for future model-independent searches, as outlined in the final chapter of this thesis.

Appendix C Calorimeter R&D for the DarkSHINE Experiment

This chapter documents the research and development of the calorimeter for the proposed electron-on-target experiment, DarkSHINE, which aims to search for dark photons^[256]. Section C.1 provides an overview of the experiment, followed by an introduction to the electromagnetic calorimeter (ECAL) system^[257], which constitutes the primary focus of this study. The design of the calorimeter and the associated simulation techniques^[258] for efficient and accurate detector response modeling are discussed in Section C.2. Furthermore, a novel approach using generative machine learning (ML)^[259] for fast calorimeter simulation is presented in Section C.3.

C.1 Overview of the DarkSHINE Experiment

Despite extensive searches, no clear evidence has been observed for weakly interacting massive particles (WIMPs) at high mass scales, up to the TeV range^[21]. This has led to growing interest in the search for low-mass dark matter in the sub-GeV range. Among the various theoretical models predicting new physics in this regime, the dark photon framework provides a well-motivated extension, as discussed in Section 2.2.4. High-luminosity accelerator-based experiments at appropriate energy scales offer a direct avenue for producing low-mass dark matter particles. However, the challenges posed by the low cross-sections and overwhelming backgrounds necessitate innovative detector technologies and experimental strategies.

The DarkSHINE experiment is designed to search for massive dark photons using an 8 GeV electron beam with a high repetition rate of up to 10 MHz, delivered by the Shanghai High Repetition-Rate XFEL and Extreme Light Facility (SHINE)^[260]. With an annual electron-on-target (EOT) count of approximately 3×10^{14} , largely consisting of single electrons, DarkSHINE will significantly enhance the sensitivity for dark photon production with sub-GeV mass^[256]. This unprecedented event rate, combined with the advanced detector design, provides substantial advantages over existing experiments operating in similar energy ranges, including NA64^[261], BELLE-II^[262], BES-III^[263], LDMX^[264] and so on.

The experimental principle of the dark photon search at DarkSHINE is illustrated in

Figure C.1. The experiment focuses on the invisible decay channel, where the dark photon manifests as missing energy and momentum in the detector. Precise measurements of electron momentum and energy are therefore crucial, motivating the use of a multi-layer silicon-based tracker^[265] and a high-resolution, LYSO crystal-based electromagnetic calorimeter (ECAL)^[257].

An incident electron interacts with the tungsten target, generating a dark photon. This process results in a recoiling electron with largely reduced energy and a significant angular deviation, as depicted in Figure C.2. The tracker system measures the electron momentum before and after the target, while track reconstruction aids in determining the recoil angle. The ECAL ensures accurate energy measurements for the electron and other final-state particles, leveraging its full absorption design and high granularity, which enhances signal-background discrimination. The primary background originates from nuclear interactions, characterized by lower energy losses and smaller recoil angles, as illustrated in Figure C.3. Additionally, the hadronic calorimeter (HCAL), constructed from plastic scintillators and steel absorbers with dimensions of $10\text{ m} \times 10\text{ m}$, is designed to detect escaping neutral hadrons and muons^[266].

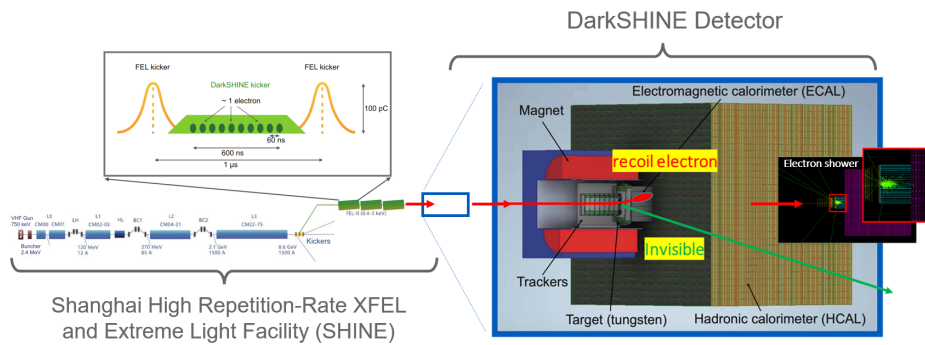


Figure C.1 Schematic illustration of the DarkSHINE experiment.

C.2 Electromagnetic Calorimeter (ECAL) Study

The ECAL is a crucial component of the DarkSHINE detector system, optimized for high-precision energy measurement with fine granularity to facilitate advanced reconstruction algorithms. Its design is illustrated in Figure C.4.

Charged particles traversing the dense crystal material deposit energy primarily via electromagnetic interactions, producing scintillation or Cherenkov light. To maximize light yield and minimize response time, LYSO crystal^[267] is chosen as the active medium, offering

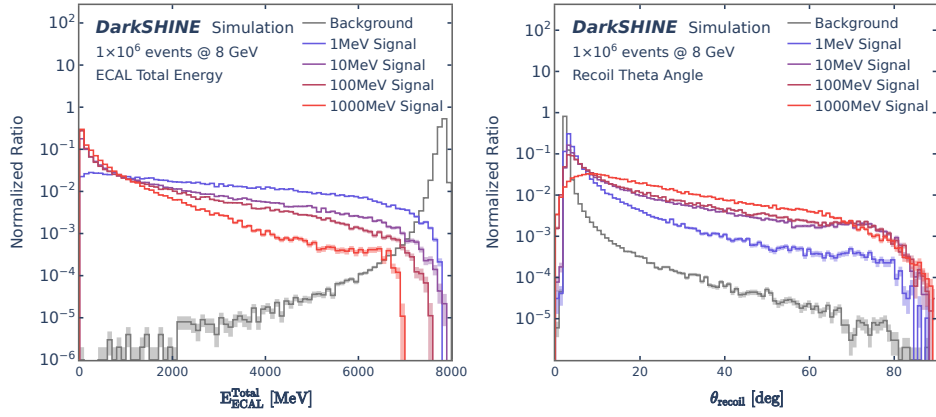


Figure C.2 Energy deposition in the ECAL and the recoil angle of the electron in the dark photon production process^[258]. Most of the energy of recoiled electron is deposited in the ECAL.

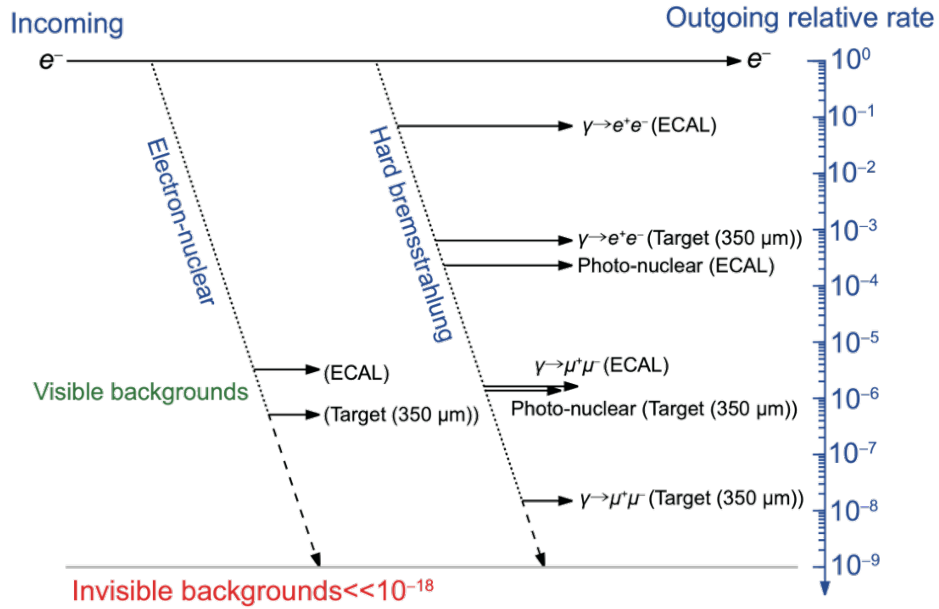


Figure C.3 Dominant background sources in the DarkSHINE experiment^[256], categorized by interaction location ("ECAL" or "Target").

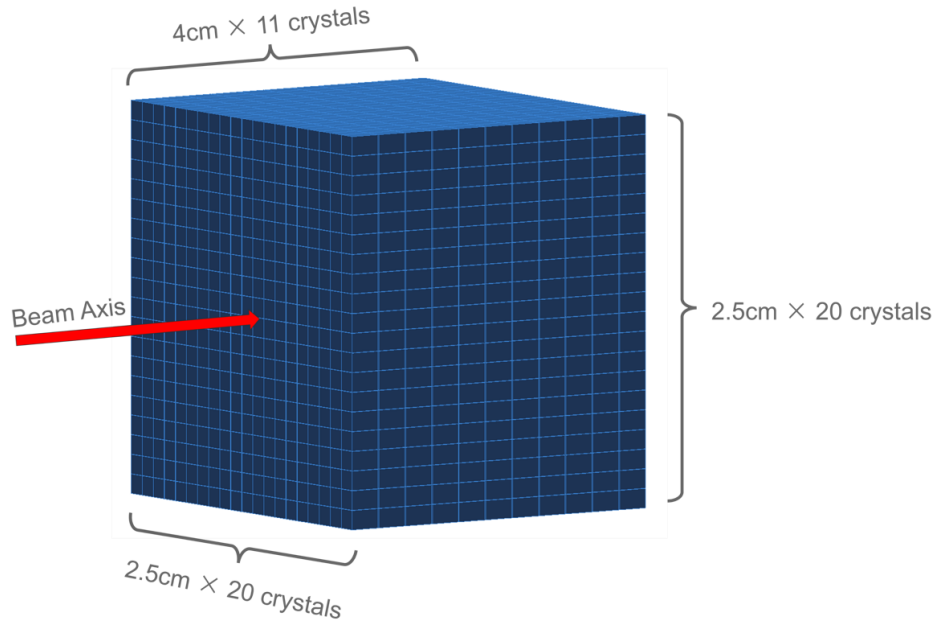


Figure C.4 Design of the electromagnetic calorimeter (ECAL).

over 30,000 photons per MeV of deposited energy and 40 ns light decay time.

Each crystal unit ($2.5\text{ cm} \times 2.5\text{ cm} \times 4\text{ cm}$) is read out by a silicon photomultiplier (SiPM) sensor, which provides high gain and fast response, connected to a pre-amplifier and readout electronics. The detector design features a high granularity of $20 \times 20 \times 11$ readout channels. To enhance light collection efficiency, each crystal unit is wrapped in Enhanced Specular Reflector (ESR) film with over 98% reflectivity and coupled to the SiPM using optical glue with a matched refractive index.

A dedicated GEANT4-based^[165] simulation framework has been developed to model particle interactions and material effects in the ECAL. The detailed structure, material properties, and geometric parameters are implemented to balance simulation fidelity with computational feasibility.

C.2.1 Optical Simulation

Light propagation and reflection within the calorimeter unit significantly influence the detector's energy resolution and timing performance. To model these effects accurately, optical simulation is enabled in the GEANT4 framework.

Optical processes—such as photon propagation, absorption, reflection, refraction, and sensor detection—are modeled independently of other physics processes, as handled by

GEANT4's Material-Property-Table (MPT)^[165]. Key optical parameters used in the simulation, including light yield, scintillation properties, refractive indices, and absorption lengths, are listed in Table C.1. Variable parameters, such as wrapper reflection and SiPM efficiency, are determined from laboratory measurements and set to nominal values in the current study.

Parameters	Value	Unit
Light Yield	(Variable)	ph/MeV
FastTimeConstant	40	ns
ScintillationPhotonDist.	0.1, 2.21, 2.58, 2.82, 2.95, 3.10, 4.00	eV
ScintillationStrength	0.0, 0.23, 0.85, 1.93, 2.15, 1.08, 0.0	-
RefractionIdx	1.85, 1.833, 1.821, 1.813, 1.809, 1.804, 1.79	-
AbsorptionLength	40(flat)	cm
WrapperSurface	dielectric_LUT/polishedtyvekair	-
WrapperReflection	(Variable)	-
SiPMSurface	dielectric_LUT/polishedvm2000glue	-
SiPMEfficiency	(Variable)	-

Table C.1 Optical parameters used in the ECAL study.

The optical simulation begins with the generation of scintillation photons, which are then tracked as they propagate within the crystal unit. Each photon undergoes reflection, refraction, or absorption based on the surface properties and material characteristics. This process is computationally intensive, particularly for high light-yield materials where millions of photons are generated per calorimeter unit. A full optical simulation of light transport within a single ECAL unit is shown in Figure C.5. The photons travel from their emission points, interacting with the boundaries and crystal material before reaching the SiPM sensor.

Since the full ECAL comprises 4400 units, running a complete optical simulation for each event is computationally impossible. To address this, a Look-Up-Table (LUT) method has been developed, significantly accelerating the simulation. The LUT approach approximates photon transport as a probability function that maps emission coordinates to detection efficiency, thereby saving the time for explicit photon tracking. This method is illustrated in Figure C.6.

The LUT is constructed using small datasets with full optical simulation, producing efficiency maps for different surface reflectivity and SiPM efficiency settings. Figures C.7 and C.9 illustrate these efficiency distributions. The LUT-based simulation produces the compatible results of the full simulation while achieving a speedup of over an order of magnitude, as demonstrated in Figures C.10 and C.11.

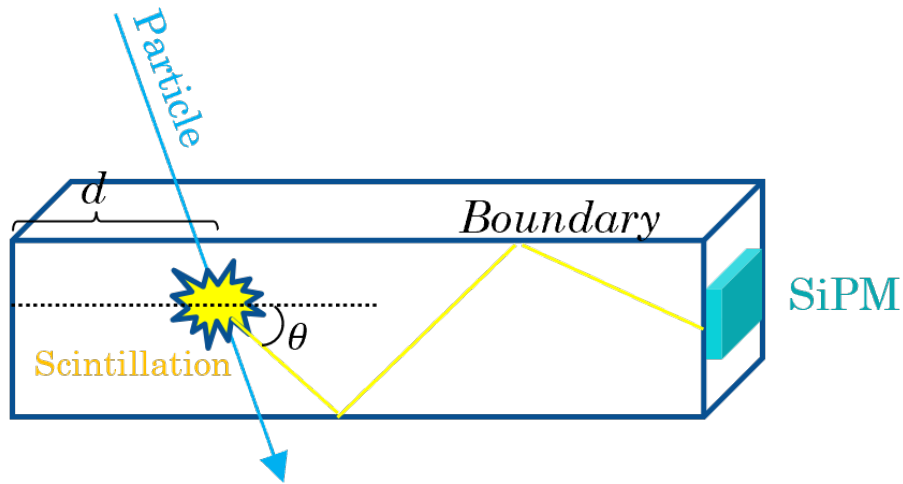


Figure C.5 Simulation of optical photon propagation within a single calorimeter unit. The parameters d and θ define the emission point and angle of the optical photon.

