
What to expect when you are expecting new physics: searches for new phenomena in multilepton final states with the ATLAS detector

Ph.D. dissertation

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*To nani, nanu, mom, dad and veenu,
from your Sone Chiraya.*



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Abstract

This dissertation describes my work on three diverse but related aspects of the ATLAS experiment at CERN. The central idea of this thesis is structured around searches for new phenomena in multilepton final states using data from proton-proton collisions at a center-of-mass energy of $\sqrt{s} = 13$ TeV recorded by the ATLAS detector at the Large Hadron Collider during Run 2. Three distinct models, covering final states with multiple light leptons, tau leptons, jets and missing transverse energy are considered. The first analysis presented is the first-ever search for flavour violating heavy Higgs bosons decaying to multilepton plus multi b -jets final states, motivated primarily by the $t\bar{t}W$ -like and $t\bar{t}t\bar{t}$ -like tensions in data reported by the ATLAS and CMS experiments. The targeted signals lead to final states with either a same-sign top-quark pair, three top-quarks, or four top-quarks. A broad excess is observed over the considered parameter space of mass and couplings, with the largest local significance being 2.8 standard deviations. The second analysis is, yet again, the first-ever direct LHC search for a doublet or singlet vector-like lepton (VLL) coupling to first and second generation Standard Model leptons, motivated by the anomalous muon magnetic moment and flavor anomalies. No significant excess is observed over the SM expectation value for any of the models under study, and to-date, the strictest limits are placed on the production of VLLs from these models. Finally, the third analysis covered as part of this dissertation presents preliminary studies for the search for VLLs preferentially coupled to third generation SM fermions, in final states with multiple light leptons, tau-leptons, b -jets and missing transverse energy. The preliminary sensitivity to the model is estimated from these channels and is competitive with that from tau-only channels at low VLL masses, which exclude VLLs up to 1 TeV. While no significant excess was seen in either of the searches, they serve as an attempt to add another piece to the jigsaw of finding a suitable extension of the SM, and a playground to build and test cutting-edge data analysis techniques for the next generation of analyses.

My work on searching for BSM physics is complemented by the other two topics covered in this dissertation, on studying the TileCal light yield degradation with the data obtained by the integrator read-out of the ATLAS TileCal during Run 2 and deriving TileCal-related uncertainties for the ATLAS luminosity measurement in Run 3. The former study not only provides valuable feedback to the TileCal Phase-II upgrade plans, but is also essential for re-processing physics data and indirectly affects the determination of jet and missing transverse energy related uncertainties. The study estimated the effect of damage and

ageing of the scintillators and wavelength shifting fibres in TileCal cells to be between 10% to 30% depending on the location of the cell from the interaction point. The latter measurement affects counting of the measured number of events of a certain theoretical process, is used by every ATLAS measurement using the dataset and is a limiting factor in precision analyses measuring physics cross-sections. The overall uncertainty in the luminosity determination in 2022 was estimated to be 2.19% (1.91% from TileCal) and in 2023 was estimated to be 2.04% (1.2% from TileCal).

Resumen

Esta disertación describe mi trabajo en tres aspectos diversos pero relacionados del experimento ATLAS en el CERN. La tesis se centra en la búsqueda de nuevos fenómenos en estados finales con múltiples leptones, utilizando datos de colisiones protón-protón a una energía en el centro de masa de 13 TeV, registrados por el detector ATLAS en el Gran Colisionador de Hadrones durante el Run 2. Se consideran tres modelos distintos, que abarcan estados finales con leptones ligeros, leptones tau, jets y energía transversa faltante. El primer análisis es la primera búsqueda de bosones de Higgs pesados con violación de sabor que decaen en estados finales con múltiples leptones y múltiples b-jets, motivada por las tensiones tipo $t\bar{t}W$ y $t\bar{t}t$ reportadas por los experimentos ATLAS y CMS. Las señales de interés producen estados finales con un par de quarks top con el mismo signo, tres quarks top o cuatro quarks top. Se observa un exceso amplio en el espacio de parámetros de masa y acoplamientos, con una significancia local máxima de 2.8 desviaciones estándar. El segundo análisis es la primera búsqueda directa en el LHC de un lepton vectorial (VLL) doblete o singlete, que acople con leptones de primera y segunda generación del Modelo Estándar, motivada por el momento magnético anómalo del muón y anomalías en el sabor. No se observa un exceso significativo sobre el valor esperado del Modelo Estándar para los modelos estudiados, y hasta la fecha, se han establecido los límites más estrictos en la producción de VLLs de estos modelos. Finalmente, el tercer análisis presenta estudios preliminares para la búsqueda de VLLs acoplados preferentemente a fermiones de tercera generación del Modelo Estándar, en estados finales con múltiples leptones ligeros, leptones tau, jets de b y energía transversa faltante. La sensibilidad preliminar al modelo se estima a partir de estos canales y es competitiva con la de los canales solo tau a bajas masas de VLL, excluyendo VLLs hasta 1 TeV. Aunque no se observó un exceso significativo en las búsquedas, éstas contribuyen a buscar una extensión adecuada del Modelo Estándar y sirven como campo de prueba para técnicas avanzadas de análisis de datos a usar en futuros estudios.

Mi trabajo en la búsqueda de física más allá del Modelo Estándar se complementa con otros dos temas en esta disertación: el estudio de la degradación del rendimiento luminoso del TileCal con datos del integrador del ATLAS TileCal durante el Run 2 y la derivación de incertidumbres relacionadas con TileCal para la medición de luminosidad del ATLAS en el Run 3. El primer estudio proporciona información valiosa para la actualización de la Fase-II del TileCal y es esencial para el reprocesamiento de datos, afectando la determinación de

incertidumbres en jets y energía transversa faltante. Se estimó que el efecto del daño y envejecimiento de los scintiladores y fibras en las celdas de TileCal varía entre 10% y 30%, según la ubicación respecto al punto de interacción. El segundo estudio afecta el conteo de eventos teóricos, utilizado en todas las mediciones del ATLAS y es un factor limitante en análisis de precisión. La incertidumbre en la determinación de luminosidad fue de 2.19% en 2022 (1.91% del TileCal) y de 2.04% en 2023 (1.2% del TileCal).

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The work done towards building this dissertation comes from a roller coaster of emotions and concepts - excitement, curiosity, patience, friendship and above all, love. I want to thank everyone who helped me feel these and bring them to life, in one form or another, in this thesis and towards building me up as a researcher and a person.

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Introduction

The discovery of the first subatomic particle [1], the electron, preceded a theoretical motivation for its existence: nature was assumed to be built of indivisible, indestructible entities called atoms. This discovery started the quest to find the building blocks of nature and build a comprehensible theory of matter and its interactions. Some of the most radical ideas of the 1900s include wave-particle duality, the development of quantum mechanics to describe matter at the smallest scales, and general relativity, to describe the behaviour of large astronomical structures.

Quantum Field theory (QFT) is a theoretical framework that extends quantum mechanics to systems with infinite degrees of freedom, while taking into account the effects of special relativity. Simply put, it postulates the existence of infinite, continuous fields that pervade the universe and the building blocks of matter as quantization of these fields. The first successful QFT was *Quantum Electrodynamics* [2] that introduced a relativistic description of the electron and photons as quantization of the electromagnetic field. The mid-1960s saw a boom in the particle zoo: a plethora of strongly interacting particles were discovered. *Quarks* [3,4] were postulated as theoretical constituents of these particles, following the rules of a QFT of the strong force called *Quantum Chromodynamics*. The *Brout-Englert-Higgs mechanism* [5–7] arose as a solution for mass generation for particles in these theories. The discovery of the Higgs boson in 2012 [8,9] completed the theoretical framework of the *Standard Model* (SM) of particle physics: the most complete, elegant and well-tested description of nature to-date.

Despite its success, the SM is not a complete theory of nature because it does not include a quantum description of gravity. Further, feedback from astrophysical and cosmological observations indicate that it describes only 5% of the known universe, lacks an explanation for the baryon asymmetry, for the hierarchical structure of masses and mixing angles for

fermions, to name a few shortcomings. Additionally, recent experimental results, such as the anomalous magnetic moment of the muon [10] and flavor anomalies [11], suggest possible physics beyond the SM. These results have motivated the development of multiple theoretical extensions to the SM, generally called *Beyond Standard Model* (BSM) theories. Hadron colliders provide an exciting avenue to search for BSM particles. The largest hadron collider built to-date, the *Large Hadron Collider* (LHC), is capable of producing not only SM particles but also potential BSM particles with mass in the TeV range. Effects of heavier BSM particles can be studied indirectly through their interactions with SM particles. In particular, events with two, three and four or more leptons provide *clean* channels to study BSM theories due to well understood and relatively low SM backgrounds. The work in this thesis has contributed to searching for a few BSM models in multi-lepton final states: searches for heavy scalar Higgs bosons from a general Two Higgs Doublet model (with the potential to explain the baryon asymmetry in the universe) and two searches for vector-like leptons (motivated by the muon $g - 2$ anomaly and/or flavor anomalies). The following publications (using the Run 2 dataset collected by the ATLAS experiment) are a result of this work:

- ATLAS Collaboration, “*Search for heavy Higgs bosons with flavour-violating couplings in multilepton plus b-jets final states in pp collisions at 13 TeV with the ATLAS detector*”, JHEP 12 (2023) 081, available at arXiv:2307.14759.
- ATLAS Collaboration, “*Search for electroweak production of vector-like leptons in tau-lepton and b-jet final states in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*”, available at ATLAS-CONF-2024-008.
- ATLAS Collaboration, “*Search for vector-like leptons coupling to first and second generation Standard Model leptons in multilepton final states in pp collisions at 13 TeV with the ATLAS detector*”, paper in preparation.

The author has also made significant contributions to SM background modelling studies in the following publications:

- ATLAS Collaboration, “*Measurement of the total and differential cross-sections of $t\bar{t}W$ production in pp collisions at 13 TeV with the ATLAS detector*”, JHEP 05 (2024) 131, available at arXiv:2401.05299.

- ATLAS Collaboration, “*Search for leptoquark pair production decaying into $t\bar{t}e^-e^+$ or $t\bar{t}\mu^-\mu^+$ in multi-lepton final states in pp collisions at 13 TeV with the ATLAS detector*”, Eur. Phys. J. C 84 (2024) 818, available at arXiv:2306.17642.
- ATLAS Collaboration, “*Search for same-sign top-quark pair production in pp collisions at 13 TeV with the ATLAS detector*”, submitted to JHEP, available at arXiv:2409.14982.

The author has been an active contributor to studies with the Minimum Bias system of the ATLAS Tile Calorimeter, leading to the following public results (using the Run 2 and part of the Run 3 datasets collected by the ATLAS experiment):

- ATLAS Collaboration, “*Operation and Performance of the ATLAS Tile Calorimeter in LHC Run-2*”, accepted by European Physical Journal C (EPJC), available at arXiv:2401.16034.
- ATLAS Collaboration, “*Preliminary analysis of the luminosity calibration of the ATLAS 13.6 TeV data recorded in 2022*”, available at ATL-DAPR-PUB-2023-001.
- ATLAS Collaboration, “*Preliminary analysis of the luminosity calibration of the ATLAS 13.6 TeV data recorded in 2023*”, available at ATL-DAPR-PUB-2024-001.
- ATLAS Tile Collaboration, “*Radiation Hardness of the Optical Instrumentation of the ATLAS/LHC Tile Calorimeter in Run 2*”, paper in preparation, available at ATL-COM-TILECAL-2024-001.

The author actively participated in detector operations in LHC Run 3, covering data-taking shifts at CALO/FWD desk in the ATLAS control room, and expert on-call shifts for the Tile Calorimeter Detector Control System. The author has also participated in the test beam campaigns at the Super Proton Synchrotron in 2023 with the support of EuroLabs Grant Agreement No. 10105751, for testing TileCal Upgrade electronics for the ATLAS experiment, with tasks ranging from assembly of the upgraded TileCal module prototype, providing feedback on optimal placement of detectors along the beamline, validation of the readouts and data-taking shifts.

Chapter 2

The Standard Model of particle physics

The Standard Model (SM) [12–14] of particle physics took birth in the 1960s as a theoretical framework built upon the principles of Quantum Field Theory (QFT). It introduces infinite, continuous fields that pervade the universe, with elementary particles as discrete fluctuations or *quanta* of these fields. In addition to obeying Poincaré symmetries (translations, rotations and Lorentz boosts in space-time), the SM is constructed to be invariant under the symmetry group:

$$SU(3)_C \otimes SU(2)_L \otimes U(1)_Y. \quad (2.1)$$

This symmetry group describes three of four fundamental forces: the strong force, the weak force and electromagnetism. The $SU(3)_C$ symmetry group governs interactions of the strong force, while the $SU(2)_L \otimes U(1)_Y$ framework governs weak and electromagnetic interactions. According to Noether’s theorem [15], each symmetry corresponds to a conserved quantity. For instance, the $SU(3)_C$ symmetry leads to the conservation of three *color charges* for the strong force, while the $SU(2)_L \otimes U(1)_Y$ symmetry is associated with the conservation of *weak iso-spin* and *weak hypercharge* for the weak and electromagnetic forces respectively. These conserved quantities, known as *quantum numbers*, are unique to each elementary particle.

Elementary particles in the SM, summarised in Figure 2.1, are categorised into two groups based on an intrinsic quantum number called *spin*: ***bosons*** and ***fermions***.

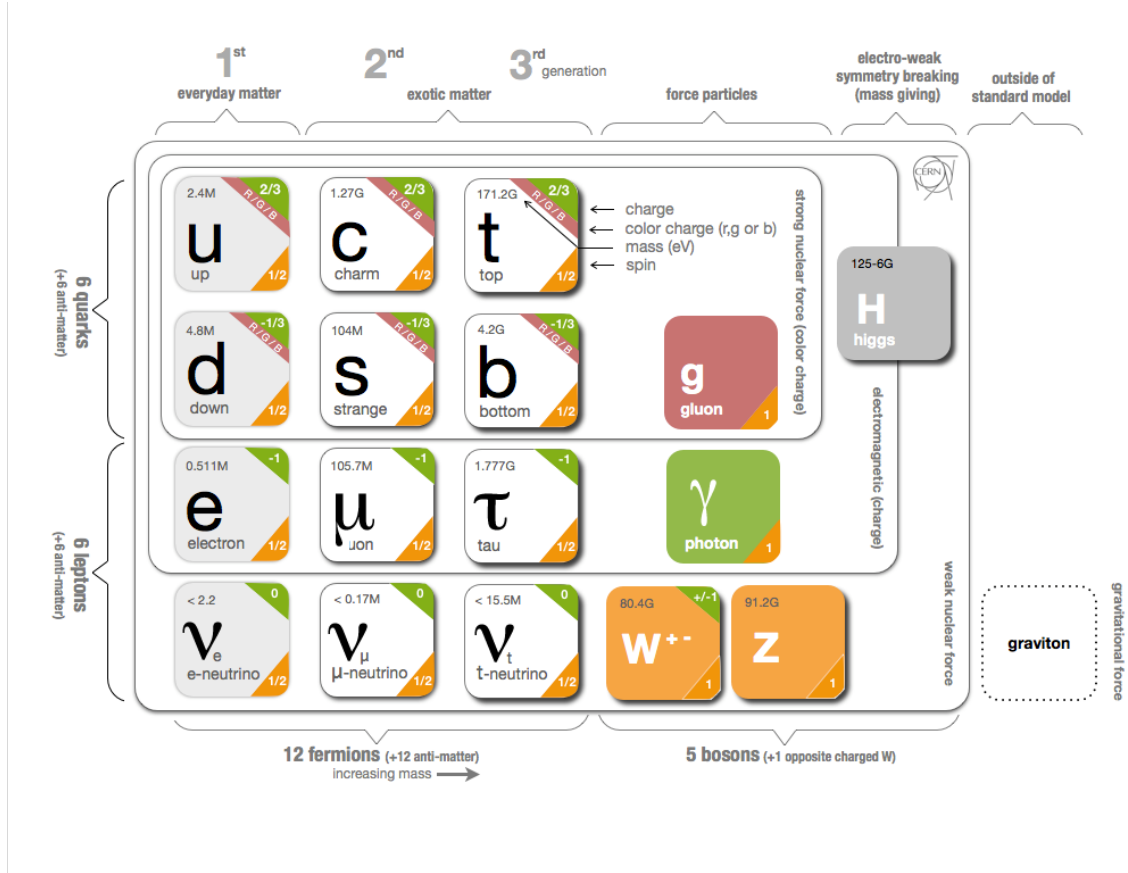


Figure 2.1: Summary of particles in the SM. Fermions are shown with black lettering, while bosons are shown with white lettering. The graviton is a hypothetical particle predicted to extend the SM to a quantum theory of the gravitational force. Figure taken from Ref. [16].

Bosons are particles with integer spin and serve as carriers of fundamental forces in the SM. *Vector bosons*, or particles with spin one, mediate the strong force (gluon: g), weak force ($W^\pm$ and Z bosons) and electromagnetism (photon: γ). The Higgs boson (H), the only spin zero particle in the SM, provides mass to the $W^\pm$ and Z bosons and charged fermions through electroweak symmetry breaking, discussed in Section 2.2.

Fermions are particles with non-integer spin obeying the Pauli exclusion principle [17]: no two fermions can simultaneously occupy the same quantum state within a quantum system. This principle allows stable fermions such as electrons, protons and neutrons to form macroscopic objects around us. In the SM, fermions are of two types:

- **Leptons** are classified into three generations, each forming left-handed iso-spin doublets based on weak flavor: the electron (e) paired with the electron neutrino (ν_e), the muon (μ) with the muon neutrino (ν_μ), and the tau (τ) with the tau

neutrino (ν_τ). Electrons, muons, and taus are electrically charged and interact via the electromagnetic force, which affects only charged particles. The SM assumes that weak interactions exhibit lepton flavor universality, implying that the interactions are independent of the specific lepton flavor involved and occur universally among all leptons. Electrons are the lightest stable leptons and a major constituent of matter around us. Neutrinos possess very low masses compared to their charged counterparts, and the mechanisms governing their mass generation are subject to debate within the SM (see Section 2.3).

- **Quarks** are represented by six fermions: up-type (u), down-type (d), strange (s), charm (c), bottom (b) and top (t). They interact via all three fundamental forces: the weak force, electromagnetic force and strong force. With the exception of the top quark which has a very short lifetime (10^{-25} seconds), quarks are only observed inside bound states known as *hadrons*. Hadrons can be further categorized into *mesons*, composed of a quark and an antiquark, and *baryons*, composed of three quarks. Experimental evidence has also confirmed the existence of particles with more than three valence quarks [18].