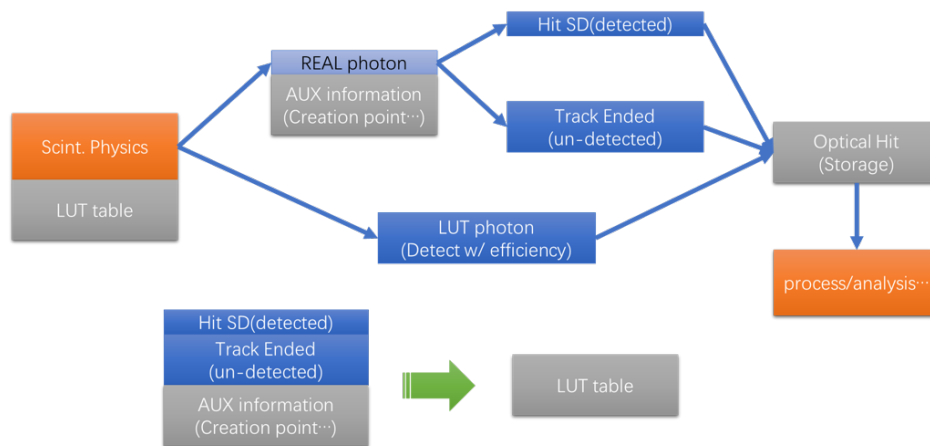


Figure C.6 Workflow of the LUT-based optical simulation. The LUT maps emission parameters (d, θ) to detection probabilities, enabling a significant reduction in computational overhead.

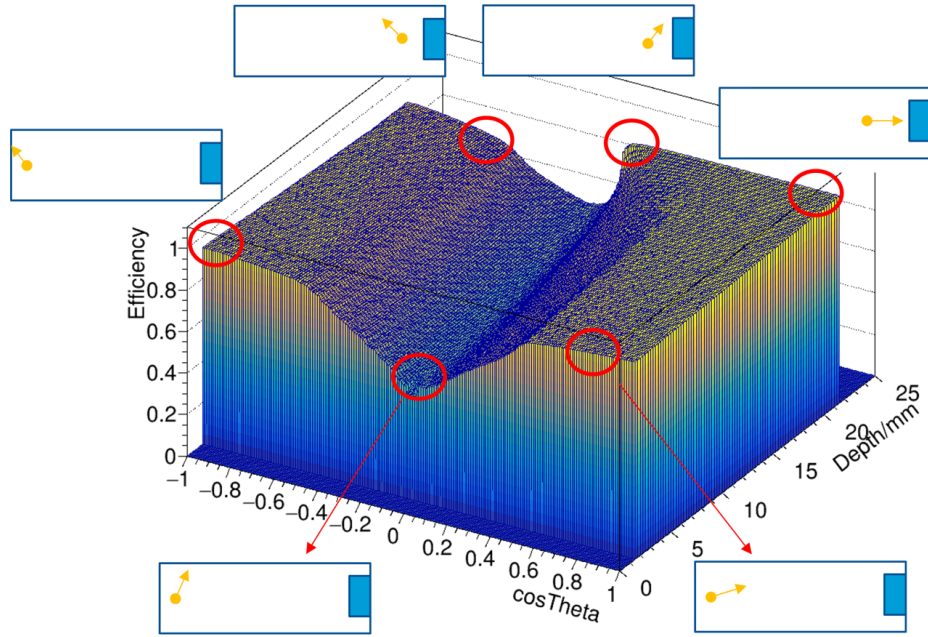


Figure C.7 Photon detection efficiency for different emission coordinates (d, θ) within a crystal unit. Simulation assumes 100% wrapper reflection and SiPM efficiency.

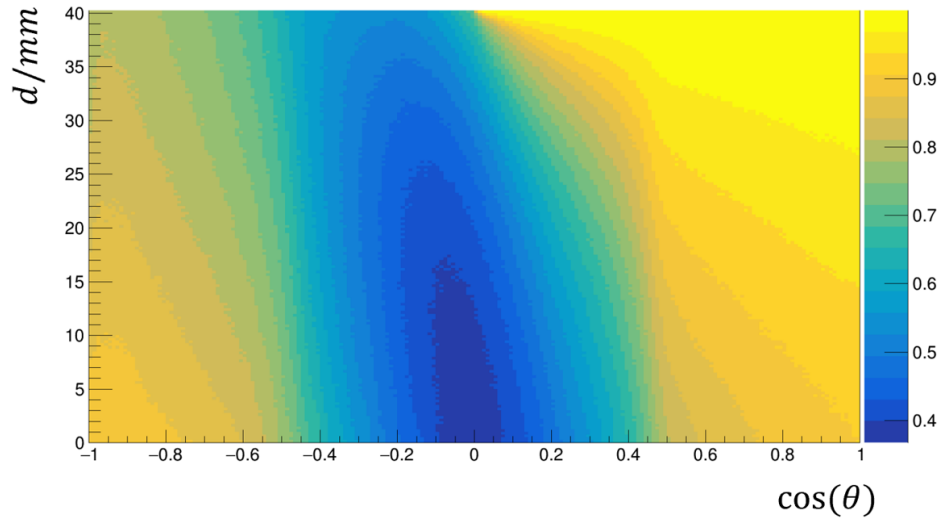


Figure C.8 Detection efficiency map for optical photons in a single calorimeter unit with 100% wrapper reflection and SiPM efficiency.

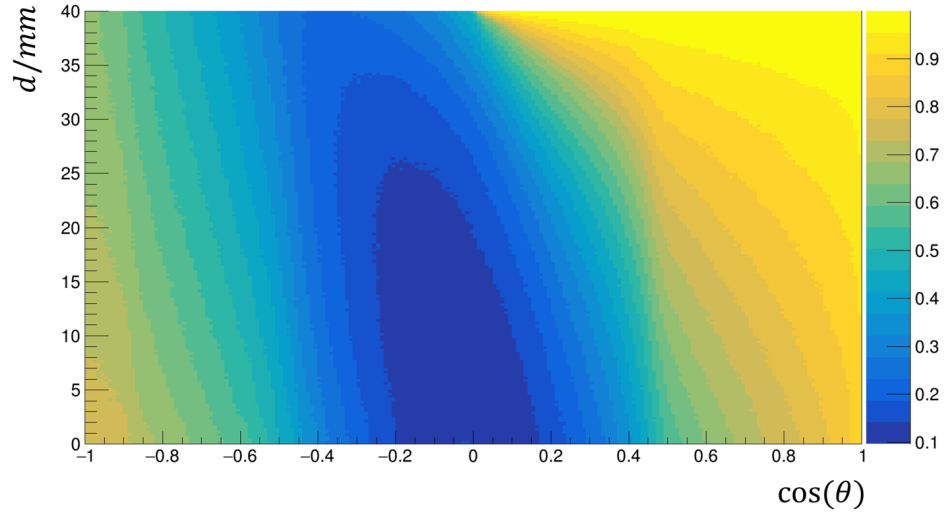


Figure C.9 Detection efficiency map for optical photons in a single calorimeter unit with 90% wrapper reflection and SiPM efficiency.

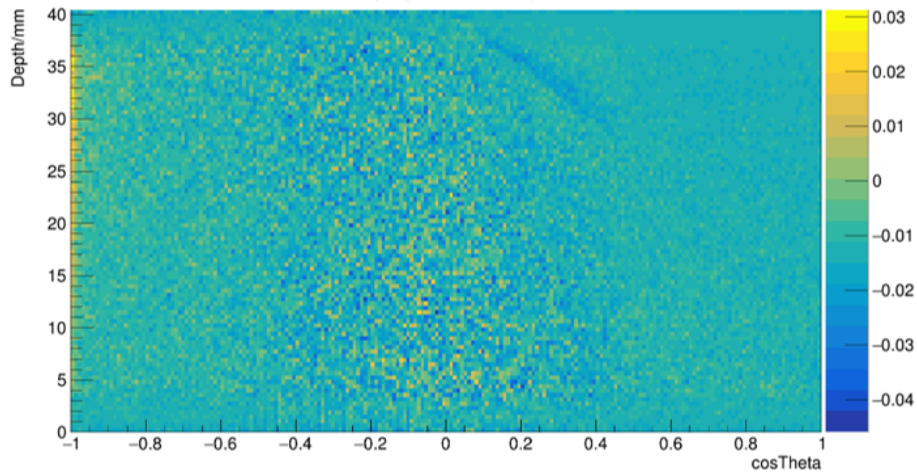


Figure C.10 Validation of the LUT-based simulation against full optical simulation. The values indicate the relative difference in photon detection efficiency.

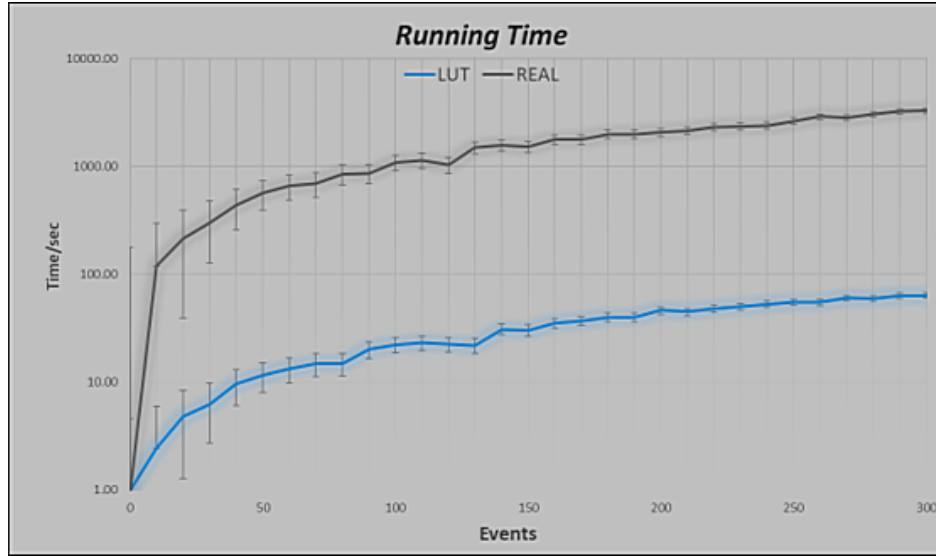


Figure C.11 Computational speedup achieved using the LUT-based optical simulation compared to the full simulation.

C.2.2 Digitization and Fast Smearing

Accurate simulation of the ECAL response requires modeling of both the optical processes and digitization effects of electronics. The digitization process involves summing the single photon pulses from the SiPM sensor, simulating the analog-to-digital conversion (ADC), including signal clamping and gain adjustments. The primary digitization parameters are listed in Table C.2.

Parameter	Value	Unit
SiPM Pixel Count	57,600	-
SiPM Pixel Recovery Time (τ)	50	ns
ADC Bit Width	12 (4096 levels)	-
ADC Sampling Interval	1.25	ns
ADC Maximum Time Window	100	ns
ADC Dynamic Range	5000	mV
ADC Noise (σ)	5	mV

Table C.2 Digitization parameters for the ECAL simulation.

To efficiently model the calorimeter response in the full detector simulation, a fast energy smearing method is implemented. The single-unit response is first simulated with the LUT-based optical simulation and digitization. The energy response is characterized by fitting log-normal functions for electrons incident at discrete energy levels (10, 20, 50, 100, 200,

500, 1000, 2000, 4000, and 8000 MeV). The fitted σ , the energy resolution, as a function of incident energy is then parameterized using the standard calorimeter resolution formula:

$$\frac{\sigma}{E} = \frac{A}{\sqrt{E}} \oplus B \oplus \frac{C}{E}. \quad (\text{C.1})$$

The extracted parameters (A , B , and C) are applied to the full-scale ECAL simulation. Energy deposition in each crystal unit, denoted as the "truth" energy, undergoes Gaussian smearing based on the fitted resolution parameters. This approach enables realistic detector response simulation while maintaining computational efficiency.

Table C.3 summarizes the four ECAL configurations considered, accounting for variations in wrapper reflectivity and crystal properties. The extracted smearing parameters are listed in Table C.4. The four setups were ultimately incorporated into the prospective study of the DarkSHINE experiment to evaluate the expected sensitivity while accounting for realistic detector effects, as discussed in Ref^[256]. Preliminary analyses based on total energy response indicate that, after calibration, the different configurations have minimal impact, confirming the robustness of the ECAL design. The effects on shower shape reconstruction and multivariate analysis are currently being investigated in follow-up studies. This work establishes an efficient simulation methodology that will support future R&D efforts.

Table C.3 ECAL unit configurations.

	Cube Dimensions	Wrapper	SiPM Size (mm^2)	Coupling $\times$ QE (%)	Yield/MeV
R90_LYSO	2.5 $\times$ 2.5 $\times$ 4 cm	Ref=90%	9	20%	30000 (LYSO)
R10_LYSO	2.5 $\times$ 2.5 $\times$ 4 cm	Ref=10%	9	20%	30000 (LYSO)
R90_S9_PWO4	2.5 $\times$ 2.5 $\times$ 4 cm	Ref=90%	9	20%	200 (PWO)
R90_S36_PWO4	2.5 $\times$ 2.5 $\times$ 4 cm	Ref=90%	36	20%	200 (PWO)

Table C.4 Extracted energy smearing parameters for the ECAL fast smearing.

	$A/\sqrt{\text{GeV}}$	B	C/MeV
R90_LYSO	1.00%	0.00%	0.0000
R10_LYSO	6.69%	0.00%	0.0851
R90_S9_PWO4	4.26%	0.70%	0.0001
R90_S36_PWO4	2.32%	0.17%	0.7051

C.3 Generative Machine Learning for Fast Calorimeter Simulation

Despite the optimizations discussed in previous sections, simulating high-granularity calorimeters remains computationally expensive, particularly for the DarkSHINE experi-

ment, which aims to detect extremely rare processes and requires large-scale event statistics. Traditional GEANT4-based simulations become increasingly resource-intensive as the energy of incident particles rises due to the need for detailed tracking of secondary particles. To address this challenge, a novel generative machine learning (ML) approach based on Vector-Quantized Variational Autoencoders (VQ-VAE), Calo-VQ^[259], has been developed to significantly accelerate calorimeter simulations.

This ML-based approach conceptualizes calorimeter response as high-dimensional data, similar to image generation in deep learning. It employs a two-stage generation strategy: first, compressing spatially structured calorimeter data into a discrete latent space, and second, generating new calorimeter responses using a transformer-based model. Extensive validation on the CaloChallenge dataset^[268] demonstrates that this method achieves a remarkable speedup of approximately 2000 times over traditional simulations, generating calorimeter showers within milliseconds while maintaining high fidelity.

C.3.1 Dataset and Calorimeter Benchmarking

The CaloChallenge dataset provides a standardized benchmark for high-energy physics calorimeter simulations. The dataset's second configuration (Dataset2^[268]) employs a cylindrical calorimeter design with a granularity comparable to the DarkSHINE ECAL, consisting of 45 layers segmented into 15 radial and 9 angular bins, resulting in 6480 readout channels. Showers induced by single electrons with energies logarithmically distributed between 1 GeV and 1 TeV are simulated using GEANT4 and stored for ML training.

C.3.2 Model Architecture

The architecture of the VQ-VAE-based generative calorimeter simulation is illustrated in Figure C.12. The first stage of the model, designed for representation learning of the calorimeter response, follows an encoder-decoder paradigm, where high-dimensional calorimeter showers (termed `calo-image`) are mapped to discrete latent representations (`calo-language`). These discrete latent codes mimic the tokenization approach used in large language models^[269] such as GPT^[270].

Vector quantization (VQ) techniques^[271] are applied to enforce discrete representations, wherein the encoder learns to compress calorimeter data into a set of representative codebook vectors. Only the indices of these quantized vectors are stored, drastically reducing data

complexity. An adversarial loss^[272] is introduced in the autoencoder training, as shown in Figure C.13, to mitigate the blurring effects common with conventional L2-loss autoencoders, thereby enhancing fidelity. To respect the cylindrical geometry of the detector, specialized convolutional operators and Fourier-based resampling techniques are incorporated to enforce rotational invariance.

In the second stage, the transformer-based generative model is trained to produce sequences of `calo-language` tokens conditioned on the incident particle's energy. The generated tokens are then decoded back into full calorimeter responses.

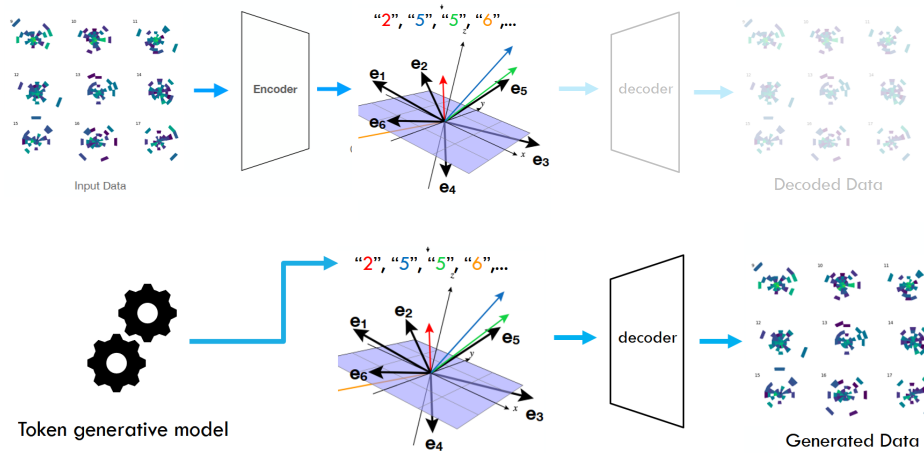


Figure C.12 Overview of the Calo-VQ algorithm. The first stage (top) performs representation learning, while the second stage (bottom) handles calorimeter response generation.

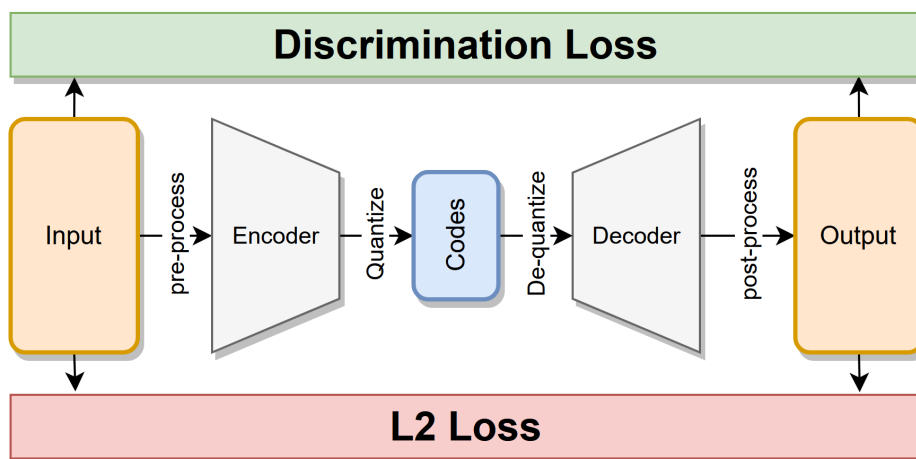


Figure C.13 Architecture of the Stage-1 VQ-VAE representation learning model.

C.3.3 Performance and Validation

The generative ML model achieves calorimeter shower generation times of less than 1 ms per event, independent of incident particle energy. This results in a speedup exceeding 2000 times compared to GEANT4-based simulations, which typically require several seconds per event especially for high energy incident. Figure C.14 compares the average energy deposition patterns between ML-generated and GEANT4-simulated showers for a representative calorimeter layer, demonstrating strong agreement.

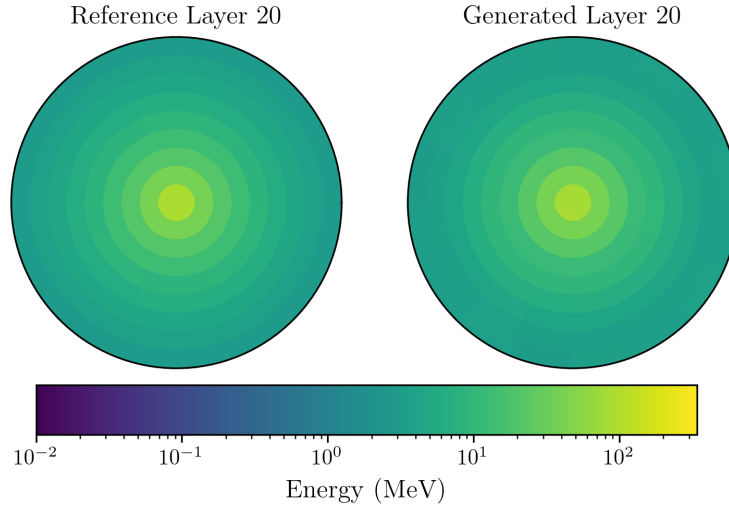


Figure C.14 Average energy deposition per calorimeter cell in layer 20 for single electron showers. Left: GEANT4 reference; Right: ML-generated response.

To quantitatively evaluate the fidelity of the generated showers, key physics observables—including the total deposited energy and spatial shower profiles—are compared against GEANT4 references. Figure C.15 shows the total energy response distribution for electron showers, where the ML-generated distribution closely matches the GEANT4 results. The separation metric, defined as

$$D = \sum_{\text{bins}} \frac{(n' - n)^2}{2(n' + n)}, \quad (\text{C.2})$$

is computed for various observables and found to be below 0.005, indicating excellent agreement. Furthermore, shower shape observables, such as energy-weighted radial and

longitudinal moments, are validated with discrepancies below 0.1 in the separation metric. Further metrics and detailed results can be found in the publication^[259].

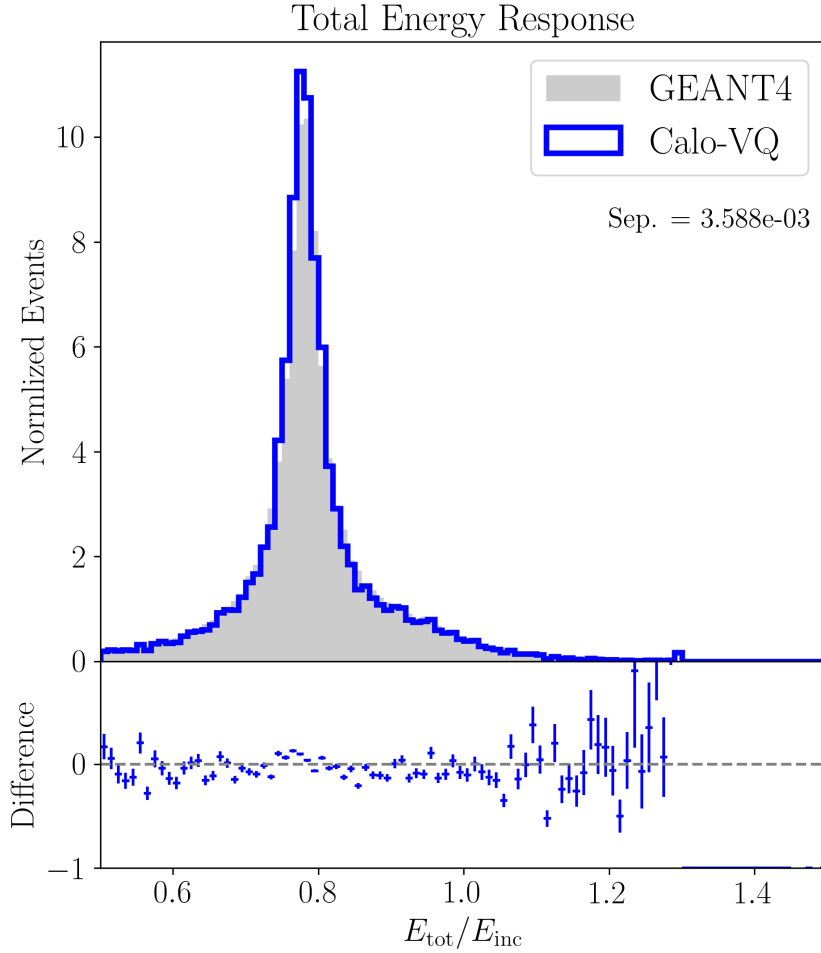


Figure C.15 Total energy response distribution for electron showers. The ML-generated distribution (orange) closely follows the GEANT4 reference (solid blue).

C.3.4 Outlook and Future Directions

The Calo-VQ algorithm represents a significant step towards leveraging generative ML models for fast, high-fidelity calorimeter simulations in high-energy physics. This approach enables large-scale event generation required for rare event searches, such as DarkSHINE, while maintaining computational efficiency. Ongoing work aims to integrate this ML-based simulation into the DarkSHINE analysis framework, ensuring its robustness across different

detector configurations and physics scenarios.

The success of ML-driven calorimeter simulations opens new avenues for experimental high-energy physics, where advanced AI techniques can complement traditional simulation pipelines. Future developments will focus on refining model architectures, expanding datasets, and optimizing inference efficiency. Ultimately, such innovations may contribute to groundbreaking discoveries in the dark sector.

Appendix D Differential Measurement of Vector Boson Scattering (VBS) $Z\gamma$

The vector boson scattering is a rare and crucial Standard Model process that provides a powerful test of electroweak (EW) symmetry breaking and serves as a sensitive probe for physics beyond the Standard Model. This analysis studies the VBS process of a Z boson and a photon, in association with two jets, and with the Z boson decays into a pair of leptons (electrons or muons). The process, denoted as $Z(\ell\ell)\gamma jj$, is measured using the full Run2 140 fb^{-1} of proton-proton collision data collected by the ATLAS detector at $\sqrt{s} = 13 \text{ TeV}$ during 2015-2018.

This section provides an overview of the measurement^[273], for which I have served as the analysis contact since 2022, with particular emphasis on the study of a new unfolding method – a key technique that enables the differential cross-section measurement of this rare process, in the presence of a large amount of backgrounds. The chapter is organized as follows: the physics motivation is presented in Sec. D.1; a summary of the analysis method and the inclusive cross-section measurements is given in Sec. D.2; and the differential measurements, together with the unfolding study, are detailed in Sec. D.3.

D.1 VBS $Z\gamma$ Process

The vector boson scattering (VBS) process is characterized by the presence of a three- or four-vector-boson vertex, as illustrated in Fig. D.1. In the Standard Model (SM), the gauge symmetry regulates the divergences in these interactions, and any new physics that modifies this regulation would lead to significant deviations of the production cross section from SM predictions. In particular, fully neutral quartic vertices such as $ZZZ\gamma$ are forbidden at the lowest order in the SM and the $WWZ\gamma$ vertex provides sensitivity to anomalous quartic gauge couplings (aQGCs). Therefore, the study of the EW production of $Z\gamma$ via VBS offers a precise probe of the gauge-boson self-interaction and the non-Abelian nature of the electroweak sector, as well as potential new physics at the TeV scale.

There are other EW non-VBS processes that can produce the same final states and cannot be uniquely separated due to unitarity, as shown in Fig. D.2. Consequently, the analysis

measures the total EW production of the $Z\gamma jj$ final state. In addition, the same final state can also arise from QCD-induced processes, such as gluon exchange or gluon radiation, as depicted in Fig. D.3. These QCD-induced events typically have a much larger cross section and exhibit enhanced hadronic activity between the two jets due to color connections, resulting in kinematic distributions that differ from those of EW-induced events. In contrast, the vector bosons tend to be produced between two quarks that are well separated in rapidity in EW events, leading to a specific topology and kinematic features such as large dijet invariant mass m_{jj} and rapidity separation Δy_{jj} . The interference between the EW and QCD contributions, arising from their identical final states, is expected to be small – at the level of about 7% in this analysis – based on theoretical calculations and previous studies^[274].