This chapter illustrates the mathematical framework of the SM, starting from the principles of gauge invariance (Section 2.1) and its application to build the theory of quantum chromodynamics (Section 2.1.1) and the electroweak force (Section 2.1.2). This is followed by a discussion on the Brout–Englert–Higgs mechanism of mass generation in the SM (Section 2.2). Each section delves briefly into relevant experimental results associated with theory. The chapter concludes with an examination of theoretical limitations of the SM, including input from particle physics and astrophysics experiments (Section 2.3), shedding light on how to build a more complete theory.

2.1 Yang-Mills theories

QFTs built on invariance under the Poincaré and $SU(N)$ *gauge* groups, where $SU(N)$ is the group of special unitary matrices of order N , are called Yang-Mills theories. Poincaré symmetries act on space-time coordinates and leave them unchanged under translations, rotations and Lorentz boosts. Gauge symmetries, on the other hand, act on fields. The SM is a Yang-Mills theory obeying the gauge group in Equation 2.1. This section briefly outlines the steps for introducing local gauge invariance in a Yang-Mills theory with massless bosons,

laying the groundwork to building a theory of the strong force (Section 2.1.1) and the electroweak force (Section 2.1.2) in the subsequent chapters.

From the principles of group theory, the basis of the $SU(N)$ group is formed by $N^2 - 1$ generators, denoted as t^k ($k = 1, \dots, N^2 - 1$), satisfying the commutation relation:

$$[t^k, t^j] = if^{kjl}t^l. \quad (2.2)$$

Here, f^{kjl} have been introduced as the structure constants of the group. A general element $\mathcal{U} \in SU(N)$ satisfies by definition, $\mathcal{U}\mathcal{U}^\dagger = 1$ and $\det(\mathcal{U})=1$, and can be expressed in terms of generators t^k of the $SU(N)$ group as:

$$\mathcal{U} = \mathcal{U}(\alpha(x^\mu)) = \exp(ig\alpha^k(x^\mu)t^k). \quad (2.3)$$

Here, g is a coupling constant (in the strictest sense, at a given energy scale) and α^k are defined in spacetime coordinates x^μ . The generators t^k can be promoted to bosonic fields A^μ as:

$$A^\mu(x^\mu) = A_k^\mu(x^\mu)t^k. \quad (2.4)$$

The form of the field A^μ can be determined by imposing the requirement that its interaction with a general N -component fermionic field Φ at one point in space-time remains independent of its interaction at any other space-time point. This is called the principle of *local gauge invariance*. A general N -component fermionic field Φ with mass m obeying the Dirac equation in $3 + 1$ dimensional spacetime (setting $\hbar = c = 1$) can be written as:

$$\Phi(\vec{x}) = \begin{pmatrix} \phi_1(x_1) \\ \phi_2(x_2) \\ \vdots \\ \phi_N(x_N) \end{pmatrix}, \quad (i\gamma^\mu\partial_\mu - m)\Phi = 0. \quad (2.5)$$

Here, γ^μ are the gamma matrices and ∂_μ is the partial derivative with respect to the spacetime coordinate x^μ . The action of $\mathcal{U} \in SU(N)$ on Φ is called a *gauge transformation* of the field Φ , and dependent on space-time coordinate if α^k are not constant. Local gauge invariance can be imposed by promoting the partial derivative to a *covariant* derivative, D^μ , which describes the kinematics of the field A^μ :

$$D^\mu = \partial^\mu - igA^\mu. \quad (2.6)$$

Thus, under the action of an element $\mathcal{U}$ on Φ :

$$\Phi \rightarrow \Phi' = \mathcal{U}\Phi \quad \implies \quad D^\mu\Phi \rightarrow \mathcal{U}D^\mu\Phi. \quad (2.7)$$

This condition sets the form of A^μ :

$$A^\mu = A_C^\mu - \alpha_A A_B^\mu f^{ABC} + \partial^\mu \alpha_C. \quad (2.8)$$

Further, the commutator of the covariant derivative defines the field tensor $F^{\mu\nu}$:

$$[D^\mu, D^\nu] = igF^{\mu\nu} \quad \implies \quad F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu - ig[A^\mu, A^\nu]. \quad (2.9)$$

Finally, the Lagrangian of locally gauge invariant Yang-Mills theory, consisting of fields A^μ and Φ , can be written as:

$$\mathcal{L}_{YM} = -\frac{1}{4}\text{Tr}[F^{\mu\nu}F_{\mu\nu}] - m\bar{\Phi}\Phi + i\bar{\Phi}\gamma^\mu D_\mu\Phi. \quad (2.10)$$

It is crucial to emphasize that requiring local gauge invariance prohibits a mass term for the bosonic field in the Yang-Mills Lagrangian. This highlights the necessity for an additional mechanism to generate mass if the corresponding boson exhibits a non-zero mass in experimental measurements. Additionally, the bosonic field exhibits self-interactions if the structure constants of the group are non-zero.

2.1.1 Quantum Chromodynamics

Quantum Chromodynamics (QCD) is a non-abelian gauge theory describing the strong interaction, based on local gauge invariance under the $SU(3)$ group. The $3^2 - 1 = 8$ generators of the group are chosen to be the Gell-Mann matrices (λ^a):

$$\begin{aligned}\lambda_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda_2 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \lambda_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ \lambda_4 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & \lambda_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, & \lambda_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ \lambda_7 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, & \lambda_8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.\end{aligned}$$

These correspond to 8 physical gluon fields: $G_a^\mu(x)$ ($a = 1 \dots 8$), building the covariant derivative in Equation 2.11 and the field tensor in Equation 2.12.

$$D^\mu = \partial^\mu - ig_s \left(\frac{t^a}{2} G_a^\mu \right). \quad (2.11)$$

$$G_a^{\mu\nu} = \partial^\mu G_a^\nu - \partial^\nu G_a^\mu + g_s f^{abc} G_b^\mu G_c^\nu. \quad (2.12)$$

Here, g_s is introduced as the QCD coupling constant at a given energy scale. Representing a quark triplet with the notation $q_f^T = (q_f^1, q_f^2, q_f^3)$ where q_i is the quark field with flavor $f = (u, d, c, s, b, t)$ and color $i = (r, g, b)$, we can build the Lagrangian for QCD (without mass terms for the quarks) as:

$$\mathcal{L}_{QCD} = -\frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} + \sum_f \bar{q}_f i \gamma_\mu D^\mu q_f. \quad (2.13)$$

The QCD Lagrangian in its extended form is shown in Equation 2.14 with interaction terms illustrated in Figure 2.2.

$$\begin{aligned}
 \mathcal{L}_{\text{QCD}} = & \underbrace{-\frac{1}{4}(\partial^\mu G_a^\nu - \partial^\nu G_a^\mu)}_{\text{gluon kinematic term}} + \underbrace{\sum_f \bar{q}_f i \gamma_\mu \partial^\mu q_f}_{\text{quark kinematic term}} + \underbrace{g_s G_a^\mu \sum_f \bar{q}_f^\alpha \gamma_\mu \left(\frac{\lambda^a}{2}\right)_{\alpha\beta} q_f^\beta}_{\text{gluon-quark interaction term}} \\
 & + \underbrace{g_s f^{abc} (\partial_\mu G_{a\nu}) G_b^\mu G_c^\nu}_{\text{three-gluon vertex}} - \underbrace{\frac{g_s^2}{4} f^{abc} f^{ade} G_b^\mu G_c^\nu G_{d\mu} G_{e\nu}}_{\text{four-gluon vertex}}
 \end{aligned} \tag{2.14}$$

Figure 2.2 illustrates the gauge interaction terms in the QCD Lagrangian. The first diagram shows the quark-gluon interaction term, which is proportional to $g_s \frac{\lambda_{\alpha\beta}^a}{2} \gamma_\mu$. The second diagram shows the three-gluon vertex, which is proportional to $g_s f^{abc}$. The third diagram shows the four-gluon vertex, which is proportional to $g_s^2 f^{abc} f^{ade}$.

Figure 2.2: Gauge interaction terms in the QCD Lagrangian (Equation 2.14). The first diagram is the quark-gluon interaction term, followed by illustrations of the three- and four-gluon vertices respectively.

Revisiting Equation 2.11, energy dependence for the coupling constant g_s arises to make QCD a renormalisable theory [19]. In experimental measurements, the coupling constant g_s is described in terms of the fine structure constant α_s :

$$\alpha_s = \frac{g_s^2}{4\pi}. \tag{2.15}$$

Energy scale (Q) dependence of α_s is calculated in a perturbative fashion [20] and at first order, expressed as:

$$\alpha_s(Q^2) = \frac{12\pi}{(11n_c - 2n_f) \log \frac{Q^2}{\Lambda^2}}. \tag{2.16}$$

Here, n_c is the number of quark colors, n_f is the number of quark flavors with mass below the energy scale Q . Λ^2 is defined as a cut-off energy after which the perturbative

approximation is valid. Equation 2.16 highlights the inverse relationship between the energy scale Q^2 and value of the coupling α_s (in a universe with less than 16 quark flavors). At high values of Q^2 , α_s is small, such as in the quark-gluon plasma produced in colliders, making the strong force vanishing small. Physically, this implies that quarks and gluons behave as nearly free particles at these scales. On the other hand, as Q^2 becomes smaller, α_s grows, leading to confinement of quarks and gluons to form bound states. This property of the strong force is called *asymptotic freedom* and won the Nobel Prize for David Gross, Frank Wilczek and David Politzer in 2004 [21].

2.1.2 Electroweak unification

The interactions of the weak and electromagnetic forces, termed the electroweak (EW) interactions, are described within a unified symmetry group $SU(2)_L \otimes U(1)_Y$. $U(1)_Y$ has a single degree of freedom and the $2^2 - 1 = 3$ generators of $SU(2)_L$ are chosen to be the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

These correspond to four fields $B^{\mu\nu}$ and $W_i^{\mu\nu}$ ($i = 1, 2, 3$):

$$\begin{aligned} W_i^{\mu\nu} &= \partial_\mu W_\nu^i - \partial_\nu W_\mu^i + gf^{abc}W_\mu^i W_\nu^j, \\ B^{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu. \end{aligned} \tag{2.17}$$

The $SU(2)_L$ symmetry introduces a conserved quantity called *weak isospin* T_3 and $U(1)_Y$ introduces *weak hypercharge* Y , related to the electromagnetic charge Q by the Gell-Mann Nishijima formula [22]:

$$Q = T_3 + \frac{Y}{2}. \tag{2.18}$$

Under $SU(2)_L$, fermions occur as left-handed doublets, acted upon by $SU(2)_L \otimes U(1)_Y$ and right-handed singlets, acted upon only by $U(1)_Y$.

$$l_L = \begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \quad \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L, \quad \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}_L$$

$$\begin{aligned}
q_L &= \begin{pmatrix} u_L \\ d_L \end{pmatrix}_L, & \begin{pmatrix} c_L \\ s_L \end{pmatrix}_L, & \begin{pmatrix} t_L \\ b_L \end{pmatrix}_L \\
\nu_R &= (\nu_e)_R, & (\nu_\mu)_R, & (\nu_\tau)_R \\
e_R &= (e)_R, & (\mu)_R, & (\tau)_R \\
u_R &= (u)_R, & (c)_R, & (t)_R \\
d_R &= (d)_R, & (s)_R, & (b)_R
\end{aligned}$$

This description of the four fields in Equation 2.17, three governed by the weak force and one by the electromagnetic force, does not yet correspond to force carriers of the electroweak field. This is because it has been observed from neutrino scattering experiments, that neutral currents have a small but non-zero component that couples to right handed fermions [20]. Correspondence with the physical fields - the photon (γ), $W^\pm$ and Z boson fields - requires a description of both forces under a unified framework, and is introduced through carefully defined covariant derivatives of $SU(2)_L \otimes U(1)_Y$:

$$\begin{aligned}
D^\mu l_L^f &= \left(\partial^\mu - ig \frac{\sigma_i}{2} W_i^\mu - ig' \frac{Y}{2} B^\mu \right) l_L^f, \\
D^\mu e_R^f &= \left(\partial^\mu - ig' \frac{Y}{2} B^\mu \right) e_R^f, \\
D^\mu \nu_R^f &= \left(\partial^\mu - ig' \frac{Y}{2} B^\mu \right) \nu_R^f.
\end{aligned} \tag{2.19}$$

Similar terms are defined for the quark fields. Coupling constants g and g' associated to the $SU(2)_L$ and $U(1)_Y$ respectively have been introduced. The electroweak Lagrangian can be written as:

$$\begin{aligned}
\mathcal{L}_{EW} &= -\frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{4} W_{\mu\nu}^i W_i^{\mu\nu} + \underbrace{\sum_f \bar{l}_L^f i\gamma_\mu D^\mu l_L^f + \sum_f \bar{q}_L^f i\gamma_\mu D^\mu q_L^f}_{\text{kinematic terms for left-handed fermions}} \\
&\quad + \underbrace{\bar{\nu}_R^f i\gamma_\mu D^\mu \nu_R^f + \bar{e}_R^f i\gamma_\mu D^\mu e_R^f + \bar{u}_R^f i\gamma_\mu D^\mu u_R^f + \bar{d}_R^f i\gamma_\mu D^\mu d_R^f}_{\text{kinematic terms for right-handed fermions}}
\end{aligned} \tag{2.20}$$

Expanding the terms in Equation 2.20 can be used to study the origin of charged and neutral currents and self interactions in the theory, while giving rise to physical force fields of the photon, $W^\pm$ and Z boson.

Charged currents

Charged currents are described by terms in Equation 2.20 corresponding to transitions in left-handed fermion doublets:

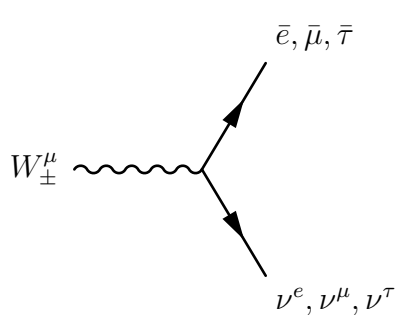
$$\mathcal{L}_{\text{Charged}} = \frac{g}{2} \sum_f \bar{l}_L^f \gamma_\mu (\sigma_1 W_1^\mu + \sigma_2 W_2^\mu) l_L^f + \frac{g}{2} \sum_f \bar{q}_L^f \gamma_\mu (\sigma_1 W_1^\mu + \sigma_2 W_2^\mu) q_L^f. \quad (2.21)$$

Physical fields associated to $W^\pm$ bosons arise on transforming to the diagonal basis $\sigma^\pm$:

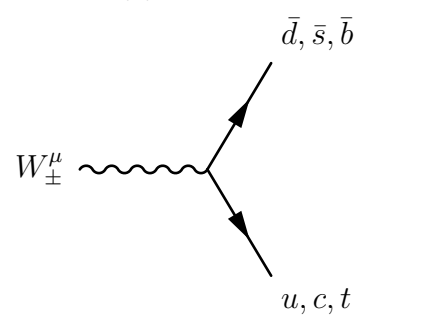
$$\sigma^\pm = \frac{1}{2}(\sigma_1 \pm i\sigma_2); \quad W_\pm^\mu = \frac{1}{\sqrt{2}}(W_1^\mu \mp iW_2^\mu). \quad (2.22)$$

Expanding the charged currents in the EW Lagrangian gives terms for lepton-neutrino and quark-quark transitions facilitated by the $W^\pm$ bosons, illustrated in Figure 2.3.

$$\begin{aligned} \mathcal{L}_{\text{Charged}} = & -\frac{g}{2\sqrt{2}} (\bar{\nu}^e, \bar{\nu}^\mu, \bar{\nu}^\tau) \gamma_5 (1 - \gamma_5) W_+^\mu \begin{pmatrix} e \\ \mu \\ \tau \end{pmatrix} \\ & - \frac{g}{2\sqrt{2}} (\bar{u}, \bar{c}, \bar{t}) \gamma_5 (1 - \gamma_5) W_+^\mu \mathcal{V}_{CKM} \begin{pmatrix} d \\ s \\ b \end{pmatrix} + \text{h.c.} \end{aligned} \quad (2.23)$$



$\propto \frac{g}{2\sqrt{2}} \gamma_\mu (1 - \gamma_5)$



$\propto \frac{g}{2\sqrt{2}} \gamma_\mu (1 - \gamma_5) \mathcal{V}_{CKM}$

Figure 2.3: Charged currents in the electroweak Lagrangian (Equation 2.20). The first diagram illustrates lepton-neutrino transitions, while the second diagram illustrates quark-quark transitions.