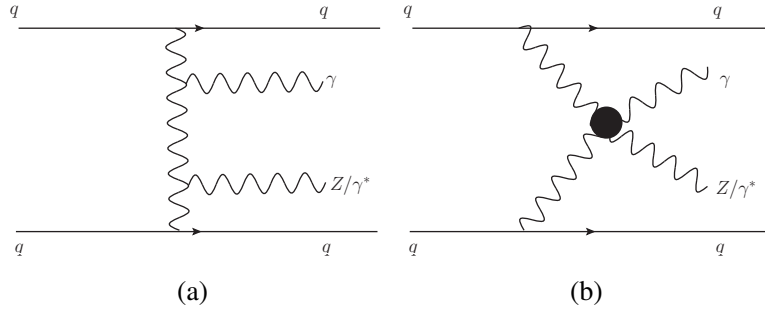


Figure D.1 Feynman diagrams of EW vertices in $Z\gamma jj$ process involving VBS subprocesses.

D.2 Analysis Methods

The analysis is designed to extract the EW $Z\gamma$ production, particularly in the high dijet mass region ($m_{jj} > 500$ GeV), which is more sensitive to potential new physics. In addition, the total EW+QCD production cross section is measured to provide reference for precise QCD studies over the full m_{jj} range ($m_{jj} > 150$ GeV). A cut-based method, developed based on the previous study^[274], is employed to separate the EW and QCD components by exploiting the distinct kinematic features between EW- and QCD-induced $Z\gamma$ processes, as well as to discriminate against other backgrounds such as fake photons and $t\bar{t}\gamma$.

D.2.1 Object and Event Selections

The following object and event selections are applied to enhance the purity of the EW $Z\gamma$ signal:

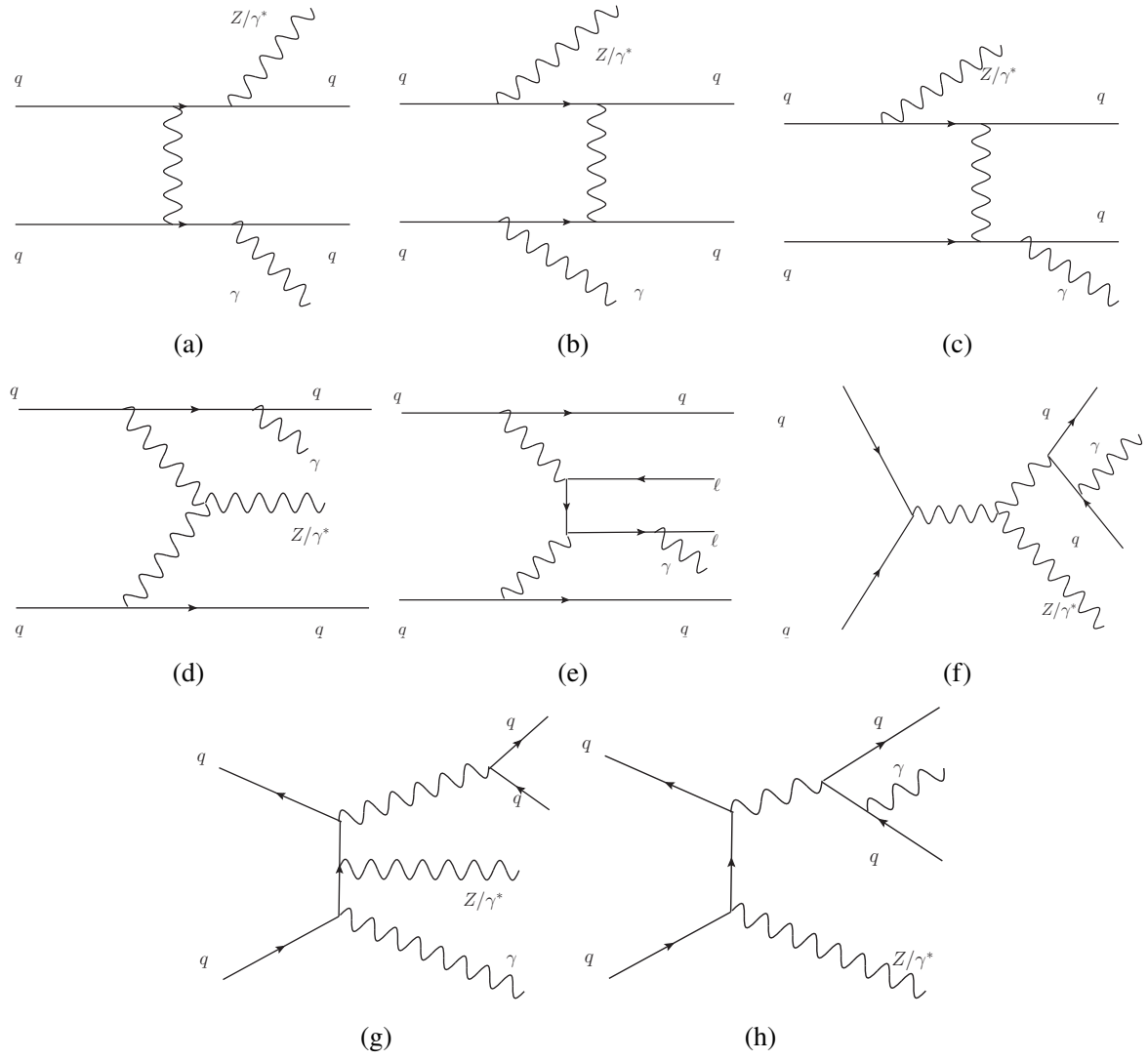


Figure D.2 Feynman diagrams of non-VBS EW vertices in $Z\gamma jj$ process.

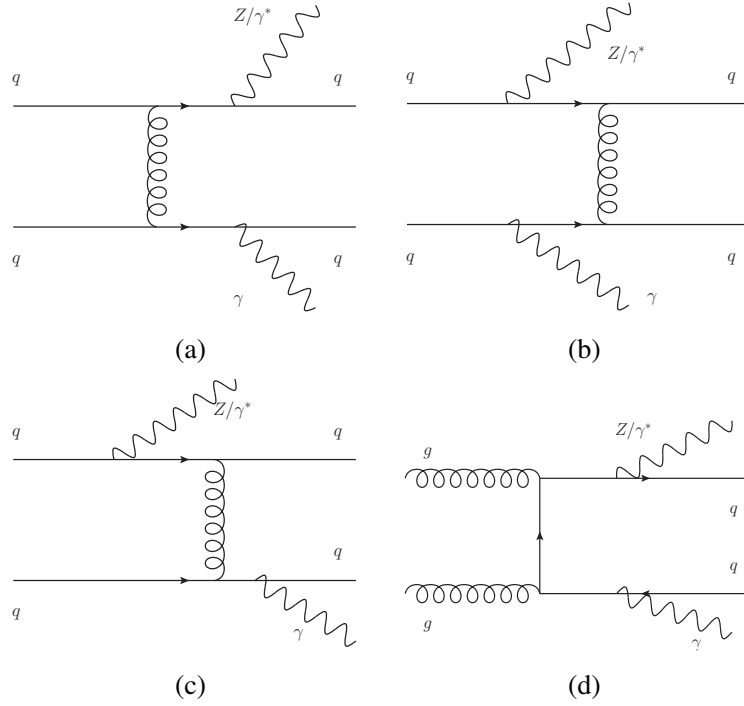


Figure D.3 Feynman diagrams of QCD vertices in $Z\gamma jj$ process.

Object selection.

- **Electrons:** $p_T > 20$ GeV, $|\eta| < 2.47$, excluding the calorimeter transition region ($1.37 < |\eta| < 1.52$). Track requirements include $|d_0/\sigma(d_0)| < 5$ and $|z_0 \sin \theta| < 0.5$ mm. The Medium identification criteria and FCLoose isolation working point are applied^[76].
- **Muons:** $p_T > 20$ GeV, $|\eta| < 2.5$, $|d_0/\sigma(d_0)| < 3$, and $|z_0 \sin \theta| < 0.5$ mm. The Medium muon identification criteria and PflowLoose_FixedRad isolation are used^[275].
- **Photons:** $p_T > 15$ GeV, $|\eta| < 2.37$, excluding the region $1.37 < |\eta| < 1.52$. Both converted and unconverted photons are included. The Loose identification working point is applied^[76].
- **Jets:** Anti- k_t jets with radius parameter $R = 0.4$, reconstructed using particle-flow inputs. Jets are required to have $p_T > 25$ GeV and $|y| < 4.4$. The LooseBad jet cleaning and the default Tight JVT requirements are applied.^[84,92]

All reconstructed objects are required to pass the standard overlap removal procedure described in Ref.^[273].

Event selection.

- Exactly two opposite-sign, same-flavor leptons are required, with the leading lepton $p_T > 30$ GeV.
- Events must contain at least two jets, with the two leading jets required to have $p_T > 50$ GeV, $|\Delta y_{jj}| > 1$, and $m_{jj} > 150$ GeV.
- The highest- p_T photon in the event is selected. It must satisfy `Tight` identification and `FixedCutLoose` isolation, with $p_T > 25$ GeV^[76].
- The dilepton invariant mass must satisfy $m_{\ell\ell} > 40$ GeV, and the sum of $m_{\ell\ell\gamma} + m_{\ell\ell} > 182$ GeV to suppress final-state radiation (FSR) events^[274].
- Events containing no unclean jets^[276].
- The centrality variable,

$$\zeta(\ell\ell\gamma) = \left| \frac{y_{\ell\ell\gamma} - (y_{j_1} + y_{j_2})/2}{y_{j_1} - y_{j_2}} \right|,$$

is required to satisfy $\zeta(\ell\ell\gamma) < 0.5$.

- No additional jet with $p_T > 25$ GeV is allowed in the rapidity interval between the two leading jets.

The corresponding particle-level selection, which defines the fiducial phase space, is summarized in Table D.1. Both Standard Model predictions and new physics models can be tested by applying this selections, and the experimental results are presented in the same fiducial region. The difference between the particle-level and reconstruction-level selections on specific observable is addressed using the unfolding procedure, which will be discussed in detail in Sec. D.3.

D.2.2 Analysis Samples

The data used in the analysis are taken using unprescaled single lepton and dilepton triggers^[58,60]. All processes are estimated using Monte Carlo (MC) simulation, except for the dominant fake-photon background, which mainly originates from Z +jets events. This background is estimated using a data-driven method, with MC samples used to evaluate associated systematic uncertainties. A dedicated $t\bar{t}\gamma$ control region is defined to validate the MC prediction, yielding a scale factor of 1.44 ± 0.22 , consistent with the previous study^[274]. All the simulated samples used in this analysis are summarized in Tables D.2 and D.3.

Three main analysis regions are defined: the EWK signal region (SR) with $m_{jj} >$

Table D.1 Particle level selection criteria.^[273]

Lepton	$p_T^\ell > 20, 30(\text{leading}) \text{ GeV}, \eta_\ell < 2.5$ $N_\ell \geq 2$
Photon	$E_T^\gamma > 25 \text{ GeV}, \eta_\gamma < 2.37$ $E_T^{\text{cone20}} < 0.07 E_T^\gamma$ $\Delta R(\ell, \gamma) > 0.4$
Jet	$p_T^j > 50 \text{ GeV}, y_j < 4.4$ $ \Delta y > 1.0$ $m_{jj} > 150 \text{ GeV}$ or $m_{jj} > 500 \text{ GeV}$ Remove jets if $\Delta R(\gamma, j) < 0.4$ or if $\Delta R(\ell, j) < 0.3$
Event	$m_{\ell\ell} > 40 \text{ GeV}$ $m_{\ell\ell} + m_{\ell\ell\gamma} > 182 \text{ GeV}$ $\zeta(Z\gamma) < 0.4$ $N_{\text{jets}}^{\text{gap}} = 0$

Table D.2 Summary of Monte Carlo generators and accuracies used for $Z\gamma$ samples.

Generator	Sample	Accuracy
MG5_AMC@NLO 2.6.5	EWK $Z(\text{ee}/\mu\mu)\gamma$	LO
SHERPA 2.2.11	QCD $Z(\text{ee}/\mu\mu)\gamma$	0,1j@NLO
SHERPA 2.2.4	QCD $Z(\text{ee}/\mu\mu)\gamma_{\text{pty}_7_ECMS}$	$\leq 3j@LO$
MG5_AMC@NLO 2.3.3	QCD $Z(\text{ee}/\mu\mu)\gamma_{\text{HT0}_125}$	$\leq 1j@NLO, 2,3j@LO$
	QCD $Z(\text{ee}/\mu\mu)\gamma_{\text{HTGT125_MjjLT150}}$	$\leq 1j@NLO, 2,3j@LO$
	QCD $Z(\text{ee}/\mu\mu)\gamma_{\text{HTGT125_MjjLT500}}$	$\leq 1j@NLO, 2,3j@LO$
	QCD $Z(\text{ee}/\mu\mu)\gamma_{\text{HTGT125_MjjGT500}}$	$\leq 1j@NLO, 2,3j@LO$
SHERPA 2.2.8	QCD $Z(\text{ee}/\mu\mu)\gamma$	$\leq 1j@NLO, 2,3j@LO$
	QCD $Z(\text{ee})\gamma$	$\leq 3j@LO$
SHERPA 2.2.10	QCD $Z(\text{ee})\gamma_{\text{CKKW15}}$	$\leq 3j@LO$
	QCD $Z(\text{ee})\gamma_{\text{CKKW30}}$	$\leq 3j@LO$
	QCD $Z(\text{ee})\gamma_{\text{QSF025}}$	$\leq 3j@LO$
	QCD $Z(\text{ee})\gamma_{\text{QSF4}}$	$\leq 3j@LO$

500 GeV and $\zeta(\ell\ell\gamma) < 0.4$, the EWK control region 1 (CR1) with $m_{jj} > 500 \text{ GeV}$ and $\zeta(\ell\ell\gamma) > 0.4$, and the total EW+QCD region with $\zeta(\ell\ell\gamma) < 0.4$. The EWK SR and CR1 are used to extract the electroweak $Z\gamma$ signal, with the CR1 serving as a control region to constrain the QCD-induced $Z\gamma$ component through a simultaneous fit. The EW+QCD region is used to measure the total EW+QCD $Z\gamma$ production cross section. Additional regions, such as the $t\bar{t}\gamma$ control region and several Z +jets validation regions, are employed to correct the $t\bar{t}\gamma$ MC normalization and to evaluate the uncertainties associated with the Z +jets data-driven

Table D.3 Summary of background samples and corresponding generators.

Sample	Generator
Zee/mumu	PowhegPythia8
QCD WZ($\ell\ell\nu$)	SHERPA 2.2.2
EW WZ($\ell\ell\nu$)	MG5_AMC@NLO 2.6.2
$t\bar{t}\gamma$	MG5_AMC@NLO 2.3.3
WW γ	SHERPA 2.2.5

background, as detailed in Refs. [\[273-274,277\]](#).

D.2.3 Uncertainties

The uncertainties in the analysis are carefully studied and categorized into the following sources:

- **Experimental uncertainties:** These arise from the reconstruction and calibration of physics objects, accounting for resolution effects, data-MC differences, and variations in experimental conditions. They include uncertainties related to jets, leptons, photons, pile-up, and integrated luminosity. Each component is evaluated according to the corresponding methods detailed in the references in the previous object section.
- **Theoretical uncertainties:** The theoretical models used to produce the MC predictions have intrinsic uncertainties, including QCD scale and parton distribution function (PDF) variations, QCD modeling (such as merging and resummation scales), and electroweak modeling (such as parton shower and underlying event variations). The interference between EWK and QCD $Z\gamma$ production is also considered.
- **Background estimation uncertainties:** The largest contribution arises from the data-driven estimation of the Z +jets fake-photon background. A 35% uncertainty on its yield is measured and assigned to account primarily for the statistical uncertainty from the sideband method, as well as systematic effects due to the correlation between photon identification and isolation selections used to construct the 2D sideband regions, where in ideal case full decorrelation is assumed. Additional uncertainty comes from the MC-based subtraction of the prompt-photon contribution in the data-driven method. The systematic uncertainty on the extracted Z +jets shape is negligible. For other backgrounds, only yield (normalization) uncertainties are considered due to their small overall contributions, with 15% assigned for $t\bar{t}\gamma$ and 20% for WZ .

- **Statistical uncertainties:** These arise from Poisson fluctuations in the data and the limited number of simulated MC events.

All systematic uncertainty terms are pruned, flattened, and smoothed to remove double counting and random biases due to statistical fluctuations, following the standard procedure described in Ref. [278].

The inclusive cross section is measured through the signal strength parameter μ , defined as the normalization factor applied to the nominal signal MC prediction. It is implemented as a free parameter that scales the yield of the targeted signal and is determined by maximum likelihood fitting, together with all systematic uncertainty terms, which are incorporated as nuisance parameters (NPs) and constrained. The methodology are well described in Sec. 5.7.

D.2.4 Signal Extraction and Results

In the extraction of the EW $Z\gamma$ process, the QCD-induced $Z\gamma$ contribution is treated as a background. An additional free parameter, μ_{QCD} , is introduced to correct its predicted yield, correlated between the EWK SR and CR1 regions. Since the QCD $Z\gamma$ component is enriched in the EWK CR1, a simultaneous fit of μ and μ_{QCD} allows the extraction of the EW signal strength while constraining the QCD contribution using data from the control region. For the total EW+QCD $Z\gamma$ measurement, single μ is applied to the total $Z\gamma$ prediction.

The fitting discriminant is defined using the binned distribution of m_{jj} , which shows distinct distributions for different physics processes. The corresponding post-fit distributions are shown in Fig. D.4.

The extracted signal strength for the EW $Z\gamma$ process is $\mu_{\text{EW}} = 1.02 \pm 0.09 \text{ (stat)} \pm 0.09 \text{ (syst)} = 1.02^{+0.13}_{-0.12}$, which excludes the background-only hypothesis with a significance well above 5σ . The corresponding fiducial cross section is measured to be $3.6 \pm 0.5 \text{ fb}$, compared to the MC prediction of $3.5 \pm 0.2 \text{ fb}$. For the total EW+QCD $Z\gamma$ production, the measured and predicted inclusive cross sections are $16.8^{+2.0}_{-1.8} \text{ fb}$ and $15.7^{+5.0}_{-2.6} \text{ fb}$, respectively. The impact of each category of systematic uncertainty is summarized in Table D.4.

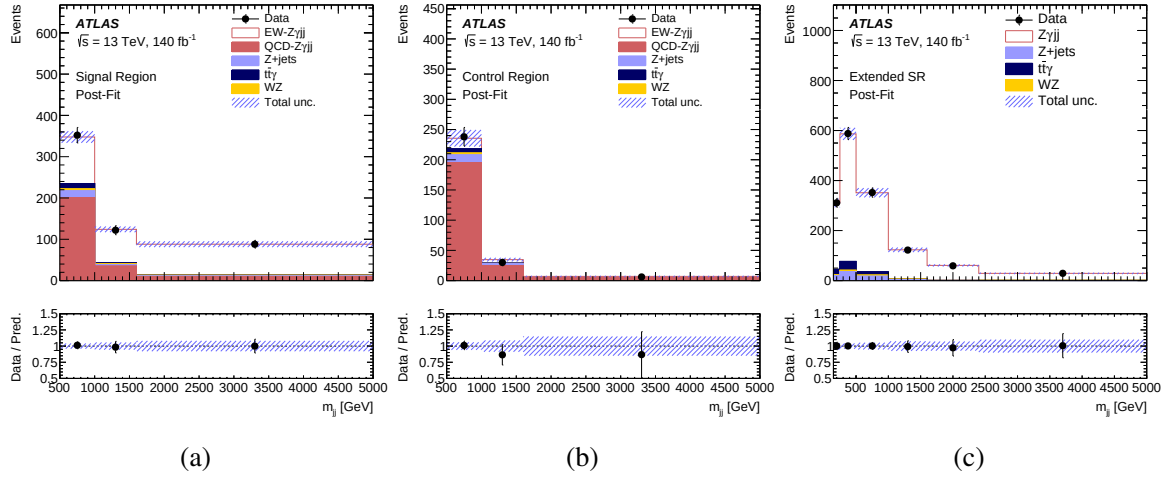


Figure D.4 Post-fit m_{jj} distributions in (a) EWK signal region (SR), (b) the EWK control region 1 (CR1), and (c) the total EW+QCD region. Overflow events are included in the last bin. The statistical uncertainty is shown as black vertical bars, while the systematic uncertainty is represented by the hatched band, including correlation determined by the fitting.^[273]

Table D.4 Summary of relative uncertainties for the EW and EW+QCD $Z\gamma$ cross-section measurements^[273].

	Data stat.	MC stat.	Background	Reco	EW mod.	QCD mod.	Total
$\Delta\sigma_{EW}/\sigma_{EW}$ [%]	± 9	± 1	± 1	± 4	$^{+8}_{-6}$	± 2	± 13
$\Delta\sigma_{Z\gamma}/\sigma_{Z\gamma}$ [%]	± 3	± 1	± 2	$^{+4}_{-3}$	$^{+7}_{-6}$	± 9	$^{+12}_{-11}$

D.3 Unfolding Study

D.3.1 Basics

The unfolding procedure is a key step in estimating the difference between the experimental results at the reconstruction level and those at the particle level (truth level). This difference arises because, in the experiment, only reconstructed observables can be accessed, which depend on the specific detector setup and its associated phase-space selections and measurement resolutions. However, theoretical predictions are usually defined at the particle level, independent of any particular detector configuration or simulation. Therefore, unfolding is developed to correct these differences by accounting for the effects of phase space cuts, and the migration of studied observable. The basic concept of the unfolding procedure is illustrated in Fig. D.5, and the three main effects it aims to correct are shown in Fig. D.6.

Unfolding can be regarded as the inverse of the detector simulation, or more specifically, $u = R^{-1}(v - \beta)$, where v is the reconstructed data, β the background, $R \equiv M \times \frac{1}{\epsilon}$ the

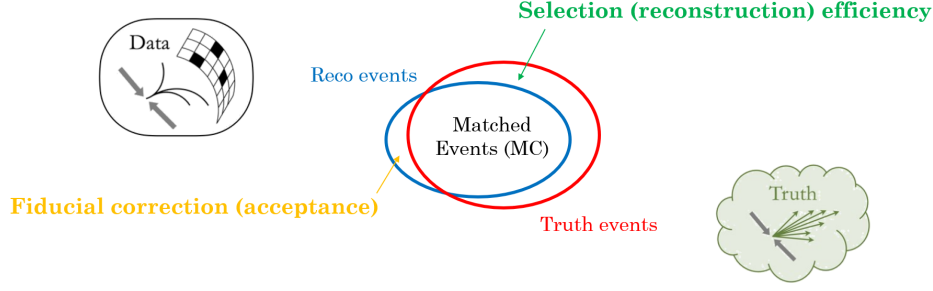


Figure D.5 Conceptual illustration of the unfolding procedure.

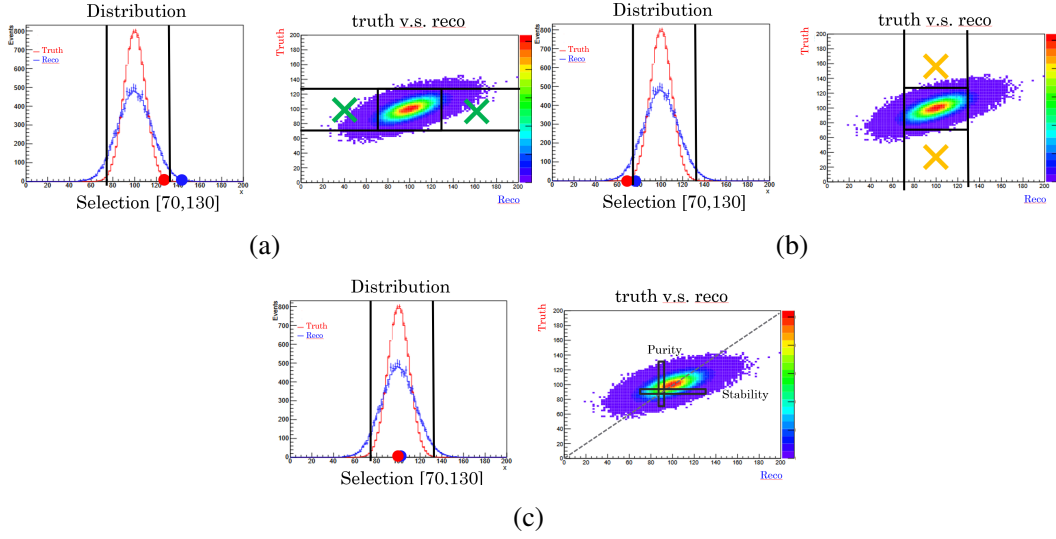


Figure D.6 Illustration of the three main effects corrected by the unfolding: (a) reconstruction efficiency, where detector effects cause events to be dropped by the cuts (ϵ); (b) fiducial correction, where events outside the fiducial phase space are reconstructed as passing the cuts (λ); and (c) bin-by-bin migration of the studied observable (M).

response function (a matrix in histogram-based studies), and u the unfolded result for the targeted signal.

The conventional method, *Iterative Bayesian Unfolding*^[279], utilizes the Bayesian approach. In this framework, u is treated as $P(\text{true})$ and v as $P(\text{reco})$, while R^{-1} is interpreted as the posterior and can be solved through Bayes' theorem. The iterative solution as shown in Equation D.1, starts with u_0 , which is initialized from the MC truth as the best prior estimate.

$$\begin{aligned}
 u^{i+1}(\text{true}) &= \int u^i(\text{true}) \frac{v(\text{obs})}{v^i(\text{reco})} P(\text{reco}|\text{true}) d(\text{reco}), \\
 v^i(\text{reco}) &= \int u^i(\text{true}) P(\text{reco}|\text{true}) d(\text{true}).
 \end{aligned}
 \tag{D.1}$$

This method is effective when the signal dominates and systematic uncertainties are treated as fully uncorrelated during unfolding. However, it encounters difficulties in the case of the EW $Z\gamma$ process, where the QCD $Z\gamma$ component must be determined simultaneously and the systematic uncertainties affect both. To address this, a new method, *Binned Likelihood Unfolding*, is employed and studied. This method treats the unfolding as a fit to sub-samples of the reconstructed distribution, where each sub-sample contains all events from one truth bin, as illustrated in Figure D.7. The method is implemented in Ref.^[278] and has proven to be efficient for handling differential measurements in the presence of large background contributions and complex systematic uncertainty correlations.

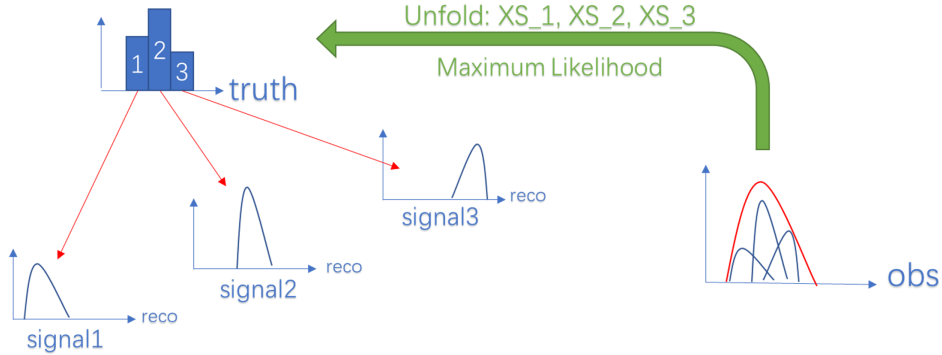


Figure D.7 Conceptual illustration of the Binned Likelihood Unfolding

D.3.2 Unfolded Variables

The observables used for the unfolding are listed in Table D.5. The unfolding procedure is repeated for each observable, in both the EW and EW+QCD analyses. The binning of each observable is optimized to include as many bins as possible for physics motivation, while satisfying the following requirements: sufficient statistics in each bin (to control both data statistical uncertainty and MC statistical uncertainty), a large signal-to-background ratio (to control background unc.), and high purity (to avoid large migration corrections). This measurement provides the most complete set of unfolded results for this signature to date.

D.3.3 Tests of Unfolding

A common shortcoming of all unfolding methods is the amplification of statistical fluctuations. Since the available statistics are often limited, and are further reduced through iterative use or sub-division, the statistical uncertainties become increasingly pronounced.