Here, $\mathcal{V}_{CKM}$ is a 3×3 unitary matrix called the *Cabbibo-Kobayashi-Masakawa (CKM) matrix* [20]. This matrix is parameterised in terms of three Euler angles $(\theta_{12}, \theta_{23}, \theta_{13})$ and a *charge-parity* (CP) violating phase angle (δ_{13}) as:

$$\begin{pmatrix} |V_{ud}| & |V_{us}| & |V_{ub}| \\ |V_{cd}| & |V_{cs}| & |V_{cb}| \\ |V_{td}| & |V_{ts}| & |V_{tb}| \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta_{13}} \\ 0 & 1 & 0 \\ -s_{13}e^{i\delta_{13}} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (2.24)$$

Here, c_{jk} and s_{jk} denote the cosine and sine of the angles. The probability of a transition from quark flavor j to k is proportional to $|V_{ij}|^2$. Parameters of this matrix are measured to great precision at multiple experimental facilities like the LHCb experiment [23]:

$$\begin{aligned} \sin \theta_{12} &= 0.22500 \pm 0.00067, \\ \sin \theta_{13} &= 0.00369 \pm 0.00011, \\ \sin \theta_{23} &= 0.04182^{+0.00085}_{-0.00074}, \\ \delta_{13} &= 1.144 \pm 0.027. \end{aligned} \quad (2.25)$$

Neutral currents

Neutral currents arise from diagonal terms in Equation 2.20:

$$\mathcal{L}_{\text{Neutral}} = \sum_f \sum_{i=q,l} \bar{\psi}_i^f \gamma_\mu \left(g T_3 W_3^\mu + g' \frac{Y}{2} B^\mu \right) \psi_i^f. \quad (2.26)$$

Mixing of neutral gauge bosons from the $SU(2)_L$ and $U(1)_Y$ groups through the *Weinberg angle* (θ_W) gives rise to the physical photon (A^μ) and Z boson (Z^μ) fields:

$$\begin{pmatrix} B^\mu \\ W_3^\mu \end{pmatrix} = \begin{pmatrix} \cos \theta_W & -\sin \theta_W \\ \sin \theta_W & \cos \theta_W \end{pmatrix} \begin{pmatrix} A^\mu \\ Z^\mu \end{pmatrix}. \quad (2.27)$$

Additionally the following quantities are defined:

$$e = g' \cos \theta_W = g \sin \theta_W, \quad (2.28)$$

$$Q = T_3 + \frac{Y}{2}, \quad (2.29)$$

$$Q_Z = \frac{1}{\sin \theta_W \cos \theta_W} (T_3 - Q \sin^2 \theta_W). \quad (2.30)$$

These substitutions allow to illustrate neutral currents in the EW Lagrangian, mediated by the photon (γ) and Z boson, illustrated in Figure 2.4.

$$\mathcal{L}_{\text{Neutral}} = \sum_f \sum_{i=q,l} e \bar{\psi}_i^f \gamma_\mu Q \psi_i^f A^\mu + e \bar{\psi}_i^f \gamma_\mu Q_Z \psi_i^f Z^\mu. \quad (2.31)$$

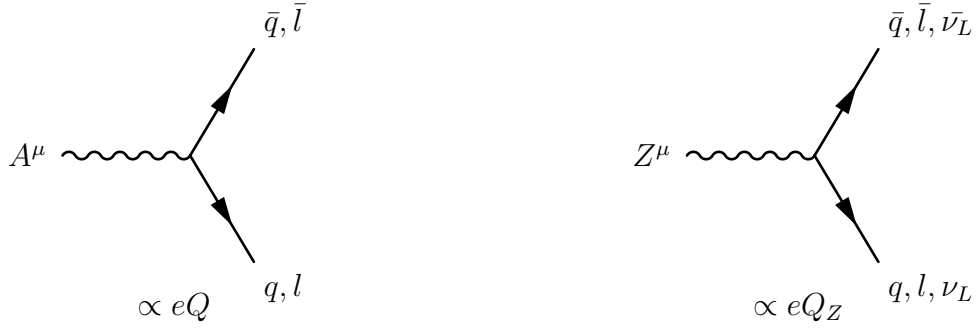


Figure 2.4: Neutral currents in the electroweak Lagrangian (Equation 2.20). The first diagram illustrates interactions of the photon, while the second diagram illustrates interactions of the Z boson.

Self interactions

Self interactions arise in Equation 2.20 by making substitutions from Equation 2.22 and Equation 2.27, illustrated in Figure 2.5.

$$\begin{aligned} \mathcal{L}_{\text{self}} = & -\frac{1}{4} [F_{\mu\nu} F^{\mu\nu} + Z_{\mu\nu} Z^{\mu\nu} + W_{\mu\nu}^+ W_{\mu\nu}^-] \\ & + ig \sin \theta_W (W_{\mu\nu}^+ W_{\mu\nu}^- A^\nu - W_{\mu\nu}^- W_{\mu\nu}^+ A^\nu + F_{\mu\nu} W_{\mu\nu}^+ W_{\mu\nu}^-) \\ & + ig \cos \theta_W (W_{\mu\nu}^+ W_{\mu\nu}^- Z^\nu - W_{\mu\nu}^- W_{\mu\nu}^+ Z^\nu + Z_{\mu\nu} W_{\mu\nu}^+ W_{\mu\nu}^-) \\ & + \frac{g^2}{2} (2g^{\mu\nu} g^{\rho\sigma} - g^{\mu\rho} g^{\nu\sigma} - g^{\mu\sigma} g^{\nu\rho}) \left[\frac{1}{2} W_\mu^+ W_\nu^+ W_\rho^- W_\sigma^- \right. \\ & \left. - W_\mu^+ W_\nu^- (A_\rho A_\sigma) \sin^2 \theta_W + Z_\rho Z_\sigma \cos^2 \theta_W + 2A_\rho Z_\sigma \sin \theta_W \cos \theta_W \right]. \end{aligned} \quad (2.32)$$

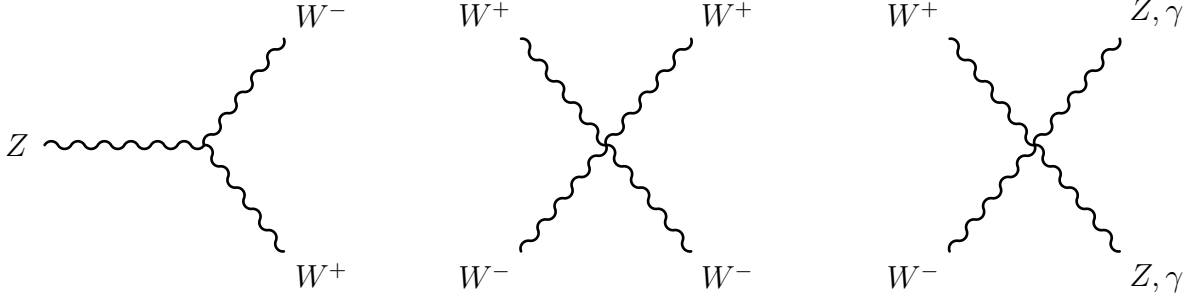


Figure 2.5: Self interaction terms in the electroweak Lagrangian (Equation 2.20).

2.2 The Brout–Englert–Higgs mechanism

The $W^\pm$ and Z bosons, described in Section 2.1.2, were observed in 1983 by the UA1 collaboration at the CERN SPS as massive vector bosons [24]. However, mass terms for gauge bosons in the EW Lagrangian are forbidden to preserve gauge invariance, underscoring the need for an additional component in the model. The *Brout–Englert–Higgs mechanism* [5–7], proposed by P. Higgs et. al. in 1964, following the work made in the context of broken symmetries in superconductivity, emerged as a solution to this problem. It involves the spontaneous symmetry breaking of a complex scalar field called the *Higgs field*, resulting in the generation of masses for the $W^\pm$ and Z bosons, while leaving the photon massless.

The Higgs field is introduced as a complex $SU(2)_L$ doublet scalar field:

$$\Phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \quad (2.33)$$

where the indices indicate the electromagnetic charge of the field. The Lagrangian for this field is constructed using the $SU(2)_L \otimes U(1)_Y$ covariant derivative for left-handed fermions (Equation 2.19), together with a potential $V(\Phi)$ of a unique form:

$$\begin{aligned} \mathcal{L}_{\text{Higgs}} &= (D^\mu \Phi)^\dagger D_\mu \Phi - V(\Phi) \\ &= (D^\mu \Phi)^\dagger D_\mu \Phi - \mu^2 \Phi^\dagger \Phi + \lambda (\Phi^\dagger \Phi)^2. \end{aligned} \quad (2.34)$$

The specific scenario where $\lambda > 0$ ensures that the potential is bounded from below. Two choices for the value of μ^2 remain, illustrated in Figure 2.6: for $\mu^2 > 0$, the only stable minima is at $|\Phi| = 0$. On the other hand, if $\mu^2 < 0$, the potential exhibits an infinite

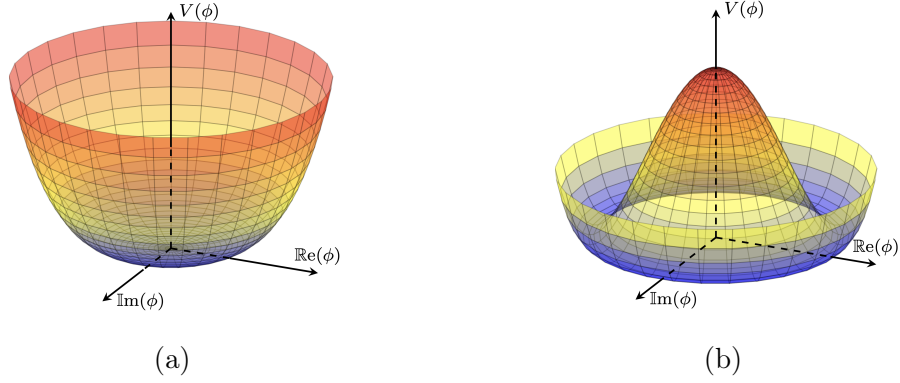


Figure 2.6: Illustration of the Higgs potential for $\lambda > 0$ and (a) $\mu^2 > 0$ (b) $\mu^2 < 0$.

number of global minima distributed along the circular path described by:

$$|\Phi|^2 = \Phi^\dagger \Phi = -\frac{\mu^2}{\lambda} \equiv \frac{\nu^2}{2}. \quad (2.35)$$

Here, ν is defined as the *vacuum expectation value* (VEV). The latter scenario illustrates the core of the Brout–Englert–Higgs mechanism: while the potential about $|\Phi| = 0$ is symmetric, choosing any point in the circular minima ($|\Phi| = \sqrt{-\frac{\mu^2}{\lambda}}$) *spontaneously* breaks symmetry. According to the Goldstone theorem [25], four massless gauge bosons occur when the $SU(2)_L \otimes U(1)_Y$ symmetry is broken. Three of these Goldstone bosons are absorbed by the $W^\pm$ and Z fields giving them mass, while the photon remains massless. The fourth Goldstone boson is the Higgs boson.

Mathematically, the minimum of the potential is chosen so that the electrically neutral field in the Higgs doublet, corresponding to the photon field, acquires a VEV:

$$\Phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ \nu \end{pmatrix}. \quad (2.36)$$

Expanding it in terms of the Goldstone fields $\theta_i (i = 1, 2, 3)$ and $H(x)$, we get:

$$\Phi = \exp \left(i \frac{\sigma_i}{2} \theta_i(x) \right) \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ \nu + H(x) \end{pmatrix}. \quad (2.37)$$

The kinematic term in Equation 2.34 can then be expanded with this new parametrization, about the VEV:

$$(D^\mu \Phi)^\dagger D_\mu \Phi = \frac{1}{2} \partial^\mu H \partial_\mu H + (\nu + H)^2 \left(\frac{g^2}{4} (W_\mu^+)^\dagger W_\mu^+ + \frac{g^2}{4} (W_\mu^-)^\dagger W_\mu^- \right) \frac{g^2}{8 \cos^2 \theta_W} Z_\mu Z^\mu. \quad (2.38)$$

The masses of the $W^\pm$, Z and Higgs bosons can be derived from the model parameters and are determined through precise experiments [20]:

$$\begin{aligned} \mathcal{M}_W &= \frac{\nu g}{2} = 80.379 \pm 0.012 \text{ GeV}, \\ \mathcal{M}_Z &= \frac{\nu g}{2 \cos \theta_W} = 91.1876 \pm 0.0021 \text{ GeV}, \\ \mathcal{M}_H &= \sqrt{2\lambda\nu} = 125.10 \pm 0.14 \text{ GeV}. \end{aligned} \quad (2.39)$$

The photon field remains massless. The Higgs potential, in terms of the Higgs field shows the self interaction terms:

$$\mathcal{V}(\Phi) = \frac{m_H^2}{2} H^2 + \frac{m_H^2}{2\nu} H^3 + \frac{m_H^2}{8\nu^2} H^4. \quad (2.40)$$

Fermion masses are provided via Yukawa interaction terms with the Higgs field:

$$\mathcal{L}_{\text{Yukawa}} = -\sum_f c_f^d (\bar{u}, \bar{d})_L \Phi d_R - \sum_f c_f^u (\bar{u}, \bar{d})_L \Phi u_R - \sum_f c_f^e (\bar{\nu}_e, \bar{e})_L \Phi * e_r + \text{h.c.} \quad (2.41)$$

which transforms after spontaneous symmetry breaking to:

$$\mathcal{L}_{\text{Yukawa}} = \frac{1}{\sqrt{2}} (\nu + H) \sum_f (c_f^d \bar{d}_f d_f + c_f^u \bar{u}_f u_f + c_f^e \bar{e}_f e_f). \quad (2.42)$$

and are thus proportional to the VEV:

$$m_{d_f} = c_f^d \frac{\nu}{\sqrt{2}}, \quad m_{u_f} = c_f^u \frac{\nu}{\sqrt{2}}, \quad m_{e_f} = c_f^e \frac{\nu}{\sqrt{2}}. \quad (2.43)$$

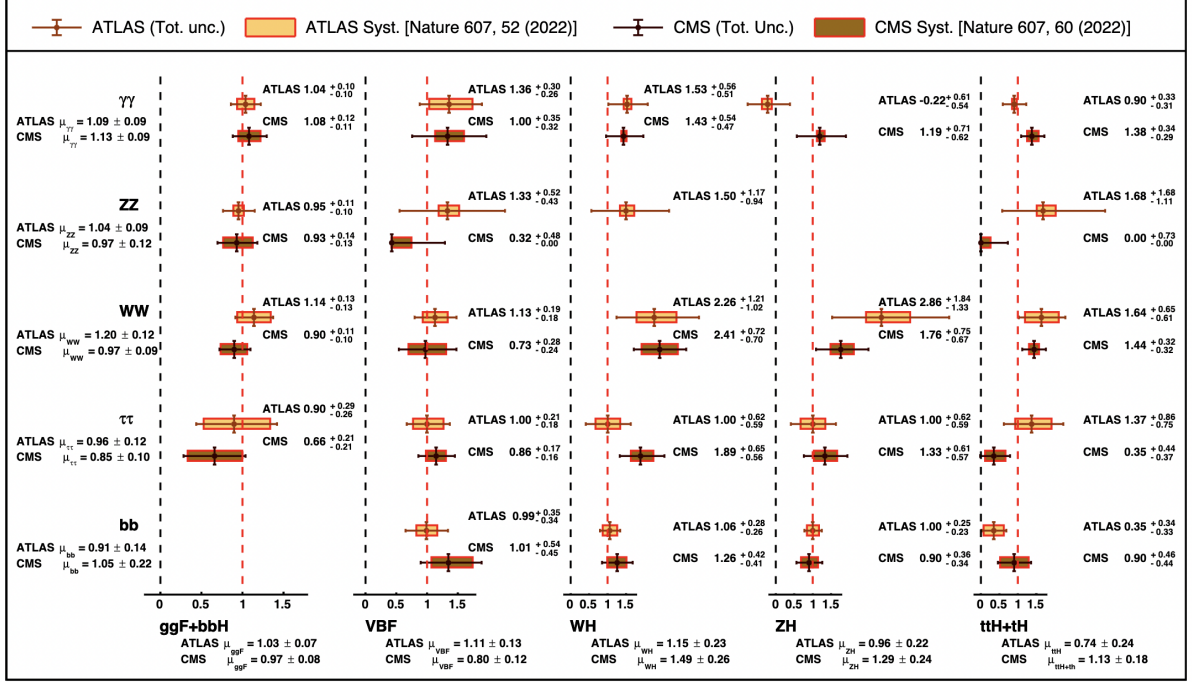


Figure 2.7: Measured production cross-sections and decay branching ratios of the discovered Higgs boson, divided by their SM predictions. Figure taken from Ref. [23].

The Higgs boson was discovered in 2012 by the ATLAS and CMS collaborations at CERN [8, 9]:

$$m_{\text{Higgs}} = 125 \pm 0.17 \text{ GeV}, \quad \nu \sim 246 \text{ GeV}. \quad (2.44)$$

Independent results from ATLAS and CMS collaborations have, since then, measured the production and decay cross-sections of the Higgs boson to be compatible with the SM prediction, illustrated in Figure 2.7.

2.3 Shortcomings of the Standard Model

The SM is the most consistent and well-tested framework for describing matter at the smallest scales. However, it fails to provide a quantum description of the gravitational force, thus failing to describe large astronomical structures in the universe where the effect of this force starts to dominate. Further, studies on the Cosmic Microwave Background (CMB) [26] have shown that only about 5% of matter in the universe can be described within the SM. Cosmological observations, such as gravitational lensing and measurements on galactic

rotation curves [27] indicate the presence of *dark matter*, interacting only through weak or gravitational interaction. Dark matter is estimated to make up about 74% of the universe and no SM particle has the properties to describe its interactions. Finally, a mysterious dark energy, predicted to make up the remaining universe and explain its accelerated expansion, lacks a description within the scope of the SM.

The SM faces further theoretical challenges, such as accounting for the wide range of particle couplings and masses that span from eV to GeV scales, and explaining the abundance of matter over anti-matter in the universe. Recent experimental results, like the anomalous magnetic moment of the muon, the Cabibbo Angle anomaly and anomalies in flavor physics, stand in tension with existing theoretical predictions. These results can be resolved with improved precision of either theoretical or experimental methods, but also potentially point at the existence of BSM particles. These challenges are highlighted in the remaining text.

Higgs mass and fine-tuning of SM parameters

The SM is defined in terms of 19 parameters that are not predicted by theory, summarised in Table 2.1.

Category	Parameter
Gauge coupling constants	$U(1)$ gauge coupling
	$SU(2)$ gauge coupling
	$SU(3)$ gauge coupling
Fermion masses	m_e, m_μ, m_τ
	$m_u, m_d, m_c, m_s, m_b, m_t$
Mixing parameters	$\theta_{12}, \theta_{23}, \theta_{13}, \delta_{13}$
QCD vacuum angle	θ_{QCD}
Higgs parameters	m_{Higgs}, ν

Table 2.1: Free parameters of the SM.

The values of these parameters are determined experimentally and used to test other predictions of the SM. The mass of the Higgs, for example, came as a surprise because higher order corrections to the Higgs mass include logarithmic contributions from fermion loops, leading to a divergent integral.

One way to regularise this is to introduce a *cut-off* mass scale (Λ_{SM}) and the correction reduces to:

$$\Delta m_{\text{Higgs}}^2 = \frac{\Lambda_{SM}^2}{32\pi^2} \left(6\lambda + \frac{1}{4}(9g^2 + 3g'^2) - y_t^2 \right) + \mathcal{O}(\ln(\Lambda_{SM})). \quad (2.45)$$

In the absence of new physics between the EW and Planck scale, Λ_{SM} is taken to be the Planck scale, leading to very large corrections to the tree-level Higgs mass. Thus, the experimentally measured value of the Higgs was unexpected and counter-intuitive, and hints at the possibility of additional new particles below the Planck scale that might cancel out the divergences.