Variable	Binning	Unit
$\zeta(\gamma)$	[0,0.075,0.15,0.225,0.3,0.4]	-
$\Delta y(j_1, j_2)$	[1,1.75,2.5,3.5,5,9]	-
$\Delta\phi(Z\gamma, jj)$	[0,2,2.95,3.2]	-
m_{jj}	[150,250,500,1000,1600,2400,5000]	GeV
$m_{Z\gamma}$	[100,150,200,250,350,700]	GeV
$p_T^{j_1}$	[50,100,175,300,500,1000]	GeV
$p_T^{l_1}$	[30,65,100,150,250,500]	GeV
$p_T^{\gamma_1}$	[25,35,50,75,150,500]	GeV
p_T^Z	[0,50,100,150,250,800]	GeV
$p_T^{Z\gamma}$	[0,50,100,150,200,500]	GeV

Table D.5 Unfolded variables and optimized binning. $p_T^{Z\gamma}$, $\zeta(\gamma)$ and $\Delta\phi(Z\gamma, jj)$ are only for EW+QCD $Z\gamma jj$ unfolding. m_{jj} binning is different for EW $Z\gamma$ unfolding due to $m_{jj} > 500$ GeV cut.

To mitigate these fluctuations, various regularization techniques specific to each unfolding algorithm are applied. However, regularization inevitably introduces potential biases, making thorough bias checks essential in any unfolding study. Significant biases should be minimized through appropriate tuning of the regularization, while any remaining deviations must be assigned as systematic uncertainties.

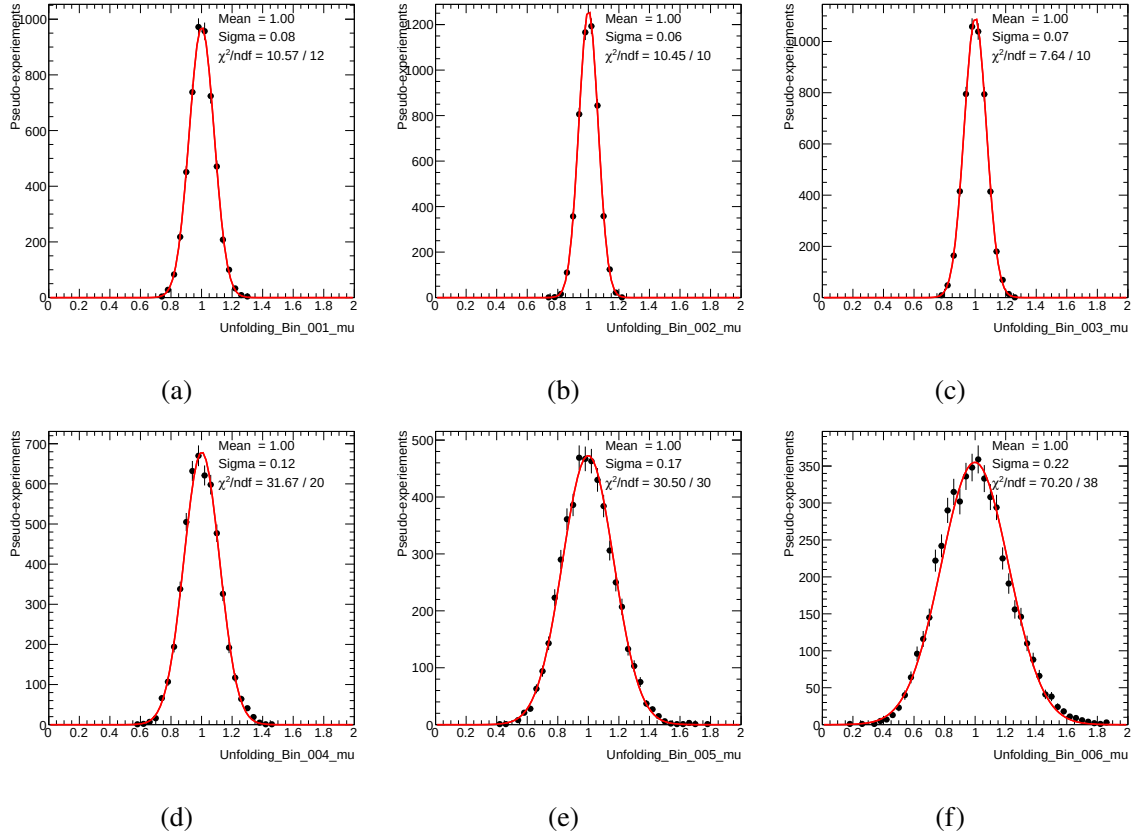
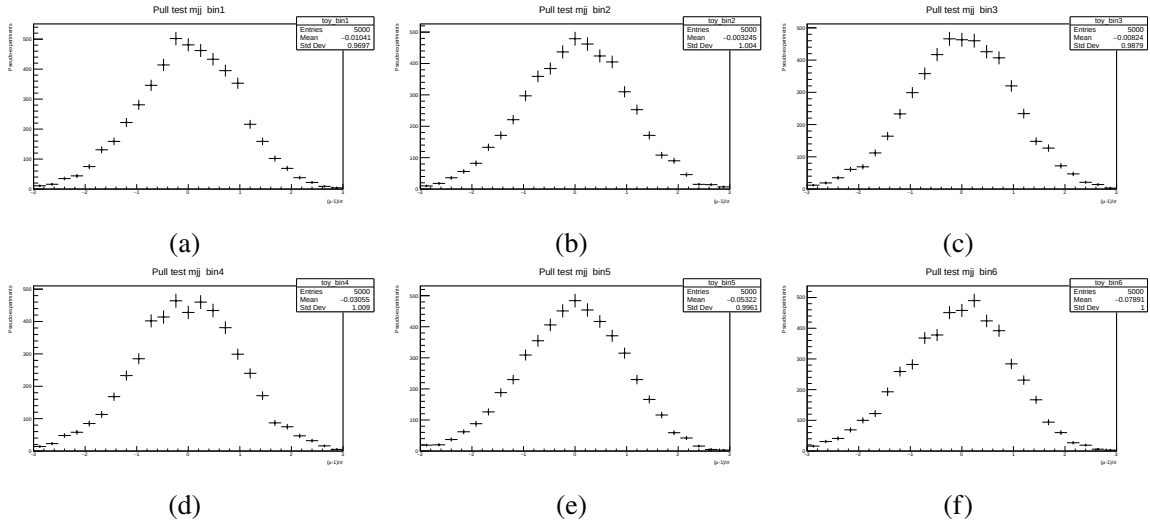
The major tests are summarized as follows. Unless otherwise stated, the pseudo-data sample, denoted as v , is constructed using MC, where the corresponding truth distribution u is known. All reweighting procedures are applied at the truth level on u , and the reconstructed pseudo-data v is modified consistently, since the truth and reconstructed events are linked within the MC sample. For events outside the fiducial truth phase space, the corresponding reconstructed events in v are used.

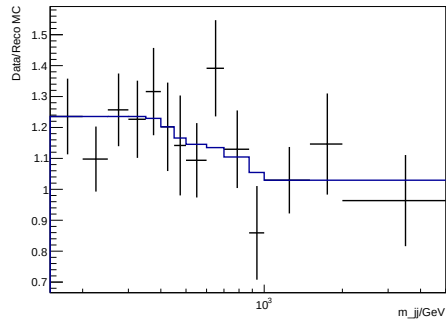
- **Closure Test with Limited Statistics:** The MC sample is randomly divided into two statistically equivalent subsets. One subset is used to estimate the response matrix R , while the other is used as pseudo-data v for testing. The unfolded result is then compared with the known truth distribution to verify the statistical stability of the unfolding procedure.
- **Pull Test:** A series of pseudo-experiments ("toys") are generated by fluctuating the reconstructed pseudo-data according to Poisson statistics. Each fluctuated dataset is unfolded independently. The ensemble of unfolded results should follow a Gaussian distribution centered at unity with a width consistent with the statistical uncertainty estimated from the maximum-likelihood fit, as shown in Figure D.8 and D.9. This test

validates whether the reported statistical uncertainties correctly describe the expected statistical behavior.

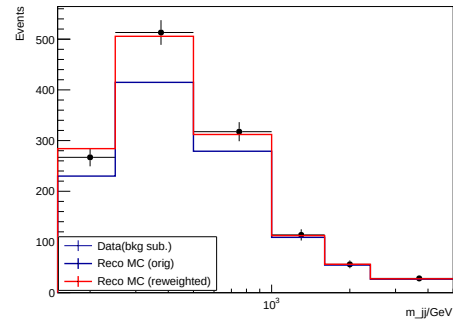
- **Functional Reweighting Test:** The pseudo-data are reweighted to mimic a potential BSM effect, for example by enhancing events in the highest m_{jj} bin. The unfolding is then performed and the unfolded result is compared to the reweighted truth distribution. This test evaluates whether the unfolding introduces any bias that could affect the sensitivity to new physics.
- **Alternative MC Test:** An alternative MC generator is used to produce pseudo-data, which are then unfolded using the nominal response matrix. The unfolded distribution is compared to the corresponding truth distribution from the alternative MC. This test assesses the robustness of the unfolding against modeling differences between generators.
- **Data-driven Closure Test:** As an ultimate validation, the pseudo-data are reweighted to match the real data distributions. The unfolding is performed, and the results are compared to the reweighted truth. This test examines whether data/MC discrepancies could create bias for unfolding. The reweighting is applied empirically by comparing data and pseudo-data in the reconstructed distribution and design the truth reweighting function for u , as shown in Figure D.10.
- **Hidden Variable Test:** Similar to the data-driven test, but performed by reweighting an observable different from the one being unfolded (e.g., a correlated kinematic variable u'). This test probes potential biases arising from data/MC differences in correlated observables.

Comprehensive tests were carried out for all observables, with representative results shown in Figure D.11, D.12 and D.13 for the m_{jj} distribution. In all cases, the observed biases and deviations are found to be negligible. Therefore, no additional systematic uncertainty is assigned to the unfolding procedure.

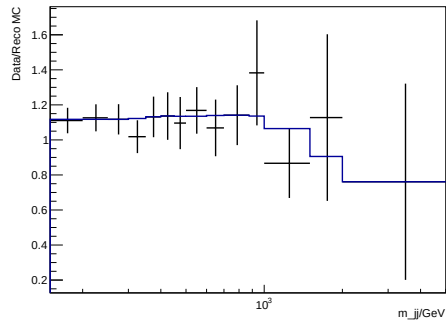
Figure D.8 Unfolded μ_i for each m_{jj} bin across all pseudo-experiments in the pull test.Figure D.9 The pull $(\mu_i - 1)/\sigma_i$ for each m_{jj} bin across all pseudo-experiments.



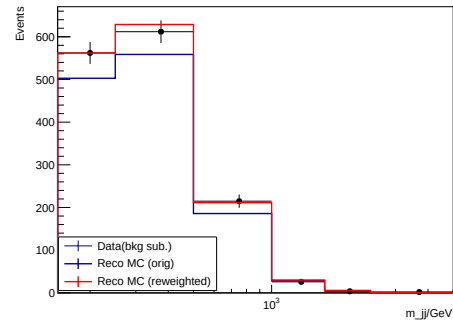
(a)



(b)



(c)



(d)

Figure D.10 Smoothed reweighting functions and reweighted reconstructed MC templates in the signal region (a,b) and control region (c,d). The reweighted MC templates better reproduce the data distributions.

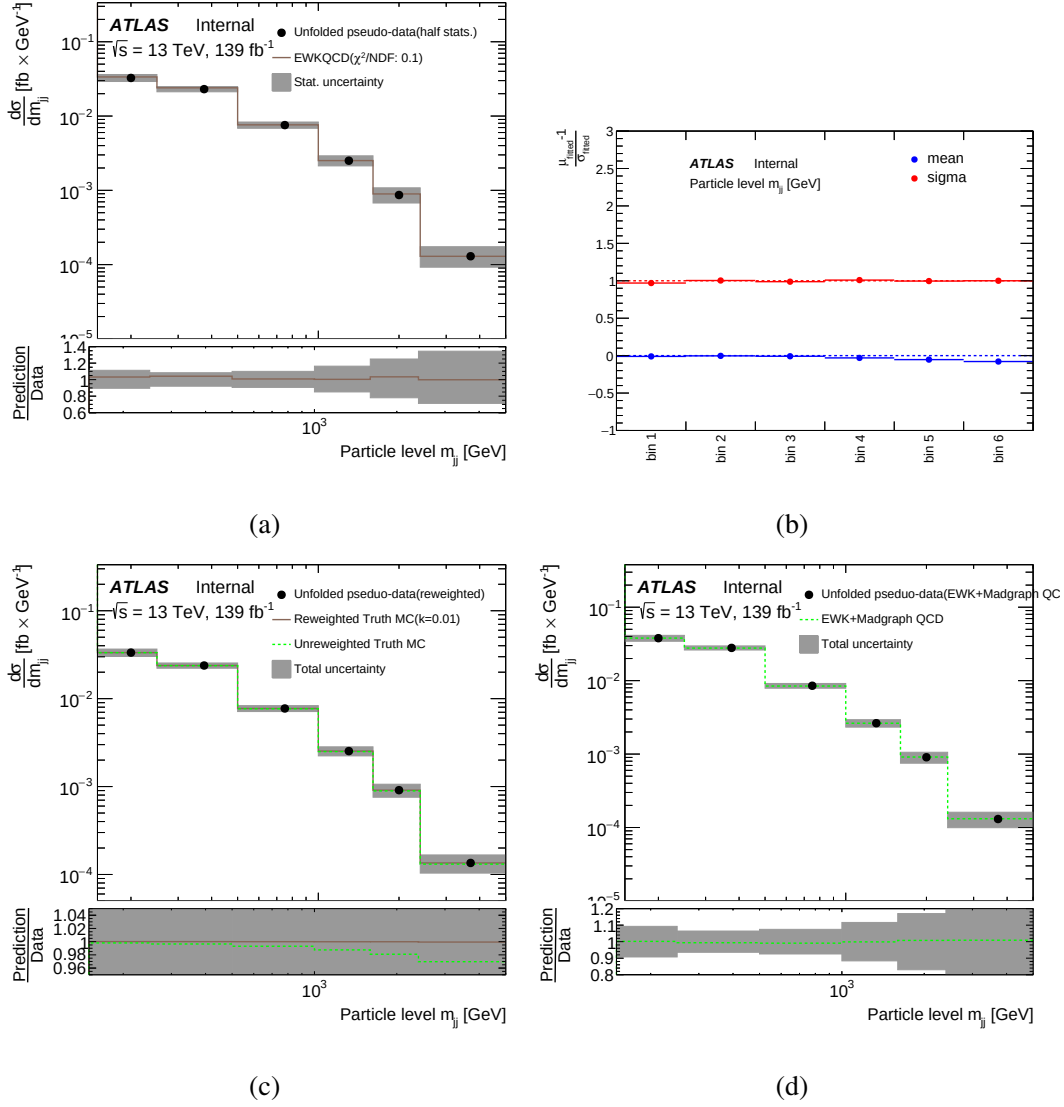


Figure D.11 Unfolding tests for the m_{jj} observable: (a) statistical test, (b) pull test, (c) functional reweighting test, and (d) alternative MC test.

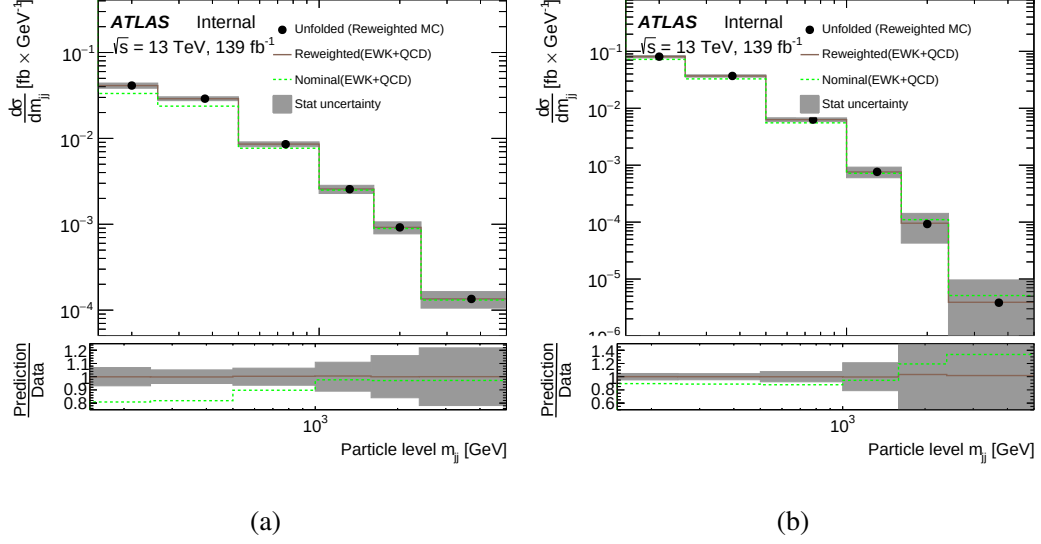


Figure D.12 Data-driven closure test of m_{jj} in the signal region (left) and control region (right). The original un-reweighted truth template is shown in dashed green for reference.

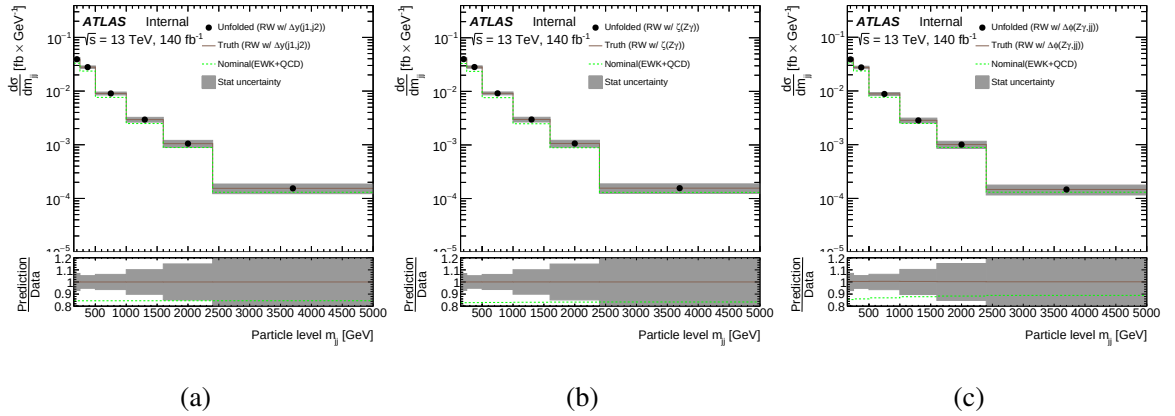


Figure D.13 Hidden-variable tests of m_{jj} using (a) Δy_{jj} , (b) $\zeta(\gamma)$, and (c) $\Delta\phi_{\ell\ell\gamma,jj}$. Pseudo-data are constructed using reweighting functions that adjust another variable (indicated as “RW w/ ...”). The un-reweighted nominal MC truth is shown as a green dashed line for reference.

D.3.4 Results of Differential Measurement

The final results of the differential measurement are shown in Figure D.14, Figure D.15 for the EW $Z\gamma$ analysis and D.16, D.17 for EW+QCD $Z\gamma$ analysis.

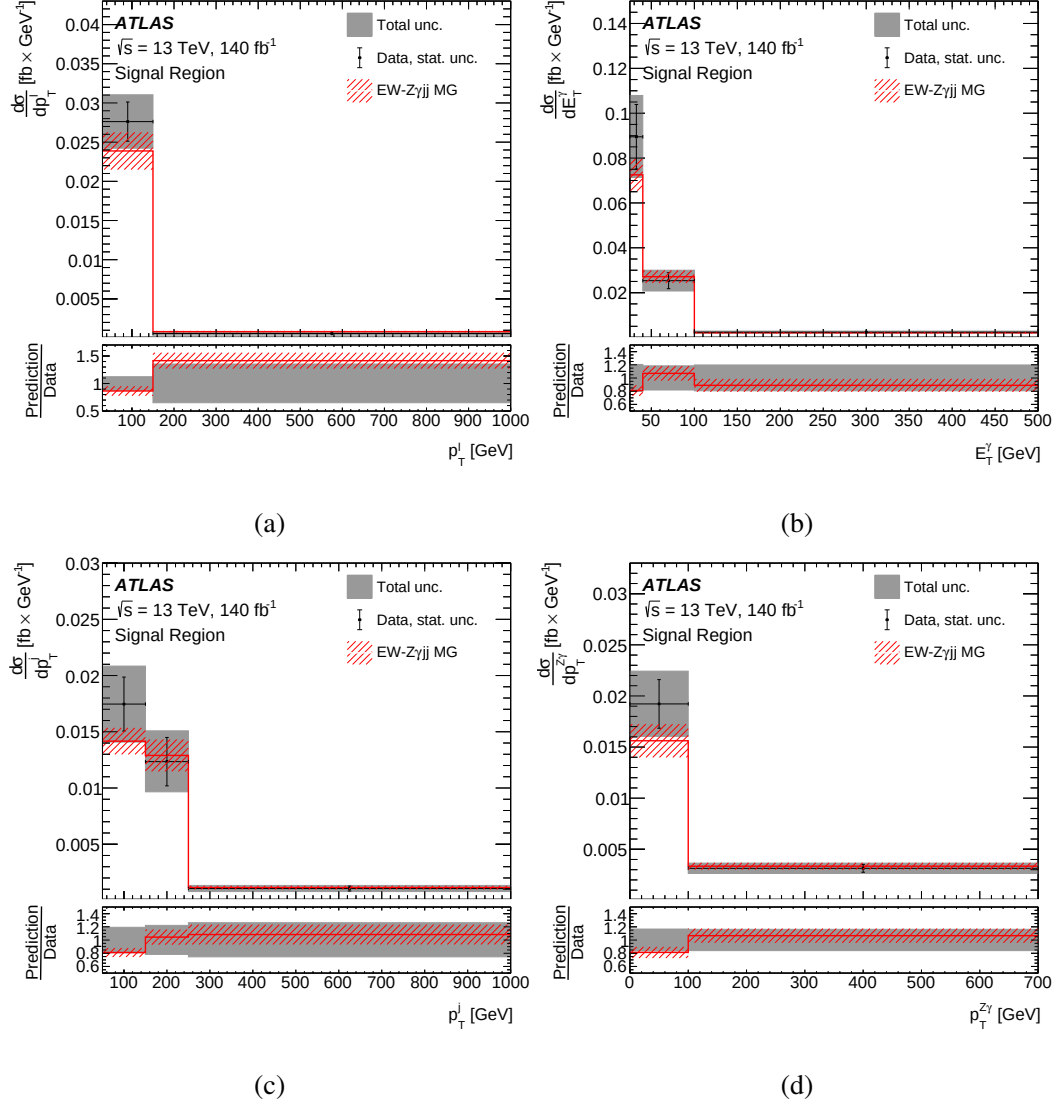


Figure D.14 The EW $Z\gamma$ differential cross-section in the EWK SR as a function of (a) the leading lepton p_T , (b) the leading photon p_T , (c) the leading jet p_T and (d) the $Z\gamma$ system p_T . The solid black line shows the unfolded differential cross-section, with statistical uncertainties indicated by vertical bars and the total uncertainty represented by the grey band. The hatched area denotes the uncertainty of the theoretical prediction. Overflow events are included in the last bin.^[274]

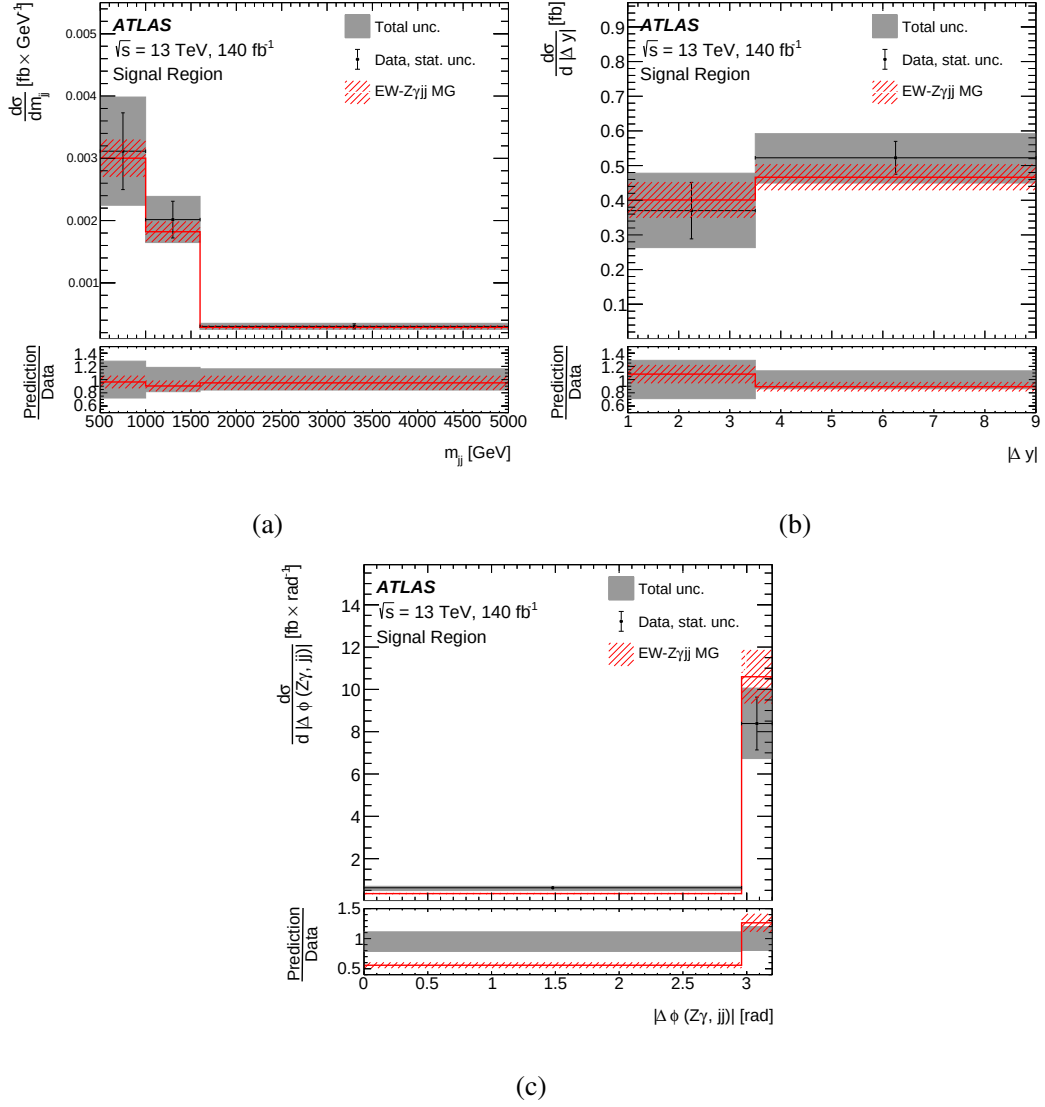


Figure D.15 The EW $Z\gamma$ differential cross-section in the EWK SR as a function of (a) the dijet invariant mass, (b) the dijet rapidity difference and (c) the $Z\gamma$ and dijet azimuthal difference. The solid black line shows the unfolded differential cross-section, with statistical uncertainties indicated by vertical bars and the total uncertainty represented by the grey band. The hatched area denotes the uncertainty of the theoretical prediction. Overflow events are included in the last bin.^[274]