Cosmological observations point to the abundance of matter over anti-matter in the universe. This is called the *baryon asymmetry* of the universe and can be introduced in the SM through two ways: the complex phase in the CKM matrix which leads to charge-parity violation in the quark sector, and a non-zero value of yet another allowed term in the QCD Lagrangian, called the *QCD vacuum angle*:

$$-\frac{g_s}{8\pi} \theta_{QCD} G_{\mu\nu}^a \tilde{G}^{\mu\nu,a}. \quad (2.46)$$

The complex phase however is not large enough to explain the observed asymmetry. On the other hand, a non-zero value of θ_{QCD} would imply a non-zero electric dipole moment of the neutron, in violation with experimental observations [23]. Thus, the abundance of matter over antimatter in the universe cannot be explained by the SM.

The Cabibbo angle anomaly

As described in Section 2.1.1, transitions between quark flavors are described at tree level by the CKM matrix. The *Cabibbo angle* is defined in terms of the $u \rightarrow d$ and $u \rightarrow s$ mixing parameters as:

$$\tan \theta_{12} = \frac{|V_{ud}|}{|V_{us}|}. \quad (2.47)$$

This angle can be measured in kaon, pion, tau and beta decays. In particular, the sensitivity to BSM effects goes as squared of $\tan \theta_C$ [28] and depends on the determination of the Fermi Constant G_F [29]:

$$G_F = 1.1663787(6) \times 10^{-5} \text{GeV}^{-2}. \quad (2.48)$$

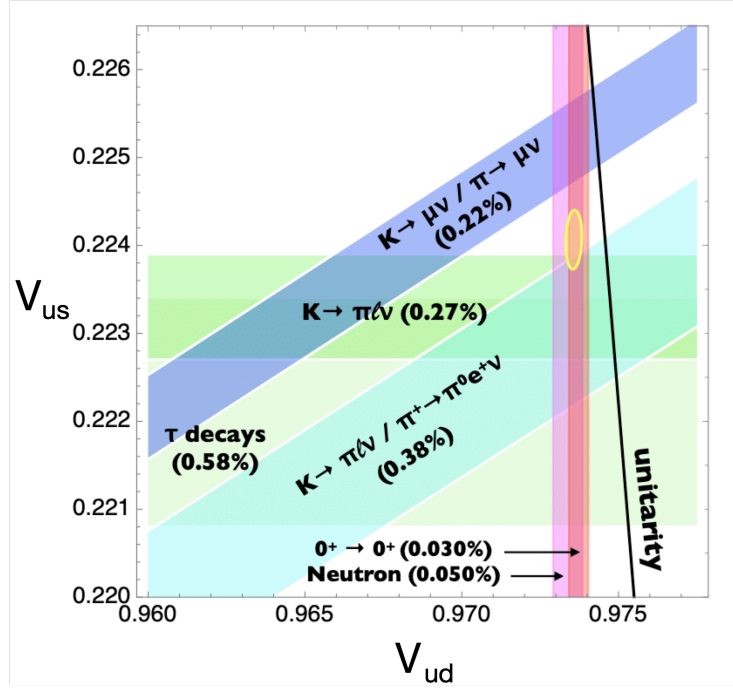


Figure 2.8: Different determinations of the CKM matrix parameters $|V_{ud}|$ and $|V_{us}|$, leading to the Cabibbo Angle Anomaly. Figure adapted from Ref. [30].

Currently, there is a $\sim 3\sigma$ deficit from unitarity in measurement of the first row of the CKM matrix, dominated by effects from $|V_{ud}|$ [31], as shown in Figure 2.8. Therefore the Cabibbo Angle anomaly can be explained by a BSM effect in beta decays ($d \rightarrow ue\nu$) transitions, but also an effect in muon decay ($\mu \rightarrow e\nu\nu$), changing the value of the Fermi constant.

Anomalous muon magnetic moment

Particles with non-zero spin (S) such as the muon carry a magnetic moment (M) defined as

$$\mathcal{M} = g_\mu \frac{e}{2m} \mathcal{S}. \quad (2.49)$$

where m is the mass of the muon, e is the electromagnetic charge and g_μ is a dimensionless factor called the g -factor. Contributions to g_μ are shown in Figure 2.9. The value of g_μ is dominated by the tree-level Dirac computation and is set to 2 [32]. Additional corrections come from QED (virtual photon, lepton and weak boson loops) and QCD (Hadronic light-light interactions and Hadronic Vacuum Polarisation). The uncertainty in g_μ is dominated by effects from Hadronic Vacuum Polarisation (HVP).

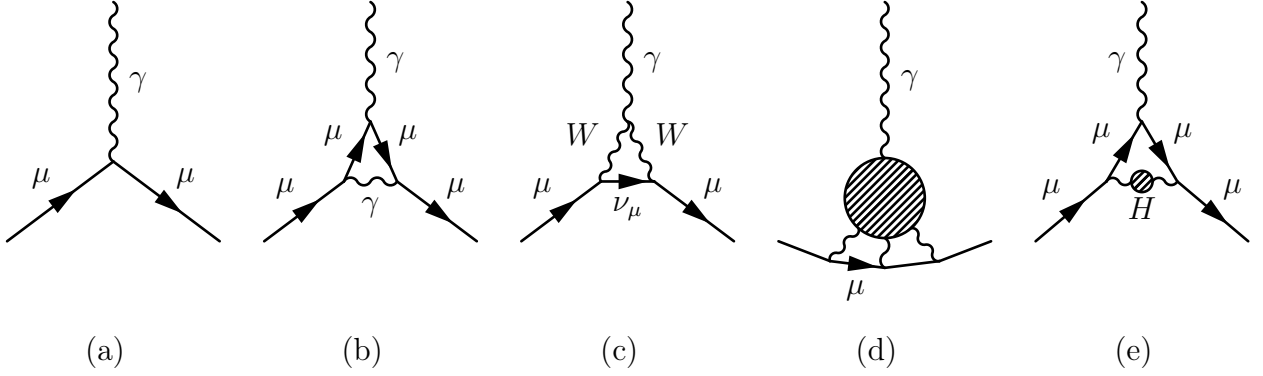


Figure 2.9: Contributions to the $g-2$ anomaly from (a) tree-level Dirac equation (b) QED (c) Electroweak effects (d) Hadronic light-by-light (e) Hadronic vacuum polarisation (HVP). The measured value is dominated by QED, while uncertainty is dominated by HVP.

It is customary to define the *anomalous* magnetic moment of the muon as its deviation from the tree-level Dirac value and calculated up to NNLO precision for HVP [32]:

$$a_\mu = \frac{g_\mu - 2}{2} = 116591830(43) \times 10^{-11}. \quad (2.50)$$

The Muon $g - 2$ Experiment at Fermi National Accelerator Laboratory (FNAL) is one of the leading facilities that can measure a_μ to great precision. The experiment uses 3.1 GeV polarised muons injected into a circular storage ring. The difference between the muon spin precession frequency and the cyclotron frequency is then used to determine the value of a_μ . The latest and most precise result to date was determined in 2023, using the data collected in 2018-20 [10]:

$$a_\mu = 116592054(22) \times 10^{-11}. \quad (2.51)$$

As seen in Figure 2.10, the experimentally measured value of a_μ differs from the SM prediction in the 2020 White Paper by $\sim 5\sigma$. Such a discrepancy can be explained by existence of heavy particles with preferential coupling to the muon. However, it is important to note that SM calculations are currently undergoing an update using Lattice QCD (also shown in Figure 2.10) and might reduce or completely remove the said discrepancy.

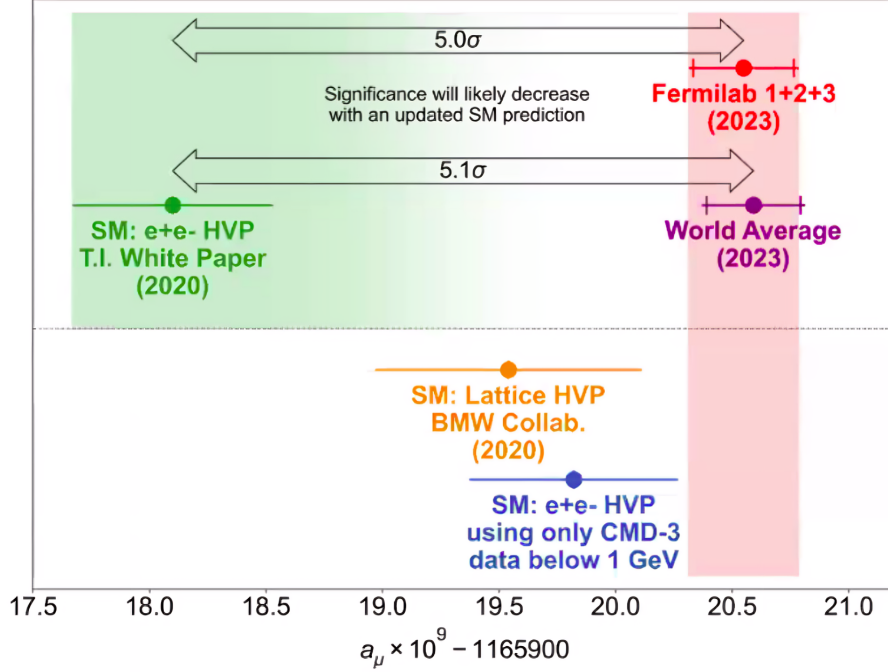


Figure 2.10: Theoretical and experimental determinations of the muon magnetic moment. Figure adapted from Ref. [10].

Flavor anomalies

Results from flavor physics experiments have reported deviations from SM predictions in semi-leptonic B -meson decays to a D -meson or D^* -meson. To reduce hadronic uncertainties, the ratio $R(D)$ is defined as:

$$R(D) = \frac{\Gamma(B \rightarrow D\tau\bar{\nu})}{\Gamma(B \rightarrow Dl\nu)}. \quad (2.52)$$

where $l = e, \mu$. Similarly, $R(D^*)$ is defined for B -meson to D^* -meson decays. The latest combination measurements of these ratios from various experiments, BaBar, Belle and LHCb, indicate a $\sim 3\sigma$ deviation from SM predictions (Figure 2.11). However, no single result taken alone is statistically significant [11]. The development of precision experiments like Belle-II will provide a vital cross-check to current estimates.

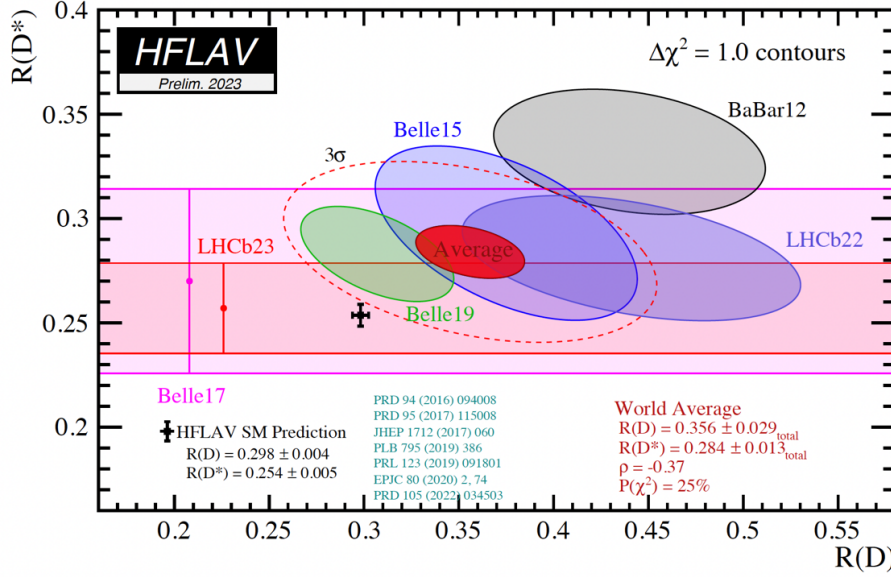


Figure 2.11: Latest combination of results of measurements of $R(D)$ and $R(D^*)$. Figure taken from Ref. [11].

2.4 Where is new physics?

The previous sections described the theoretical framework of the SM of particle physics and motivations which suggest that it is an approximation of a more fundamental theory. One paradigm assumes that such a theory lies above the electroweak mass scale and has sizeable interactions with the SM, leading to modifications in production or decay cross-sections of SM particles. Figure 2.12 shows the total production cross section measurements for measured by ATLAS and CMS: for example, the measured cross-section of $t\bar{t}W$ and $t\bar{t}t\bar{t}$ may be enhanced by decays from particles of the new theory.

The searches for new physics highlighted in this thesis focus on final states with two, three or four or more leptons. Backgrounds in these channels are well-understood or easily corrected. Section 9 highlights a search for additional Higgs bosons from a general two Higgs Doublet model, which has the potential to explain excesses in $t\bar{t}W$ and $t\bar{t}t\bar{t}$ cross-section measurements while also providing a mechanism for generation of baryon asymmetry in the universe. Chapter 10 highlights searches for vector-like leptons coupling to second generation SM leptons, which have the potential to explain the $(g-2)_\mu$ and flavor anomalies. Finally, Chapter 11 highlight the search for vector-like leptons preferentially coupled to third generation SM fermions, which have the potential to explain the hierarchy problem

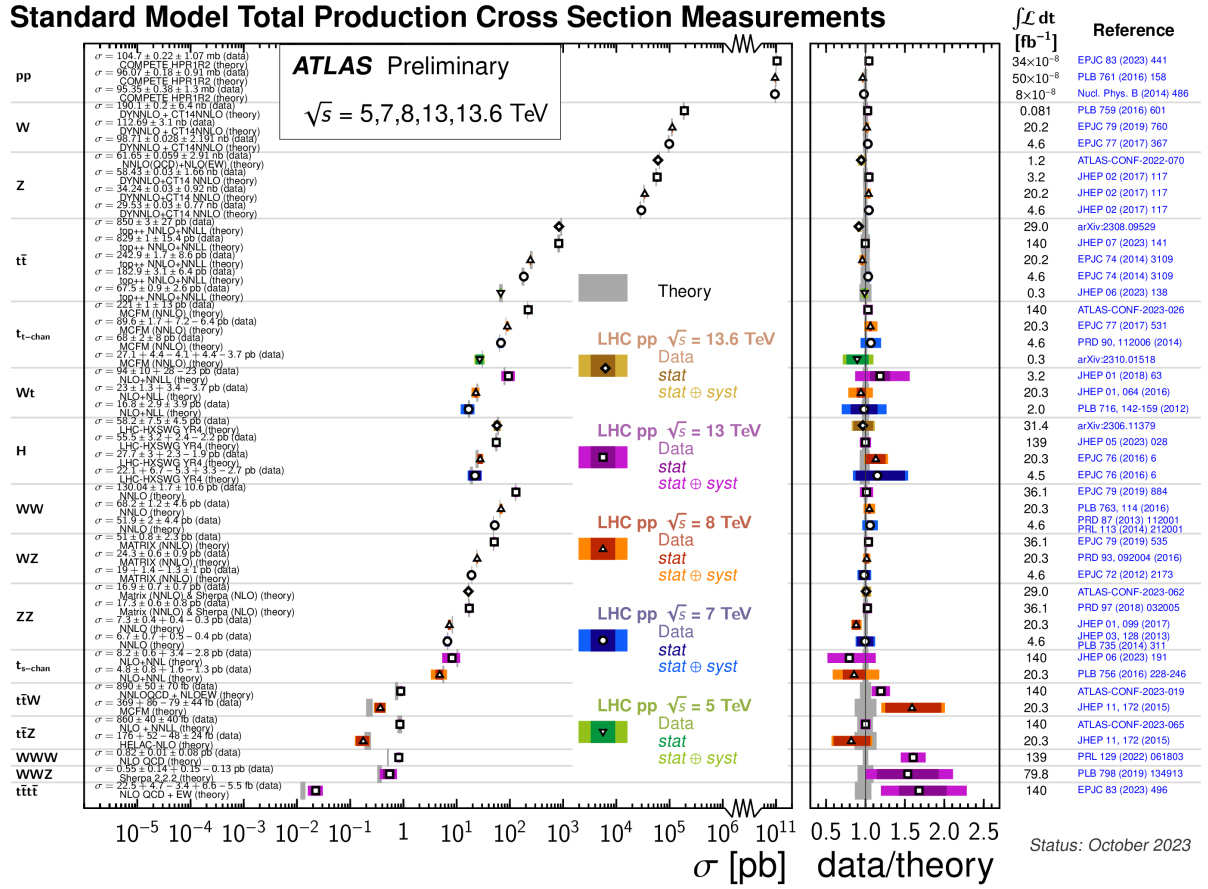


Figure 2.12: Total production cross-section measurements for some SM processes. Figure taken from Ref. [33].

and flavor anomalies. While no significant excess was seen in either of the searches, they serve as an attempt to add another piece to the jigsaw of finding a suitable extension of the SM, if not complete it.

The ATLAS experiment at the Large Hadron Collider

3.1 The Large Hadron Collider

The Large Hadron Collider (LHC) [34] at CERN is the most powerful hadron collider ever built, at the time of writing this thesis. It resides in a 27 km circular tunnel located 100 m beneath ground at the Franco-Swiss border near Geneva, Switzerland. It is a state-of-the-art machine with two superconducting rings, designed to provide proton beams up to 7 TeV. The operational periods of the machine, known as *Runs*, are alternated with periods of maintenance and upgrades referred to as *Long Shutdown (LS)*. The LHC's first Run occurred from 2010 to 2012 (Run 1), operating at a center-of-mass energy of $\sqrt{s} = 7$ and $\sqrt{s} = 8$ TeV, followed by a three-year Long Shutdown (LS1). The second Run spanned from 2015 to 2018 (Run 2), marked by data collection at a significantly higher center-of-mass energy of $\sqrt{s} = 13$ TeV. The data utilized for physics analyses in this thesis originates from Run 2. LS2 finished in 2021 and marked the start of Run 3 at a center-of-mass energy of $\sqrt{s} = 13.6$ TeV, ongoing at the time of writing this thesis.

The LHC is the final stage of a multi-stage accelerator system shown in Figure 3.1. The collider chain is initiated by extracting protons from a bottle of hydrogen gas by stripping it off electrons. These protons are accelerated to 50 MeV in a linear accelerator (LINAC 2), followed by a Booster circular accelerator where they exit with an energy of 1.4 GeV. The Proton Synchrotron (PS) and Super Proton Synchrotron (SPS) provide additional boosts up to 25 GeV and 450 GeV each and finally enter the LHC. The SPS also provides the beam to experiments located in the CERN North Area.

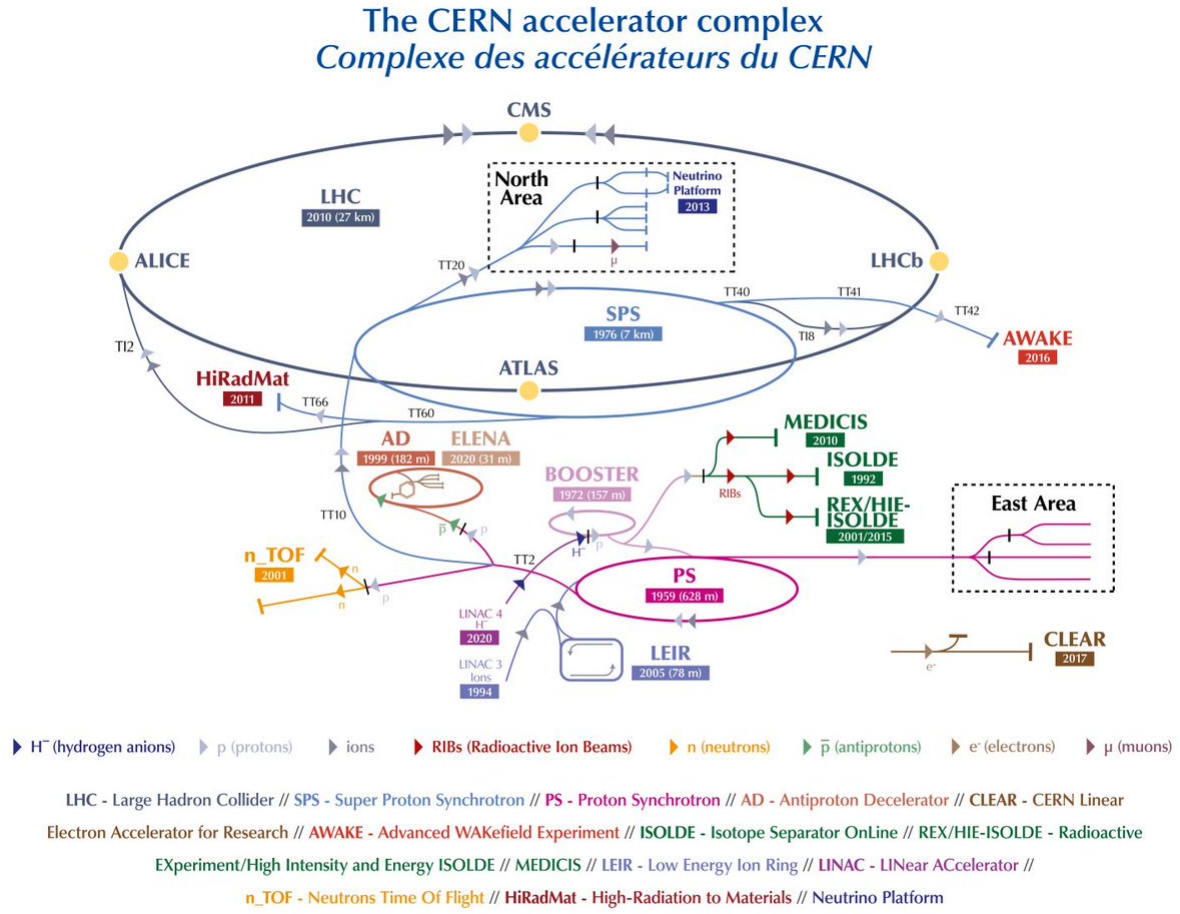


Figure 3.1: Schematic of the accelerator complex at CERN. Figure taken from Ref. [35].

Proton beams are accelerated in opposite directions in the LHC and brought to collision at four specific interactions points (IPs) where experiments are located:

- The ATLAS (A Toroidal LHC ApparatuS) [36] and CMS (Compact Muon Solenoid) [37] are general-purpose experiments positioned at opposite sides of the LHC ring. They are built to test the SM with unprecedented precision and probe new physics models.
- The LHCb (LHC-beauty) [38] experiment is a single arm forward spectrometer aimed at measuring CP violation in the quark sector and rare decays of hadrons containing bottom and charm quarks.
- ALICE (A Large Ion Collider Experiment) [39] is dedicated to study properties of

the quark-gluon plasma, believed to have existed in the early universe shortly after the Big Bang. For these studies, the LHC dedicates special runs in which lead-lead ion collisions take place to create the quark-gluon plasma. The ATLAS and CMS experiments also participate in these runs.

The LHC is divided into eight straight sections, containing 16 Radio Frequency (RF) cavities [40] for longitudinal acceleration and focusing. A total of 1232 dipole magnets are used to bend the beam into a circular trajectory, while 858 quadrupole magnets are used to focus the beam [41]. The magnets are maintained at very low temperatures (1.9 K) using a complex cryogenics system [42] of liquid nitrogen and helium.

Protons beams in the LHC have a bunch structure, with up to 2808 proton bunches and about 1.1×10^{11} protons per bunch, separated from each other by 25 ns. The instantaneous luminosity ($\mathcal{L}$) is a measure of the number of interactions in the collider per second, and is defined in terms of the number of protons in each bunch (n_1, n_2), the revolution frequency f and the overlap of the beam in the transverse plane (Σ_x, Σ_y):

$$\mathcal{L}_{\text{inst}} = f_{LHC} \frac{n_1 n_2}{2\pi \Sigma_x \Sigma_y}. \quad (3.1)$$

Luminosity blocks (LBs) are defined as sections of time where the instantaneous luminosity is approximately constant. Typically, LBs last about 60 s. The integrated luminosity, denoted by $\mathcal{L} = \int \mathcal{L}_{\text{inst}}(t) dt$, refers to the instantaneous luminosity accumulated over a certain time interval dt . Thus, the total number of events associated to a certain quantum process with cross-section σ can be expressed as:

$$\mathcal{N} = \sigma \times \int \mathcal{L}_{\text{inst}} dt. \quad (3.2)$$

In fact, multiple proton-proton (pp) interactions can occur in addition to the primary interaction of interest during a bunch crossing. These interactions are termed *pileup* and estimated using the mean of the Poisson distribution of the number of interactions per crossing in each bunch μ :

$$\mu = \frac{\mathcal{L}_{\text{inst}} \sigma_{\text{inel}}}{f_{LHC}}. \quad (3.3)$$

where, σ_{inel} is the total inelastic cross-section, corresponding to 80 mb for 13 TeV pp collisions. Pileup can involve interactions happening simultaneously during a single bunch crossing (*in-time* pileup) or from previous or subsequent bunch crossings (*out-of-time*

pileup). These effects can generally be mitigated using the tracker or calorimeter cells of the detector and are important to improve the performance of the detector.

Equation 3.4 can be generalised to beams consisting of bunches of finite length Σ_s , crossing each other at a finite angle ϕ by multiplying a reduction factor S :

$$S = \frac{1}{\sqrt{1 + \left(\frac{\Sigma_x}{\Sigma_s} \tan \frac{\phi}{2} \right)^2}}. \quad (3.4)$$

The LHC is designed to deliver collisions to ATLAS and CMS with an instantaneous luminosity of $10^{34} \text{ cm}^{-2}\text{s}^{-1}$. The total integrated luminosity recorded by the ATLAS experiment in Run 2 is shown in Figure 3.2, together with the average number of interactions per bunch crossing in Run 2.

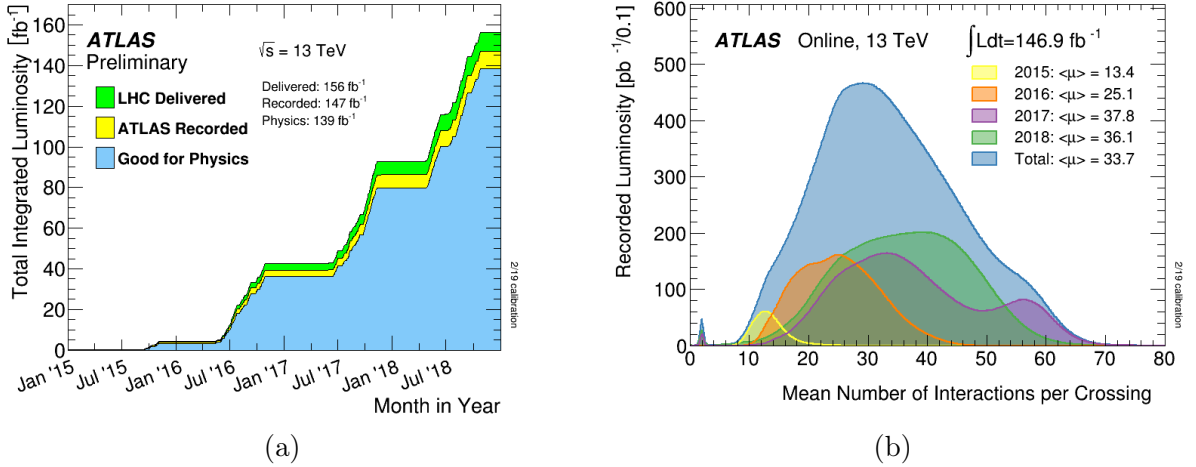


Figure 3.2: (a) Integrated luminosity versus time delivered to (green) and recorded by (yellow) the ATLAS detector in stable beam collisions of the LHC Run 2. (b) Average number of interactions per bunch crossing recorded in stable beam collisions of the LHC Run 2. Figures taken from Ref. [43].

Table 3.1 shows an overview of the operation parameters of the LHC during Run 2 and Run 3.

	Run 2				Run 3	
	2015	2016	2017	2018	2022	2023
Centre of mass energy (TeV)	13	13	13	13	13.6	13.6
Bunch spacing (ns)	25	25	25	25	25	25
Peak instantaneous luminosity ($10^{34} \text{ cm}^{-2} \text{ s}^{-1}$)	0.5	1.38	2.09	2.1	2.2	2.0
Integrated luminosity (fb^{-1})	4.2	38.5	50.2	63.4	31.4	27.58
Average interactions per bunch crossing	13.4	25.1	38.7	36.1	42.0	51.0

Table 3.1: Overview of the operation parameters of the LHC during Run 2 [44] and Run 3 [45].

3.2 The ATLAS experiment

ATLAS (A Toroidal LHC Apparatus) [36] is a 44 m long, 25 m high cylindrical general-purpose particle detector built for probing physics with pp and lead ion collisions at the LHC. The collision point is located approximately at the centre of the cylinder. ATLAS is designed to be robust under the high radiation environment of the LHC, while collecting data for precision tests of the standard model and searches for new physics up to the TeV scale. It has a layered structure of subdetectors arranged around the interaction point in a concentric manner, shown in Figure 3.3:

- The inner detector is positioned closest to the interaction point. It comprises of layers of radiation-hard, high-resolution semiconductor pixel and strip detectors and straw-tube tracking detectors arranged cylindrically around the beam-pipe, immersed in a 2 T solenoid magnetic field. The inner detector is essential for reconstructing the trajectory and momentum of charged particles, enabling the reconstruction of pp interaction vertices.
- The Liquid Argon (LAr) sampling calorimeter, located after the ID, is designed for electron and photon identification.
- Following the LAr layer is the Tile hadronic sampling calorimeter, made of alternating layers of scintillating tiles and steel absorbers. This layer is essential for accurate jet and missing transverse energy measurements. Hadronic calorimeters based on

LAr technology are also present in the end-caps to cover almost the entire azimuthal range.

- The muon spectrometer surrounds the calorimeters and consists of three layers of trackers for muon identification and momentum resolution. The toroid system, comprising a long barrel and two end-cap magnets, envelops the entire system, minimizing the effects of multiple scattering and contributing to the improvement of muon momentum resolution.

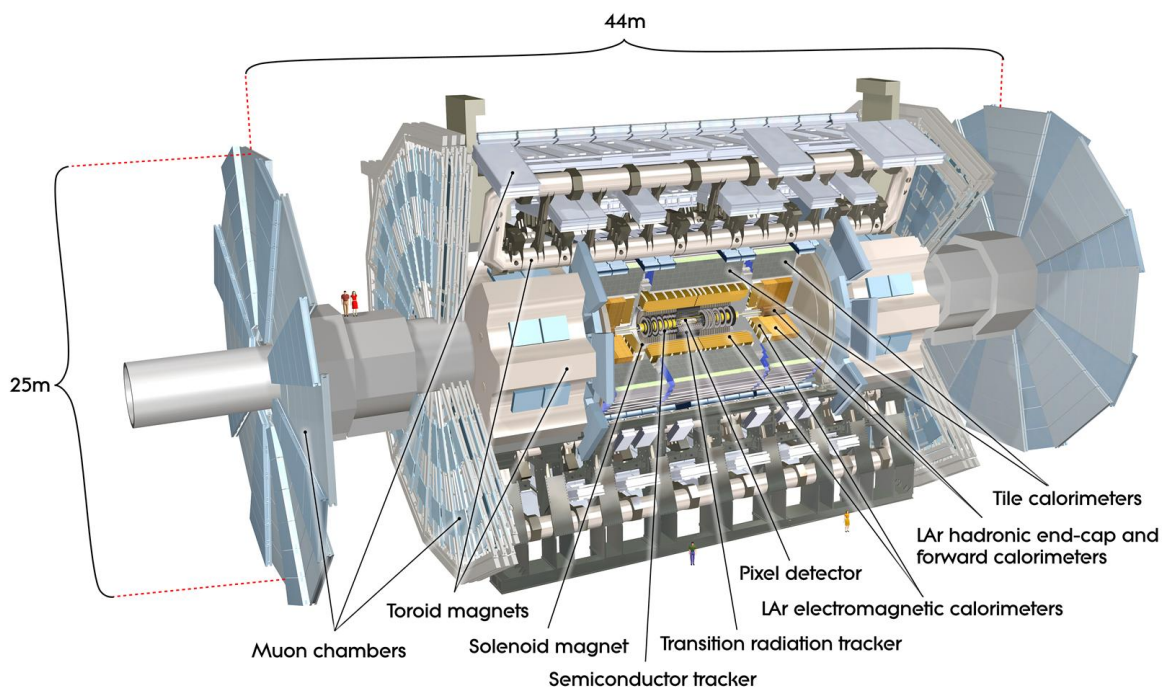


Figure 3.3: Illustration of the ATLAS detector, emphasizing its layered structure composed of numerous subdetectors. Figure taken from Ref. [36].

ATLAS has established a right-handed coordinate system to characterize particles originating from pp collisions, shown in Figure 3.4. The nominal interaction point is taken as the origin of the coordinate system, with the z -axis aligned along the beam direction. The xy plane lies perpendicular to the z -axis, with the x -axis pointing towards the centre of origin and the y -axis directed upwards. The detector is divided into side A (towards positive z) and C (towards negative z). Cylindrical coordinates are employed to further simplify discussion. The polar angle ϕ describes deviation from the beam axis in the anti-clockwise

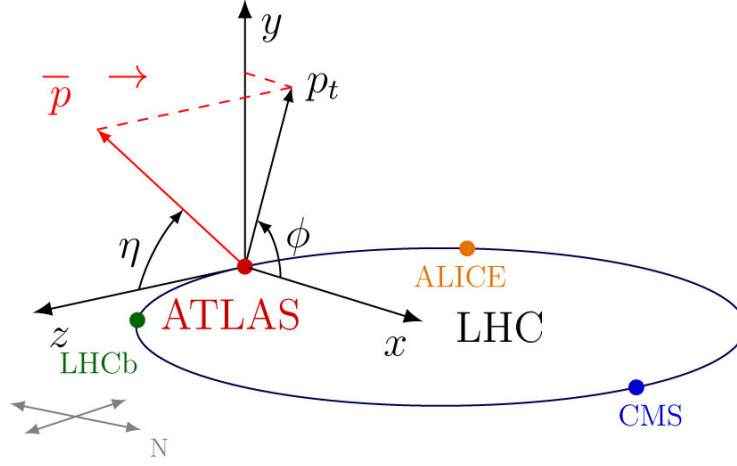


Figure 3.4: Schematic of the coordinate system used in the ATLAS experiment. Figure taken from Ref. [46].

direction in the xy -plane and is used to define the transverse momentum (p_T) and the transverse energy (E_T) of a detector object are defined in the xy plane as:

$$p_T = p \sin \theta = \sqrt{p_x^2 + p_y^2}, \quad (3.5)$$

$$E_T = E \sin \theta = \sqrt{m^2 + p_T^2}. \quad (3.6)$$

These quantities are invariant under longitudinal Lorentz boosts. Further, another Lorentz invariant quantity, *rapidity* (y) can be defined as:

$$y = \frac{1}{2} \ln \frac{E + p_z}{E - p_z}. \quad (3.7)$$

In the relativistic limit where the mass of the particle can be neglected ($E \sim |\mathbf{p}|$), Equation 3.7 can be related to the polar angle θ , measured from the positive z -axis in the yz plane, as:

$$\eta = \frac{1}{2} \ln \frac{|\mathbf{p}| + p_z}{|\mathbf{p}| - p_z} = -\ln \tan(\theta/2). \quad (3.8)$$

A distance metric (ΔR) is defined in the η - ϕ space as:

$$\Delta R = \sqrt{(\Delta \eta)^2 + (\Delta \phi)^2} \quad (3.9)$$

It quantifies the angular separation between two objects reconstructed in the detector and plays a crucial role in the reconstruction of jets.

The general performance goals of the ATLAS detector for resolution and coverage are listed in Table 3.2.

Detector component	Required resolution	η coverage	
		Measurement	Trigger
Tracking	$\sigma_{p_T}/p_T = 0.05\%p_T \oplus 1\%$	± 2.5	
EM calorimeter	$\sigma_E/E = 10\%/\sqrt{E} \oplus 0.7\%$	± 3.2	± 2.5
Hadronic calorimeter			
barrel and end-cap	$\sigma_E/E = 50\%/\sqrt{E} \oplus 3\%$	± 3.2	± 3.2
forward	$\sigma_E/E = 100\%/\sqrt{E} \oplus 10\%$	$3.1 < \eta < 4.9$	$3.1 < \eta < 4.9$
Muon spectrometer	$\sigma_{p_T}/p_T = 10\%$ at $p_T = 1\text{TeV}$	± 2.7	± 2.4

Table 3.2: General performance goals of the ATLAS detector. p_T and E represent the transverse momentum and energy of the physics object respectively in units of GeV. Table adapted from Ref. [36].