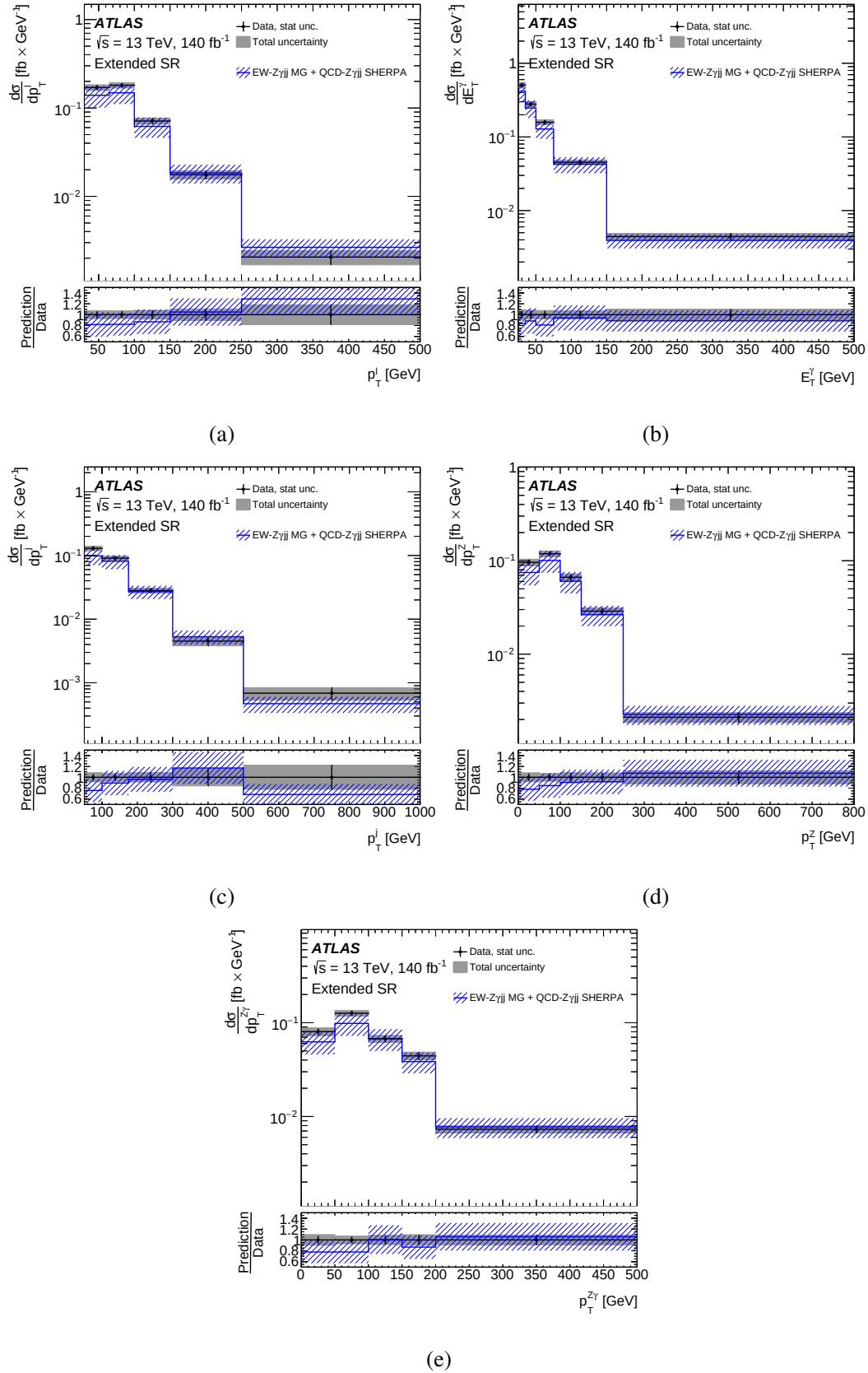


Figure D.16 The EW+QCD $Z\gamma$ differential cross-section in the EW+QCD region as a function of (a) the leading lepton p_T , (b) the leading photon $p_T^{\gamma 40}$, (c) the leading jet p_T , (d) the Z boson p_T and (e) the $Z\gamma$ system p_T . The solid black line shows the unfolded differential cross-section, with statistical uncertainties indicated by vertical bars and the total uncertainty represented by the grey band. The hatched area denotes the uncertainty of the theoretical prediction. Overflow events are included in the last bin.^[274]

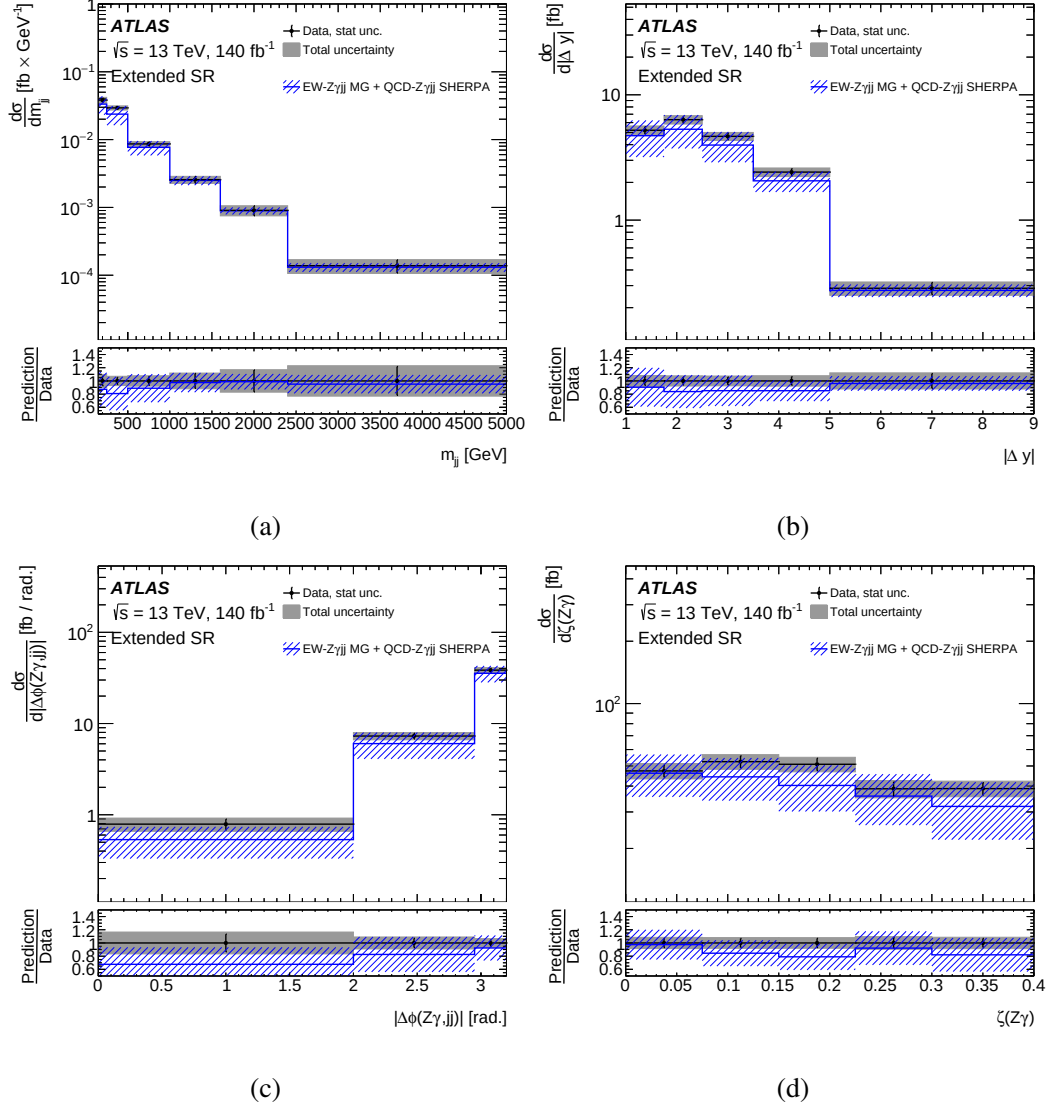


Figure D.17 The EW+QCD $Z\gamma$ differential cross-section in the EW+QCD region as a function of (a) the dijet invariant mass, (b) the dijet rapidity difference, (c) the $Z\gamma$ and dijet azimuthal difference and (d) the centrality of the system $\zeta(Z\gamma)$. The solid black line shows the unfolded differential cross-section, with statistical uncertainties indicated by vertical bars and the total uncertainty represented by the grey band. The hatched area denotes the uncertainty of the theoretical prediction. Overflow events are included in the last bin.^[274]

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List of Research Achievements

ATLAS Collaboration Publications with my major contributions

- [1] ATLAS Collaboration. Search for dark matter produced in association with a dark Higgs boson in the $b\bar{b}$ final state using pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector[J]. **Physical Review Letters**, vol. **134**, **121801**. Main contrib. *EB request talk and Paper Approval talk*. Signal interpretation, Xbb tagging, framework, sample production, experimental uncertainty.
- [2] ATLAS Collaboration. Combination of searches for Higgs boson decays into a photon and a massless dark photon using pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector[J]. **Journal of High Energy Physics**, vol. **2024**, no. **153**. Main contrib. *Exotics Group Approval talk*. Primary developer of framework and NP correlation scheme.
- [3] ATLAS Collaboration. Measurement of the cross-sections of the electroweak and total production of a $Z\gamma$ pair in association with two jets in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector[J]. **Physics Letters B**, vol. **846**, p. **138-222**. Main contrib., *Analysis contact. Internal Note Editor. Presented Paper Approval talk*. Sample preparation, framework author, uncertainty and unfolding.

Other Publications

- [1] ATLAS Collaboration. Transforming jet flavour tagging at ATLAS[J]. **arXiv:2505.19689**, accepted by **Nature Communications**. MC samples production.
- [2] ATLAS Collaboration. Combination and summary of ATLAS dark matter searches interpreted in a 2HDM with a pseudo-scalar mediator using 139 fb^{-1} of $\sqrt{s} = 13$ TeV pp collision data[J]. **Science Bulletin**, **2024**, **69(19)**: **3005-3035**. Statistical study of $m_A - m_a$ scan.
- [3] ATLAS Collaboration. Efficiency corrections for a tagger for boosted $H \rightarrow b\bar{b}$ decays in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector[J]. **Tech. Rep., ATL-PHYS-PUB-2021-035**. Main contrib. Author of $t\bar{t}$ calibration framework.
- [4] ATLAS Collaboration. Combination of searches for Higgs boson pair production at $\sqrt{s} = 13$ TeV[J]. **Conference Note, CONF-HIGP-2024-36**. Internal Note editor. Fitting study.
- [5] Design of a LYSO Crystal Electromagnetic Calorimeter for DarkSHINE Experiment[J]. **Nucl. Sci. Tech.** **36**, **41** (2025). *Co-first author*. Simulation, geometry optimization, smearing effect, analysis.
- [6] Calo-VQ: Vector-Quantized Two-Stage Generative Model in Calorimeter Simulation[J]. **arXiv:2405.06605**. *First author*. Development of Calo-VQ algorithm.
- [7] CaloChallenge 2022: A Community Challenge for Fast Calorimeter Simulation[J]. **arXiv:2410.21611**, accepted by **Rep. Prog. Phys.**, Development of Calo-VQ algorithm.

- [8] Prospective study of light dark matter search with a newly proposed DarkSHINE experiment[J]. **Sci. China Phys. Mech. Astron.**, vol. 66, no. 211062. Geant4 simulation, ECAL smearing effect, rare background bias factor.

Selected International Conference Talks

- [1] Learning powerful jet representations via self-supervision[J]. *16th International Workshop on Boosted Object Phenomenology, Reconstruction, Measurements, and Searches at Colliders (BOOST 2024)*, Genova, 2024 Aug.
- [2] Searches for dark matter at ATLAS[J]. *29th International Symposium on Particles, Strings and Cosmology (PASCOS2024)*, Quy Nhon, 2024 Jul.
- [3] Latent Generative Model for Fast Calorimeter Simulation[J]. *ML4Jets 2023*, Hamburg, 2023 Nov.
- [4] Unfolding Techniques[J]. *ATLAS Standard Model Workshop 2023*, Prague, 2023 Sep.
- [5] Latent Generative Models for Calo Simulation with VQ-VAE[J]. *CaloChallenge Workshop*, Frascati, Italy, 2023 May.
- [6] The Dark SHINE Experiment (Lightening Talk)[J]. *Dark Matter 2023: From the Smallest to the Largest Scales*, Santander, Spain, 2023 May.
- [7] Boosted W/Z boson and top tagging in ATLAS[J]. *11th International Conference on New Frontiers in Physics (ICNFP2022)*, Crete, 2022 Sep.
- [8] Multiboson production (ATLAS+CMS)[J]. *QCD@LHC 2022*, Orsay, 2022 Nov.
- [9] Zgamma VBS measurements with ATLAS full Run2[J]. *Multi-boson interactions 2022 (MBI202)*, Shanghai, 2022 Aug.
- [10] Search for Dark Matter Produced in Association with a Dark Higgs Boson Decaying to two b-quarks Using full Run-2 data set from the ATLAS detector[J]. *American Physical Society(APS)'s April Meeting*, Online, 2022 Apr.

Selected Domestic Conference Talks

- [1] Recent ATLAS results of Dark Matter combination and Dark Higgs search[J]. *10th China LHC Physics Conference (CLHCP2024)*, Qingdao, 2024 Nov.
- [2] Search for Dark Matter Produced in Association with a Dark Higgs Boson Decaying to two b quarks at ATLAS and the potential to utilize the novel Dxb tagger[J]. *8th China LHC Physics Conference (CLHCP2022)*, Nanjing/Online, 2022 Nov.
- [3] Efficiency corrections for a tagger for boosted Hbb decays in ATLAS[J]. *7th China LHC Physics Conference (CLHCP2021)*, Nanjing/Online, 2021 Nov.

ATLAS Collaboration Approval Talks

- [1] 2024: MonoS($b\bar{b}$) Search: Paper Approval Talk. Presented to the ATLAS Collaboration.

- [2] 2024: CDM Dark Photon Combination, EXOT Approval Talk. Presented at the Exotic Plenary Meeting.
- [3] 2023: VBS $Z\gamma$ Measurement, Paper Approval Talk. Presented to the ATLAS Collaboration.

Honors, Prizes, and Academic Appointments

- [1] 2022: Excellence Award, School of Physics and Astronomy, Shanghai JiaoTong University, Shanghai, China. 3rd WeiYu College Student Science and Technology Innovation Competition. DarkSHINE Experiment Simulation R&D on Siyuan-1 HPC.
- [2] 2021, 2023: Excellent Student, Key Laboratory for Particle Astrophysics and Cosmology, Ministry of Education, Shanghai, China.
- [3] 2023-present: Monte Carlo and Physics Modeling Contact, ATLAS Flavor Tagging Group.
- [4] 2022-2024: Analysis Contact, VBS $Z\gamma$ Measurement.