3.2.1 Magnet system

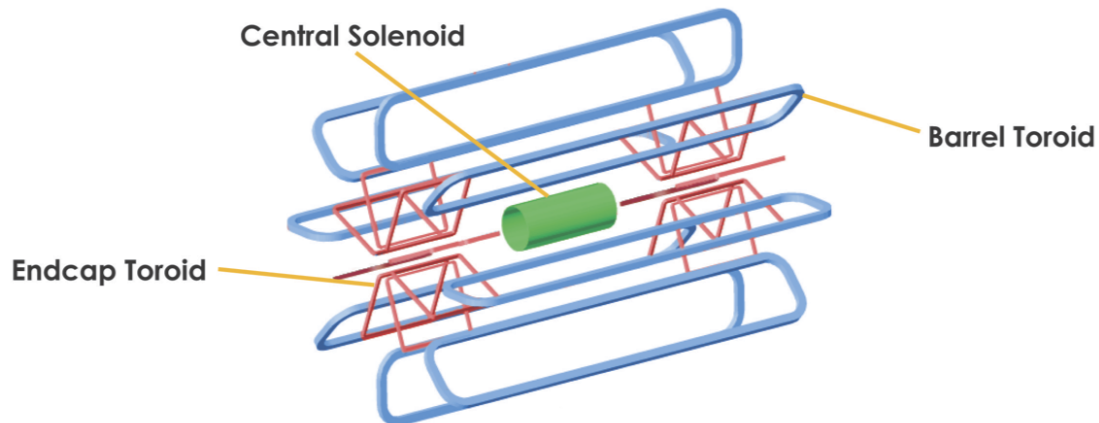


Figure 3.5: Schematic of the ATLAS magnet system showing the 2 T central solenoid field for the Inner detector and about 4 T toroid magnetic field for the muon spectrometer in the barrel and end-caps. Figure taken from Ref. [47].

The ATLAS magnet system [47] consists of four large superconducting magnets, shown in Figure 3.5:

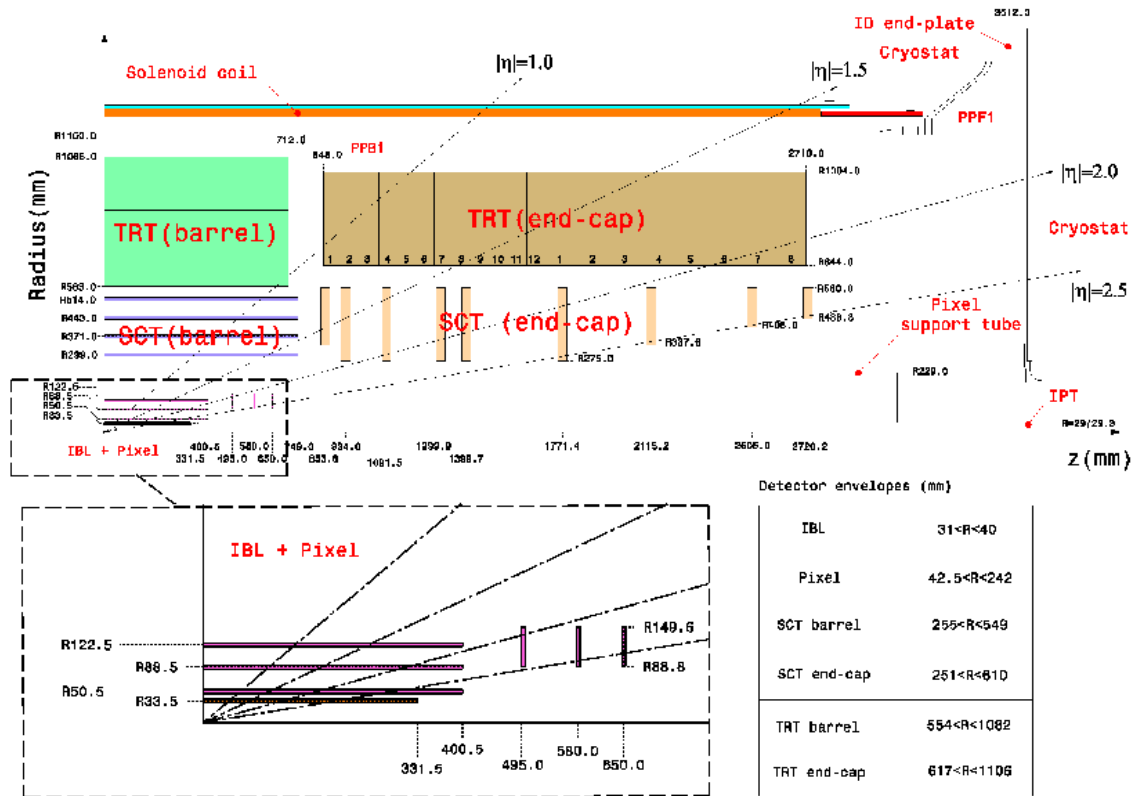


Figure 3.6: Schematic of the ATLAS Inner Detector showing the Pixel and SCT detectors in the barrel and end-cap and the TRT end-cap straw layers [48].

- A solenoid magnet surrounds the inner detector, providing a 2 T axial magnetic field. It is 5.8 m in length and consists of a single-layer coil made of a high strength aluminum-stabilized niobium-titanium conductor.
- The toroid system provides magnetic field to the muon spectrometer and is made of three parts: a set of eight magnets in the barrel, and eight in each of the end-caps. The magnetic field in the barrel is about 3.9 T and in the end-caps is 4.1 T. The toroid magnets are made of aluminum-stabilized niobium-titanium or copper conductors, wound into pancake-shaped coils to optimize spatial efficiency, followed by vacuum impregnation for insulation.

3.2.2 Inner detector

The ATLAS Inner detector (ID) [36] is 7 m long cylindrical layer with a radius of 1.15 m. It is located closest to the beampipe and immersed in a 2 T axial magnetic field from the

solenoid. The ID serves to perform pattern recognition for charged particle trajectory and momentum reconstruction down to 100 MeV, thereby aiding in reconstruction of interaction vertices in the volume $|\eta| < 2.5$. The ID is made of three distinct yet complementary subdetectors: the *Pixel* detector, *Semiconductor tracker (SCT)* and *Transition Radiation Tracker (TRT)*.

The Pixel and SCT detectors are used at inner radii for high-resolution pattern recognition. In the barrel region, they are arranged in concentric circles around the beam-pipe and as discs in the end-cap, perpendicular to the beam direction. There are 1744 pixel sensors, $250\ \mu\text{m}$, thick with dimensions between $50 \times 400\ \mu\text{m}$ (90% of the sensors) and $50 \times 600\ \mu\text{m}$ (remaining 10%, in regions close to the front-end chips on the modules). They are made of oxygenated n -type wafers with readout pixels on the n^+ implanted side. Oxygen treatment enhances radiation tolerance to charged hadrons while the doping configuration ensures good charge collection. The detectors are operated at a temperature of -5°C to -10°C to minimize radiation damage and at a bias voltage ranging from 150–600 V depending on the position of the sensor, to sustain charge collection efficiency over ten years of operation.

An additional pixel layer called the *Insertable B-Layer (IBL)* [49], was added around the LHC beampipe during the LS1 to improve flavor tagging performance. It consists of fourteen carbon fibre staves of dimensions $2 \times 64\ \text{cm}$, tilted by 14° , covering $|\eta| < 3.0$. It is based on two different silicon sensor technologies: planar n^+ -on- n pixels positioned in the central part of each staff and 3D pixels in the forward regions of both ends of the staff.

The SCT is made of 15,919 strip sensors segmented in ϕ - z and arranged in four cylindrical layers in the barrel region and nine disk layers in each end-cap. They are based on p -in- n strip technology, and have a thickness of $285\ \mu\text{m}$. These sensors are operated at voltages between 250–350 V.

The outermost part of the ID is the TRT. It is made of 52544 polyamide drift tubes, 1.5 m long and 4 mm in diameter, filled with a xenon-based gas mixture. These tubes run parallel to the beam axis in the barrel ($|\eta| < 1.0$) and are arranged radially in wheels in the end-caps ($1.0 < |\eta| < 2.0$). The centre of each drift tube has a gold-plated tungsten wire kept at ground potential, while the tube walls are kept at -1.5 kV. Charged particles passing through the tube interact with the gas to produce electrons that are captured by the wire to produce a signal. The space between the TRT straws are filled with transition radiation materials which produce X-rays depending on the type of charged particle. These are used to detect electrons and provide complementary assistance to the electron identification in the calorimeters. The TRT operates at room temperature.

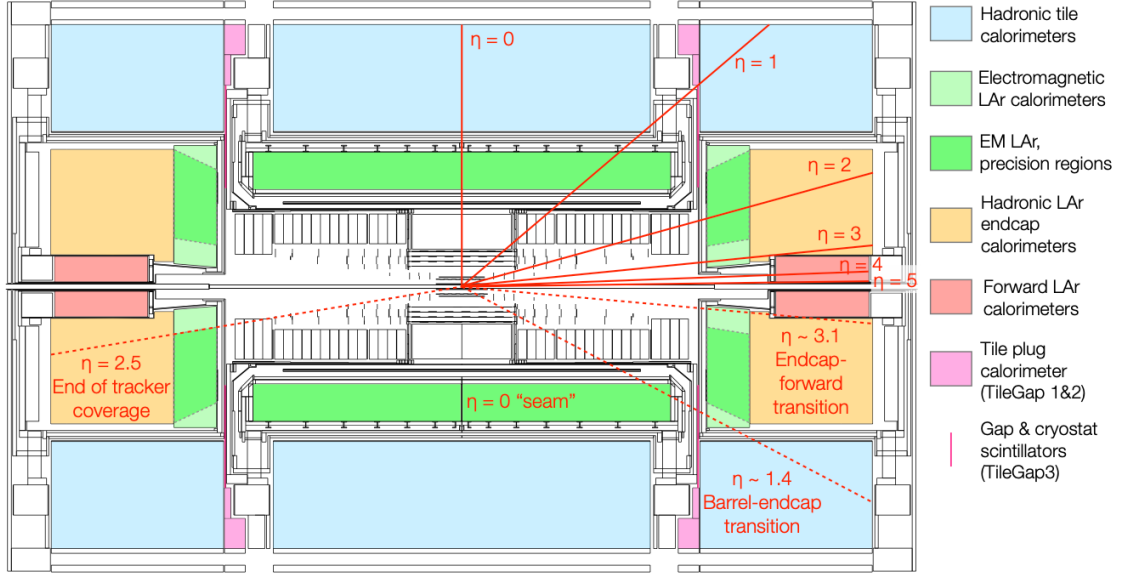


Figure 3.7: Schematic of the ATLAS calorimeter system [50].

3.2.3 Calorimeters

A set of sampling calorimeters with ϕ symmetry covering $|\eta| < 5.0$ are present after the ID to measure particles energies. These calorimeters are of two types, shown in Figure 3.7. In the barrel region, there is:

- An electromagnetic calorimeter containing Liquid Argon (LAr), providing energy measurements for electrons and photons.
- A hadronic calorimeter made of alternating layers of scintillating tiles and steel, to allow energy measurement for hadrons.

In the end-caps, sampling calorimeters based on LAr technology are used for both hadronic and electromagnetic calorimetry.

The resolution of the calorimeters can be parameterised for a particle with energy E as:

$$\frac{\sigma(E)}{E} = \frac{S}{\sqrt{E}} \oplus \frac{N}{E} \oplus C\% \quad (3.10)$$

Here, the stochastic term S accounts for energy fluctuations due to the randomness of particles in the shower; the noise term N describes the effect of noise from pileup and readout electronics and the constant term C has contributions from non-uniformities in response related to imperfect detector calibration and inactive material. Their values are

estimated to be $S = 10\%(50\%)$, $N = 0.1\%(1\%)$ and $C = 0.7\%(3\%)$ for the electromagnetic (hadronic) calorimeter [51, 52].

The Liquid Argon calorimeter

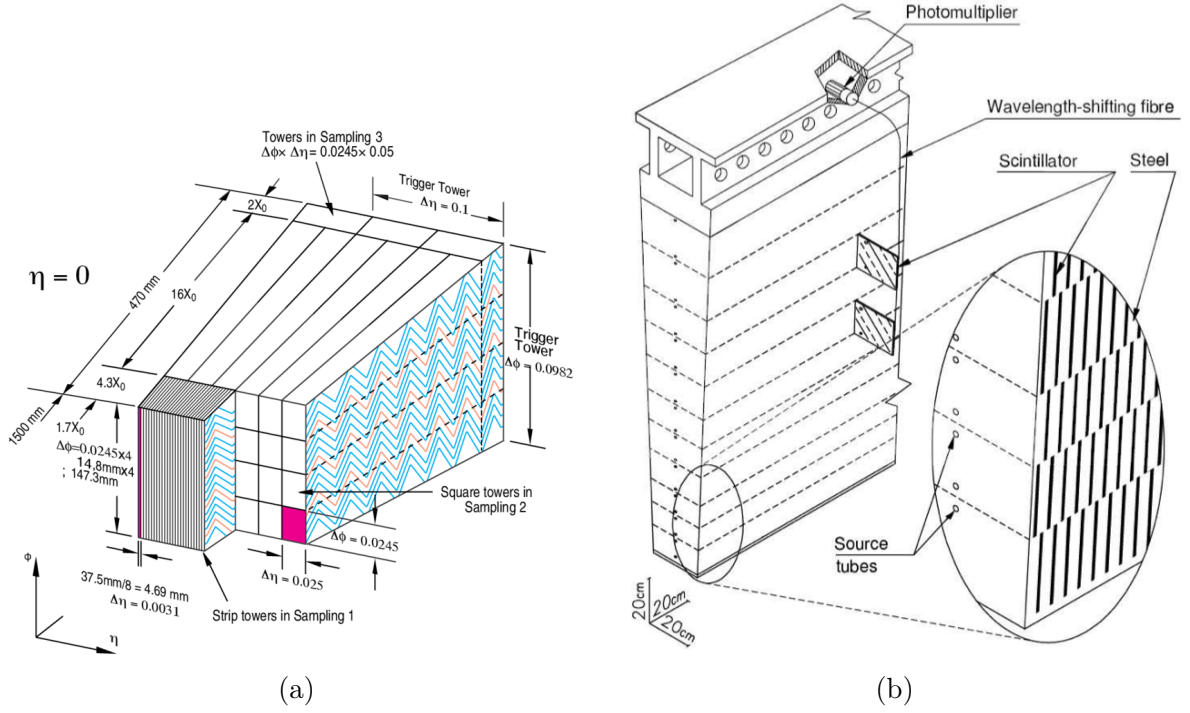


Figure 3.8: (a) Section of a LAr barrel module and (b) section of a Tile calorimeter module. Figures taken from Ref. [36].

The ATLAS electromagnetic calorimeter is a LAr sampling calorimeter featuring accordion-shaped absorbers interleaved with readout electrodes. It is composed of two subdetectors: the barrel EM calorimeter (EMB) and two end-cap calorimeters (EMEC).

The barrel EM calorimeter (EMB) is 6.4 m long and has an inner (outer) diameter of 2.8 m (4 m) and covers $|\eta| < 1.475$. In this section, the accordion waves run along the ϕ direction, adjusting folding angles with radius to maintain a consistent liquid argon gap. An example of a LAr module is shown in Figure 3.8, and the typical thickness is between 22 to 33 interaction lengths (χ_0). Each module is segmented into (η, ϕ) in three layers. The layer closest to the ID has the fine segmentation of (0.0031×0.098) for identification of neutral pions and photons. The second layer captures the largest fraction of the electromagnetic shower and has a segmentation of 0.025×0.025 , followed by coarser segmentation in the final layer (0.05×0.025) .

An additional layer made of 8 modules of active LAr called the *presampler* is present in $|\eta| < 1.8$. Each presampler module has a constant granularity of 0.2 in η , except at the end of the barrel, where the granularity reduces to 0.12 to correct for energy loss in material upstream of the calorimeters.

The end-cap calorimeters (EMEC) are 63 cm thick and segmented into three longitudinal layers covering $1.375 < |\eta| < 3.2$. In this region, the accordion waves run axially, parallel to the radial direction. Each EMEC is mechanically split into two coaxial wheels - an outer wheel spanning $1.375 < |\eta| < 2.5$ and an inner wheel covering $2.5 < |\eta| < 3.2$. Each of the four wheels comprises 32 identical wedge-shaped modules, maintaining perpendicular orientation to their axes. The front wheels exhibit a finer sampling fraction compared to the rear ones: the front modules comprise 24 copper plates, each 25 mm thick along with a 12.5 mm thick front plate. Conversely, the rear wheel modules consist of 16 copper plates, each 50 mm thick, and a 25 mm thick front plate. Consequently, the resulting sampling fractions for the front and rear wheels stand at 4.4% and 2.2%, respectively.

The Tile calorimeter

Hadronic calorimetry in central region ($|\eta| < 1.7$) of ATLAS is provided by the Tile calorimeter (TileCal). It is a cylindrical structure located above the LAr EM calorimeters. It is symmetrical about the y -axis, and divides the TileCal into sides A and C. The central long barrel (LBA and LBC) is 5.8 m in length and covers $|\eta| < 1$. It is flanked on either side by extended barrels (EBA and EBC) each 2.9 m in length and covering $0.82 < |\eta| < 1.7$.

The TileCal is made of alternating layers of plastic scintillators and steel absorbers. It is divided in ϕ into 64 modules with a radial depth of approximately 7.4 interaction lengths. An example of a Tile module is shown in Figure 3.8. Each module is further segmented radially: the first two layers, A and B(C) have a segmentation of $\eta = 0.1$, while the outermost layer (D) has a coarser segmentation of $\eta = 0.2$. When a particle travels through a Tile module, scintillating light proportional to the energy lost by the particle is produced and conducted from the tiles to the photo-multiplier tubes (PMTs) by wavelength shifting fibres on both sides of the module. Each cell in the barrel region is readout by two PMTs. Special counters made of bare scintillators are present in the gap region between the central and extended barrel to allow partial recovery of energy lost in this region of the detector. The cells formed by these modules are called *E-cells* and are readout by a single PMT each. Calorimeter signals are received in the form of an analogue pulse proportional to the energy of the incident particle. These are shaped by 3-in-1 cards, present in the

PMT block, in high and low gain settings. The signals are digitised every 25 ns by 10-bit *Analog to Digital Converters* (ADC) and stored till a Level-1 accept is received. A total of seven samples centered around the pulse peak are obtained. The high gain setting is used by default unless any of the samples saturates the ADC, in which case the low gain signal is transmitted. Each PMT is equipped with an integrator-based readout in addition to the fast readout. The integrator-based readout forms the Minimum Bias (MinBias) monitoring system of the TileCal. It integrates signals over an extended period of time (10-20 ms) thus allowing to monitor the entire readout chain of the TileCal and provide a secondary measurement of ATLAS luminosity. The integrator circuit has a low-pass DC amplifier that receives about 99% of the PMT current and is digitised by a 12-bit ADC card that saturates at 5V. Extensive work has been done in this thesis on both aspects using data collected by the Tile MinBias readout in Run 2 and Run 3. These studies are discussed in Chapter 4.

EndCap hadronic calorimeters

Forward calorimeters (FCAL) based on LAr technology are used to provide calorimetric coverage in $3.1 < |\eta| < 4.9$. These detectors are located approximately 4.7 m from the interaction point and housed in the same cryostats as the EMECs. Each FCAL is split into three modules 45 centimeters in depth: one electromagnetic modules (FCAL1) with copper absorbers for resolution optimization and heat dissipation, and two hadronic modules (FCAL2 and FCAL3) with tungsten absorbers to enhance containment and minimize lateral spread of hadronic showers. A shielding plug made of copper alloy is installed behind FCAL3 to reduce backgrounds in the end-cap muon system.

3.2.4 Muon spectrometer

The muon spectrometer (MS) [36] is the outermost component of the ATLAS detector responsible for detecting charged particles not stopped at the calorimeters within $|\eta| < 2.7$ (with trigger chambers covering $|\eta| < 2.4$). It is designed to measure muon momenta down to ~ 3 GeV and provide momentum resolution of 10% for 1 TeV muons.

The MS is immersed in a magnetic field of about 4 T provided by the toroid. In the barrel, precision-tracking chambers reflect the ϕ symmetry of the toroid system: they are arranged in eight octants consisting of three concentric layers (at radii 5 m, 7.5 m and 10 m approximately from the beam axis) between and on the eight coils of the barrel toroid

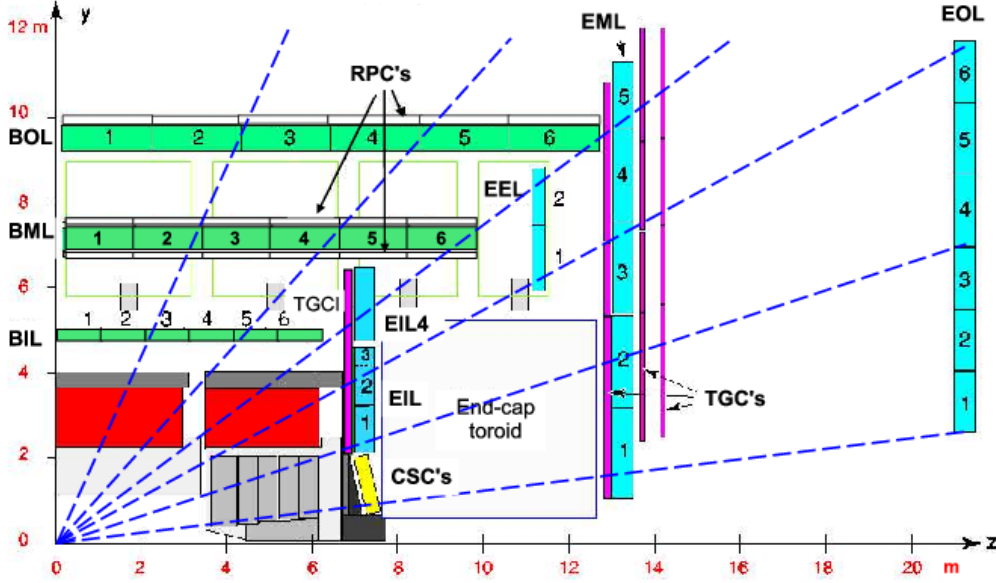


Figure 3.9: Transverse schematic of the ATLAS Muon Spectrometer showing the subdetectors. Figure taken from Ref. [53].

magnet. Each octant is further divided in the azimuthal direction with slightly different lateral extensions, providing full coverage in ϕ . In the end-cap, muon chambers form large wheels, located in front and behind the end-cap toroid magnets (approximately $|z| = 7.4$ m, 10.8 m, 14 m and 21.5 m from the interaction point). A gap in the chamber coverage is present at approximately $|\eta| \sim 0$ to facilitate access for servicing the solenoid magnet, calorimeters and the inner detector.

Monitored Drift Tube chambers (MDTs) are located in $|\eta| < 2.7$ ($|\eta| < 2.0$ in the innermost end-cap layer for precision muon measurement). They consist of three to eight layers of drift tubes operated at an absolute pressure of 3 bar, which achieve an average resolution of $80 \mu\text{m}$ per tube. Cathode Strip Chambers (CSC) are located in the innermost tracking region in $2 < |\eta| < 2.7$ due to their higher rate capability and time resolution, which translates into an spatial resolution of $40 \mu\text{m}$ in the bending plane and approximately 5 mm in the transverse plane.

The precision tracking chambers are complemented by a system of fast trigger chamber to trigger on muon tracks. In $|\eta| < 1.05$, Resistive Plate Chambers (RPCs) are used while in $1.05 < |\eta| < 2.4$, Thin Gap Chambers (TGCs) are employed. The trigger chambers measure both η and ϕ of the passing track and deliver track information within a few tens

of nanoseconds after the passage of the particle.

3.2.5 The LUCID detector

LUCID [36] (LUminosity measurement using Cerenkov Integrating Detector) is located at ± 17 m from the interaction point and detects inelastic pp collisions in the forward region for online monitoring of instantaneous luminosity delivered to ATLAS and beam conditions. It consists of elements that produce Cerenkov light detected by Photomultiplier Tubes (PMTs), enabling measurement of the number of particles in each bunch collision. Signals from PMTs are readout through custom front-end cards and directed to Field Programmable Gate Arrays (FPGAs), which utilize different algorithms to calculate luminosity for each bunch crossing, generating and storing a singular scalar value per algorithm per bunch crossing.

3.2.6 Trigger and Data Acquisition

The significant number of collisions occurring at the LHC presents challenges in both recording and storing the data, as well as in allocating computational resources for subsequent offline analysis. The Trigger and Data Acquisition (TDAQ) system is a crucial component that decides whether an event should be stored for offline physics analysis. The ATLAS TDAQ system in Run 2 was operating based on decisions taken on two distinct levels, shown in Figure 3.10: a hardware-based Level-1 (L1) system, followed by a software-based High-Level Trigger (HLT) system.

The Level-1 Trigger

The L1 Trigger [55] is a hardware-based four-component system with both on-detector and off-detector components. It is designed to reach selection decisions in less than $2.5 \mu\text{s}$, reducing the data input rate from 40 MHz to 100 kHz. The first two subsystems of L1 operate on inputs from the calorimeters (L1Calo) and the muon spectrometer (L1Muon). L1Calo reads the inputs from $\eta \times \phi$ *trigger towers* formed separately for the electromagnetic and hadronic layers. These trigger towers measure 0.1×0.1 in the barrel and 0.4×0.4 in the end-caps. Trigger towers in the central region ($|\eta| < 3.2$) are used to form jets, hadronic taus, electrons and photons, while those in the forward region are used to form forward jets. Information from all trigger towers is used to calculate global variables like the missing transverse energy (E_T^{miss}) in an event. Fast muon reconstruction in L1Muon is performed

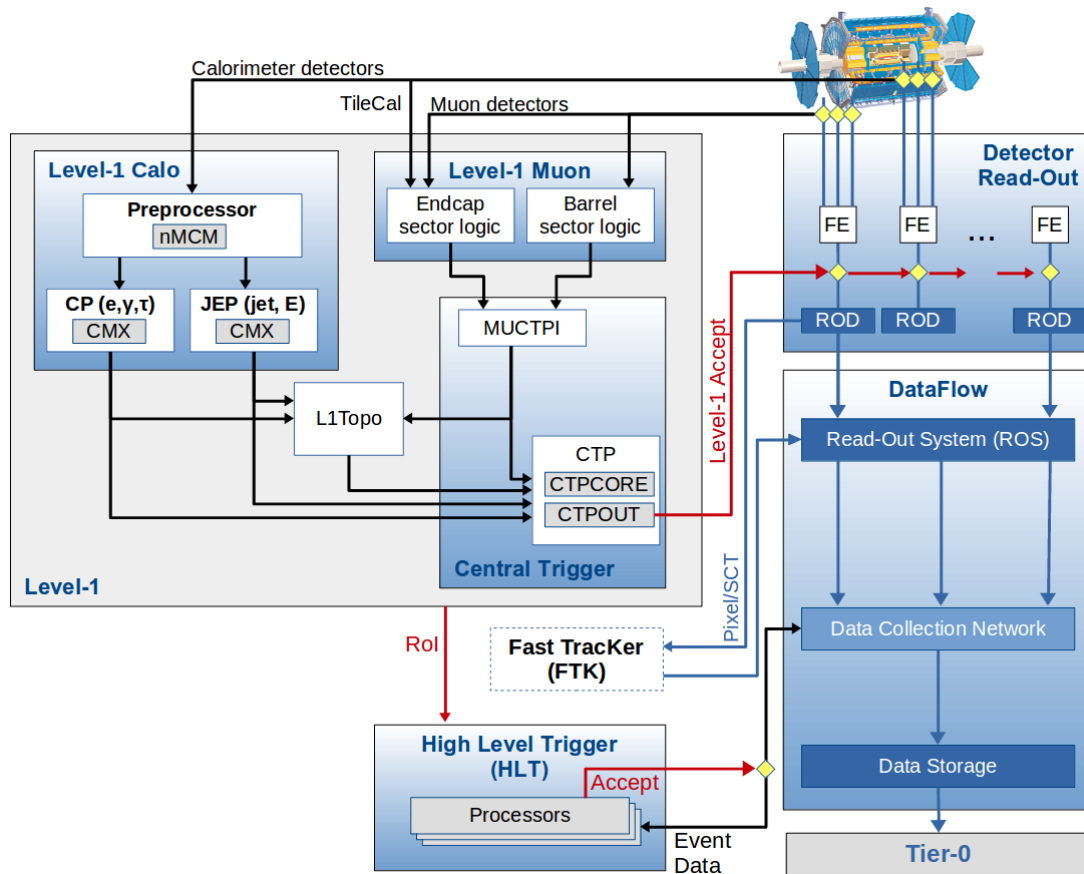


Figure 3.10: Schematic of ATLAS TDAQ system in Run 2, showing the Level-1 (L1) and High-Level Trigger (HLT) systems [54]. The FastTracker (FTK), a hardware-based system for inner-detector track reconstruction, was under commissioning in Run 2 and not used for trigger decisions.

using RPCs and TGCs. Interesting fragments of detector readout are used to form *Regions of Interest (RoI)*, from which object candidates called *trigger objects (TOBs)* are identified and sent to a third system called the *Level-1 Topological trigger*. This system computes decisions by applying more complex topological cuts, such as angular separation or invariant masses to the TOBs. The *Central Trigger Processor* collects information from all three subsystems and issues a *L1-Accept* signal, streaming down the accepted events to the HLT. Events are stored in readout buffers while waiting for the L1 trigger decision.

The High-Level Trigger

The HLT is a software-based trigger operated on a CPU farm of 28000 CPU cores located at ATLAS Point-1. It uses offline-like reconstruction algorithms with full detector

granularity and partial track reconstruction based on the L1 RoIs for more sophisticated object and event reconstruction. It reduces the input rate from 100 kHz down to 1 kHz. During Run 2, events recorded by the HLT were organised into five streams depending on the selections satisfied by the event:

- *Physics streams*: events for offline physics analysis.
- *Express stream*: subset of events from physics streams for real-time reconstruction and monitoring.
- *Debug streams*: events neither accepted nor rejected by the trigger system for identification of potential problems with the TDAQ system.
- *Calibration streams* for subdetector or HLT calibration.
- *Trigger-Level Analysis streams* containing low-level information from reconstructed TOBs physics analysis at the trigger stage for physics analyses that rely on reducing bias from online trigger selections.

In addition, monitoring streams were available for online monitoring tools during data-taking without recording. Events recorded by the HLT are transferred to the CERN Tier-0 facilities for offline processing and permanent storage.

Tile Calorimeter scintillator ageing

A brief introduction of the ATLAS TileCal is presented in Section 3.2.3. This chapter provides an overview of the calibration systems of the TileCal and focus on studies on TileCal scintillator ageing with data obtained from the MinBias readout in Run 2.

4.1 Tile calibration systems

The ATLAS TileCal is equipped with calibration systems used to monitor the readout chain, account for effects due to irradiation, ageing and faults and maintain constant Tile response over time. These systems are illustrated in Figure 4.1 and their function is briefly described in the following text.

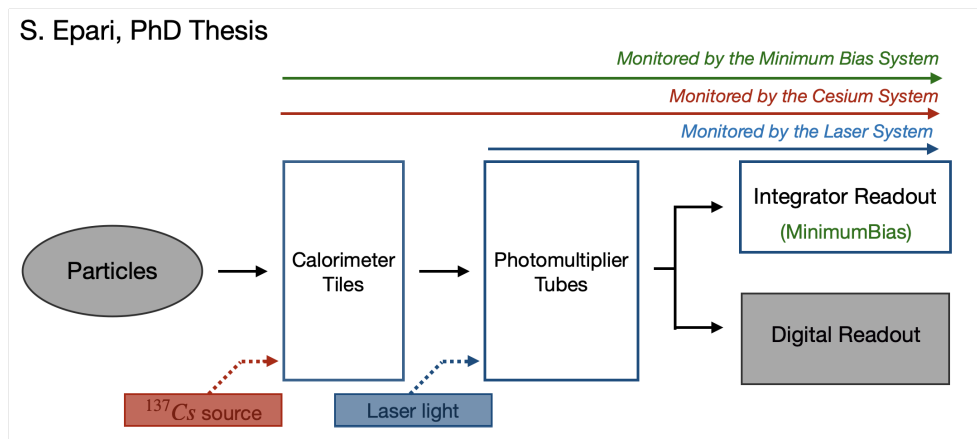


Figure 4.1: A schematic of the TileCal calibration systems. The Cesium (^{137}Cs) system is used to monitor the stability of the optical components, whereas the laser system monitors the TileCal PMTs.

The *Cesium* (Cs) system consists of a radioactive ^{137}Cs source that is moved through the tiles of the calorimeter using hydraulic control [56]. The Cs source deposits a known amount of energy to the calorimeter cells and the corresponding variation in PMT current is used to monitor optical quality of the scintillator tiles and PMTs, to equalise the response of all read-out cells to about 0.5% and monitor each TileCal cell over time. Cs calibration *scans* are performed several times per year of data-taking.

The *Laser system* monitors the stability and linearity of the TileCal PMTs [57]. In dedicated laser calibration runs, high-intensity light pulses of a known energy are sent to the TileCal PMTs via a network of optical fibres. The laser pulses maybe of very high amplitude, similar to signals generated by high energy jets, or with very low amplitude, similar to that expected from muons.

The *Charge Injection System (CIS)* injects a calibrated charge into each TileCal channel to establish the relative calibration between different readout channels to a precision of 1% [58]. CIS scans are used to calibrate and monitor the fast readout electronics and to derive pC/ADC conversion factors for the digital readout. CIS scans are performed between LHC fills, during an LHC fill in the missing bunch interval and in maintenance periods.

The rate of inelastic pp collisions at low momentum transfer, called *Minimum Bias events*, is measured by the integrator-based readout of each PMT, as discussed in Section 3.2.3. This readout forms the *Minimum Bias (MinBias) integration system*. The rate of MinBias events is proportional to the instantaneous luminosity and produce signals in all PMTs, distributed uniformly in ϕ about the interaction point. MinBias data is, thus, used to monitor both the TileCal readout and the LHC machine performance, in the form of *online* and *offline* luminosity. The procedure used to convert raw ADC counts (1 ADC = 1 mV) recorded by the MinBias readout to PMT currents is described in Section 4.2, followed by the measurement of TileCal scintillator ageing using the established procedure.

4.2 Measurement of the MinBias current

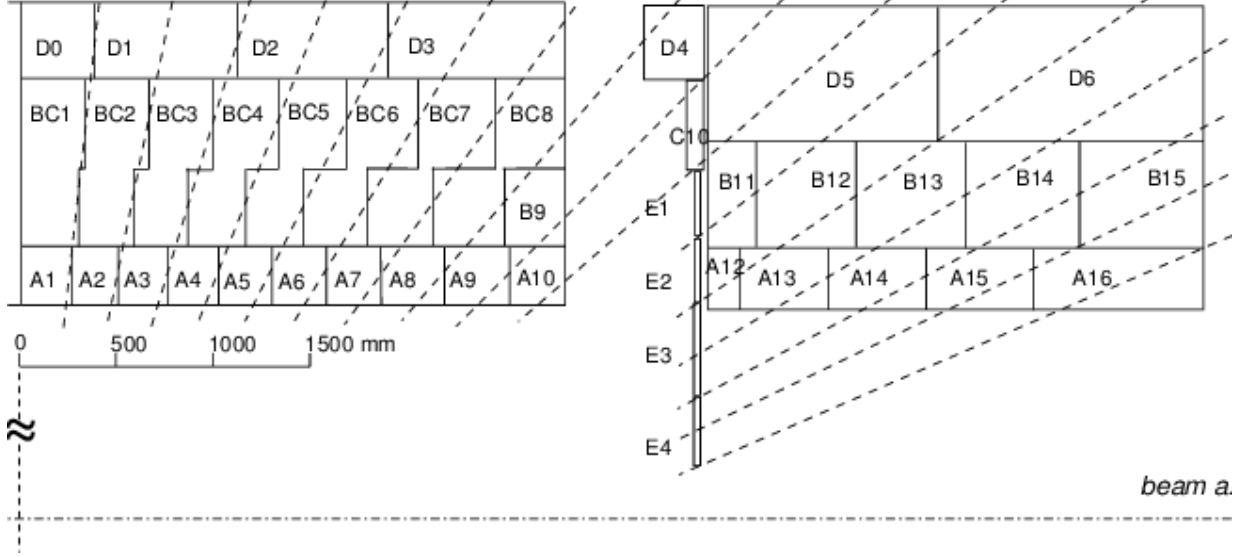


Figure 4.2: Illustrative sketch of the TileCal cells. Modules from all cells except those composed of gap/crack scintillators (E1 - E4) are readout by two PMTs each. Figure taken from Ref. [59].

As described in Section 3.2.3, each TileCal barrel is divided radially into 64 modules and further, horizontally to form *cells*. The layout of TileCal cells is shown in Figure 4.2. Modules from all cells except those composed of gap/crack scintillators (E-cells/E1 - E4) are readout by two PMTs each, termed *L* and *R*. In the case of E-cells, due to a single PMT reading out each module, the two terms may be used interchangeably. Signals recorded by the MinBias readout of a PMT are stored in the form of ADC counts. This signal is sensitive to the amount of background activity in the TileCal or surrounding material in the absence of collisions and is called the *pedestal*. The pedestal can have non-flat shapes especially in the case of activated material surrounding the Tile which produces slow and fast decaying radioactive isotopes. Example of ADC counts from a module of cell E3 from the extended barrel A for a given run is shown in Figure 4.3, together with the pedestal.

The number of ADC counts (N_{ADC}) are converted to the average PMT current ($\langle I_{\text{PMT}} \rangle$) by subtracting the pedestal (p) and dividing by the gain (G) of the integrator as shown in Equation 4.1.

$$\langle I_{\text{PMT}} \rangle = \frac{N_{\text{ADC}} - p}{G} \left[\frac{\text{V}}{\Omega} \right]. \quad (4.1)$$

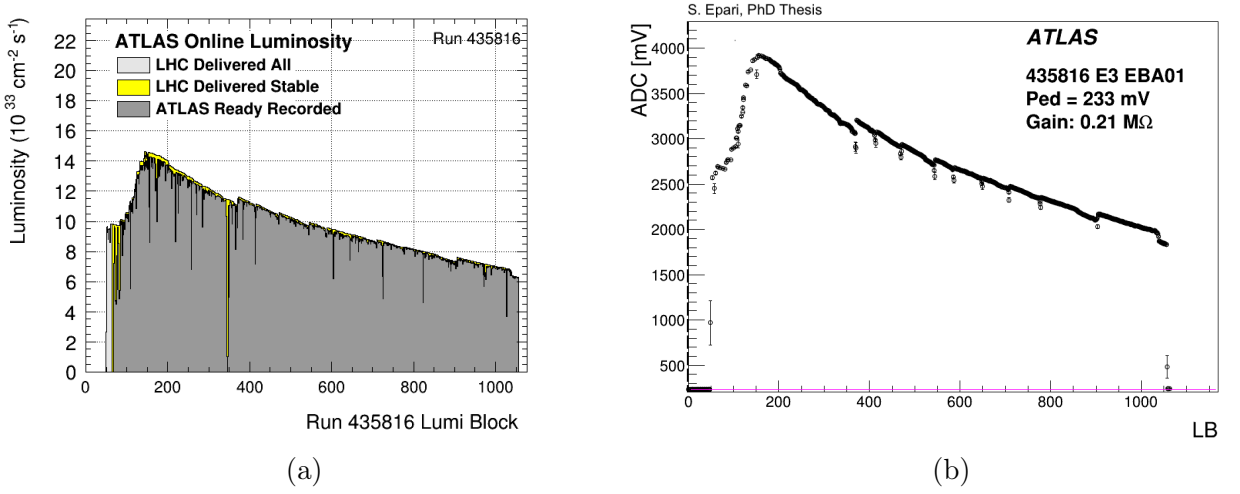


Figure 4.3: (a) Luminosity profile for run 435816 with (b) ADC counts measured by module 01 of cell E3 in the extended barrel A. The pink line shows the pedestal estimated as the mean of ADC counts before stable beams are declared ($\sim$ LB 50), as a function of the luminosity block number.

For simplicity, MinBias analyses estimate pedestal as the mean of the ADC counts in the luminosity blocks (LBs) before stable beams are declared by the LHC. At this step, LBs with ADC counts above 4095 mV, leading to saturation in the PMT measurement are removed. Additionally, modules with noisy measurements, saturation over part of (or entire) run, burnt integrator cards or those that were power-cycled during the run, leading to loss of MinBias measurement, are removed by manual inspection of plots. A module deemed *bad* in a run is removed from all runs in the dataset. Examples of such bad modules are shown in Figure 4.4. In case of signal from only one PMT reading out a module, only that measurement is used. Otherwise, the average of measurement from the two PMTs is used.

PMT currents provide an absolute measurement of cell response but are studied with respect to a reference measurement. Previous analyses [60] relied on the measurement from cells D5 and D6 as a reference because these cells are well shielded from radiation damage while providing a reasonable signal. Alternatively, D1 and D2 cells were a popular choice due to great stability over long periods but they yield a low signal in low luminosity runs. The analysis in this section uses track-counting luminosity as a reference to study MinBias data because it provides a reliably luminosity measurement over a large period of time and wide range of luminosity. The average of the measurement of all good modules for a cell, averaged over sides EBA and EBC (or LBA/LBC, depending on the location of the cell)

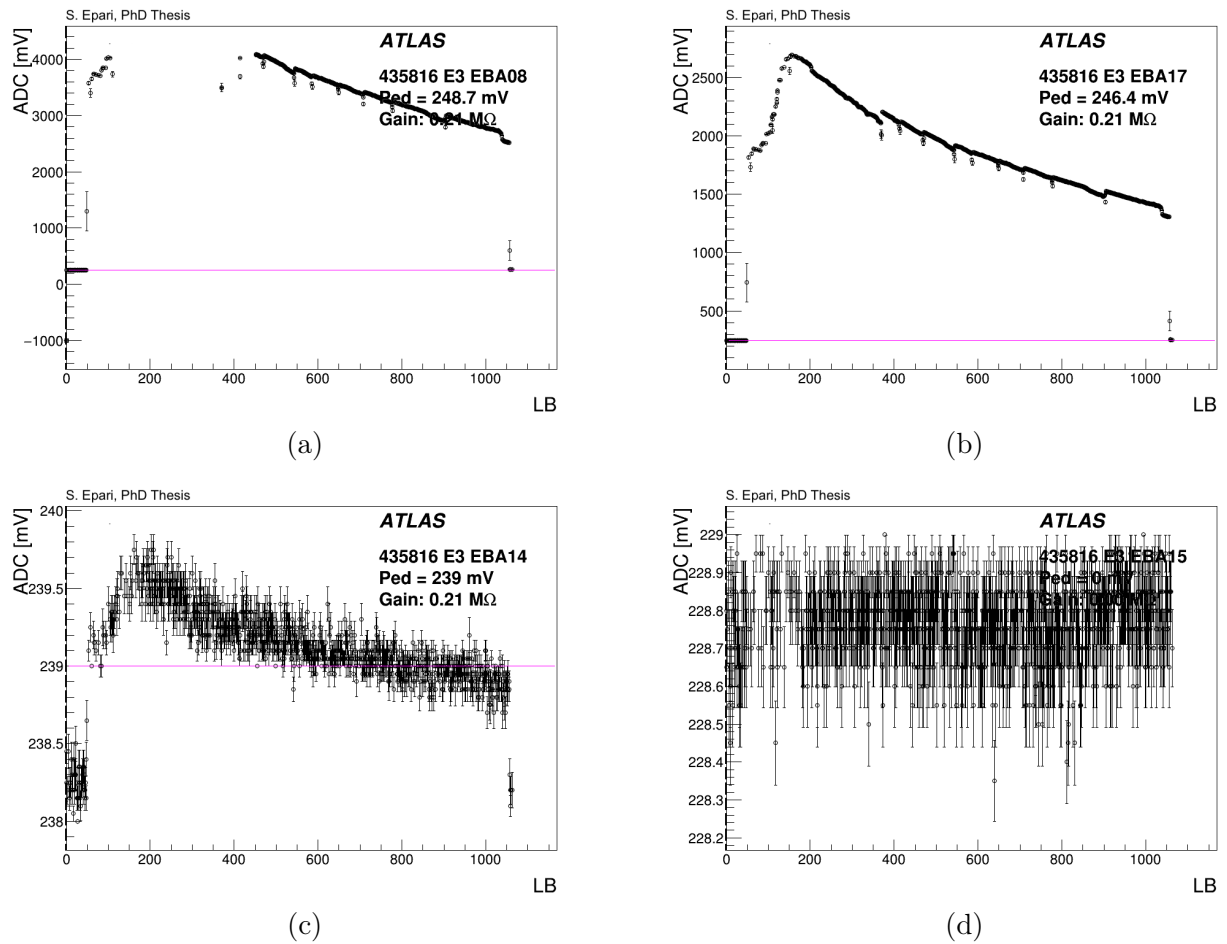


Figure 4.4: Examples of modules deemed *bad* and removed from MinBias analyses. (a) This module shows saturation in the highest luminosity LBs. (b) Compared to (a), this module has a response half of the expected value, hinting towards a burnt 3-in-1 card. (c) This module has a noisy output and (d) shows a module with no signal in the PMT. A module deemed *bad* in a run is removed from all runs in the dataset.

for a run, scaled by the reference measurement is used as the measurement from the cell for analysis.

Correcting for PMT instability

Instability in PMT response can arise from two main effects during the course of data taking: (a) ageing of the PMT due to exposure to radiation which reduces the PMT response over time and (b) PMT gain variation due to dependence on PMT current. Dedicated calibration runs are used to account for or estimate both effects. The former corrections, termed *run-to-run laser corrections* are calculated from laser calibration runs taking between consecutive LHC fills. Briefly put, a correction factor in a given run (R^i) is computed for each PMT i with respect to a reference laser run (R_{ref}^i) using the combined method [61]:

$$f_{\text{Laser}}^i = \frac{R_{\text{ref}}^i}{R^i}. \quad (4.2)$$

In the reference run, the average PMT gain variation over ± 10 days is used to normalise the PMT current for greater precision and stability of the estimate. The code and documentation for these calculations is stored in the TUCS framework [62]. The channels with corrections above 4% from the mean are removed for each PMT. Additionally, channels masked during laser data taking are also removed. Overall, run-to-run laser corrections can provide up to 0.5% effects in the PMT current measurement.

The corrections for PMT gain variation with current, termed *in-gap laser corrections*, are computed using dedicated calibration runs where laser pulses are fired in the abort gap during a run [57]. This correction is affected by the kind of High Voltage (HV) divider used in the readout of the cell: for majority of TileCal including A-cells, passive dividers are used. These exhibit a linear gain dependence with current, as shown in Figure 4.5 for 2018 estimates. On the other hand, active HV dividers are used for E-cells which significantly improve the cell response linearity, as shown in Figure 4.5.

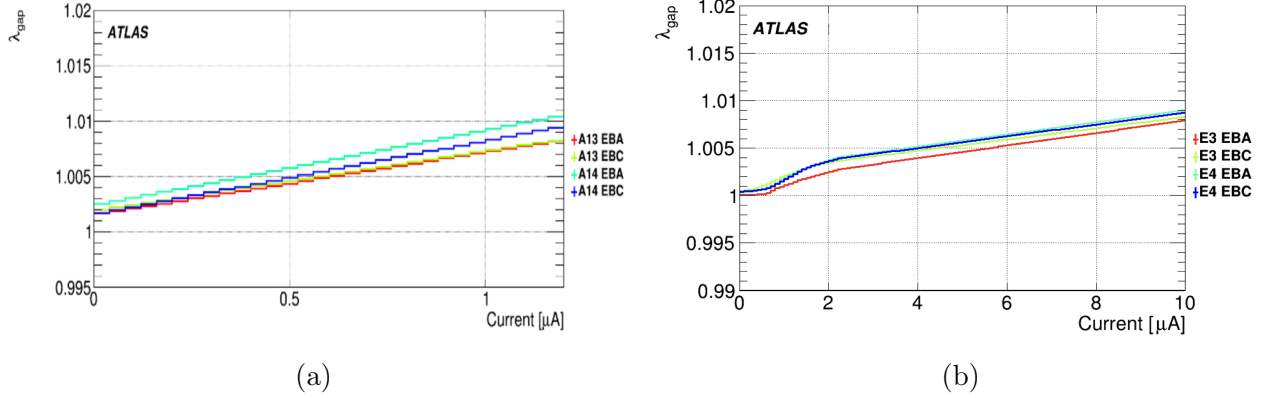


Figure 4.5: In-gap corrections computed for the 2018 dataset for (a) passive dividers which are equipped in most of TileCal including A-cells and (b) active dividers which reside in E-cells. Figures taken from Ref. [57].

4.3 Results

The first study for estimating the effect of TileCal scintillator ageing in Run 2 (2015-2018) uses MinBias data from runs in the period, using the method described in Section 4.2. The total delivered luminosity this period is 156 fb^{-1} . A total of 40 runs with good MinBias data, approximately equally spaced through each of the four years in Run 2 were chosen for the study. Cell A13, located in the inner layer of the Extended Barrel, covering the region $1.2 < |\eta| < 1.3$, was chosen as a representative for cells with moderate levels of radiation. Cells E1, E2, E3, E4, located in the gap region of the Extended Barrel, were chosen to study the effect of radiation damage of scintillators located closest to the pp interaction point. No laser corrections were applied to the Tile data. Instead, the run-to-run laser data collected in calibration runs close to the MinBias runs, were compared to the MinBias data which accounts in addition for the effect of scintillator ageing. For cell A13, Cs data was used as a cross-check to the MinBias measurement. Thus, the difference of the calorimeter response to the laser versus the MinBias or Cs systems is interpreted as the effect of damage and ageing of the scintillators and wavelength shifting fibres.

4.3.1 Response variation of cell A13

The variation of the average response to Laser, Cs, and MinBias for the cell A13 in the inner layer of the Extended Barrel, covering the region $1.2 < |\eta| < 1.3$, as a function of time is shown in Figure 4.6. The Laser, Cs and MinBias data cover the period from July

2015 till November 2018. The MinBias data are normalised to the first run (16th July 2015) while the Laser data are normalised to the average of runs taken in two weeks since 17th July 2015. The down-drifts in the Laser data relate to the degradation of the PMT response coinciding with the collision periods, while up-drifts are observed during technical stops and at the end of the pp data-taking. The Cesium and MinBias systems complement each other and are sensitive to changes in the PMTs, fibres, and scintillators. The difference of the calorimeter response to the Laser versus the MinBias or Cs systems is interpreted as the effect of damage and ageing of the scintillators and wavelength shifting fibres and is about 10%.

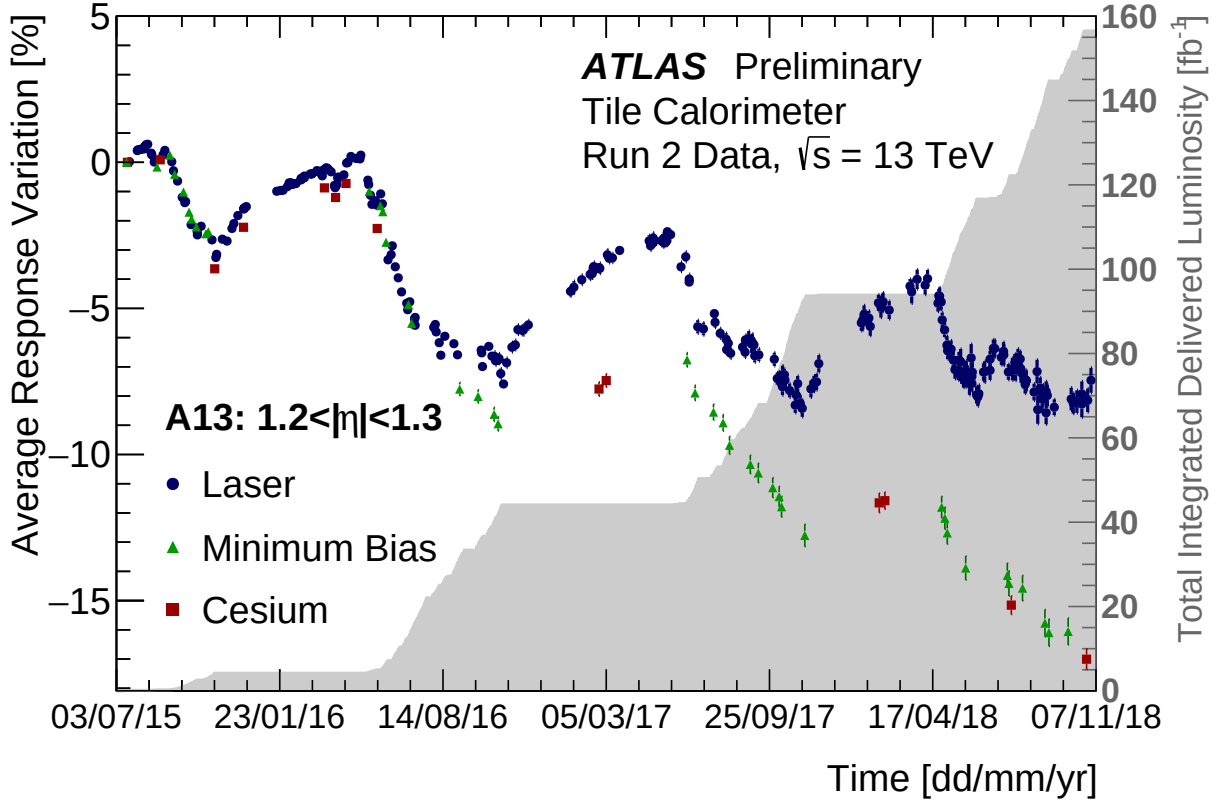


Figure 4.6: The variation of the average response to Laser, Cs, and MinBias for the cell A13 in the inner layer of the Extended Barrel, covering the region $1.2 < |\eta| < 1.3$, as a function of time, for the pp collision period of 2015-2018 (Run 2). The difference of the calorimeter response to the Laser versus the MinBias or Cs systems is interpreted as the effect of damage and ageing of the scintillators and wavelength shifting fibres and is about 10%. Figure taken from Ref. [63].

It is interesting to note the discrepancy in the trend between the last Cs scan in the end-of-year shutdown of 2017 and the first MinBias run of the year in Figure 4.6. Further, minor offsets from the trend predicted by Cs in 2016 and 2018 are seen for the respective MinBias runs. The source of these discrepancies were studied by repeating the analysis with a different reference cell for the MB data: D1L (LBC) and D6R (EBC). The results of this study are shown in Figure 4.7.

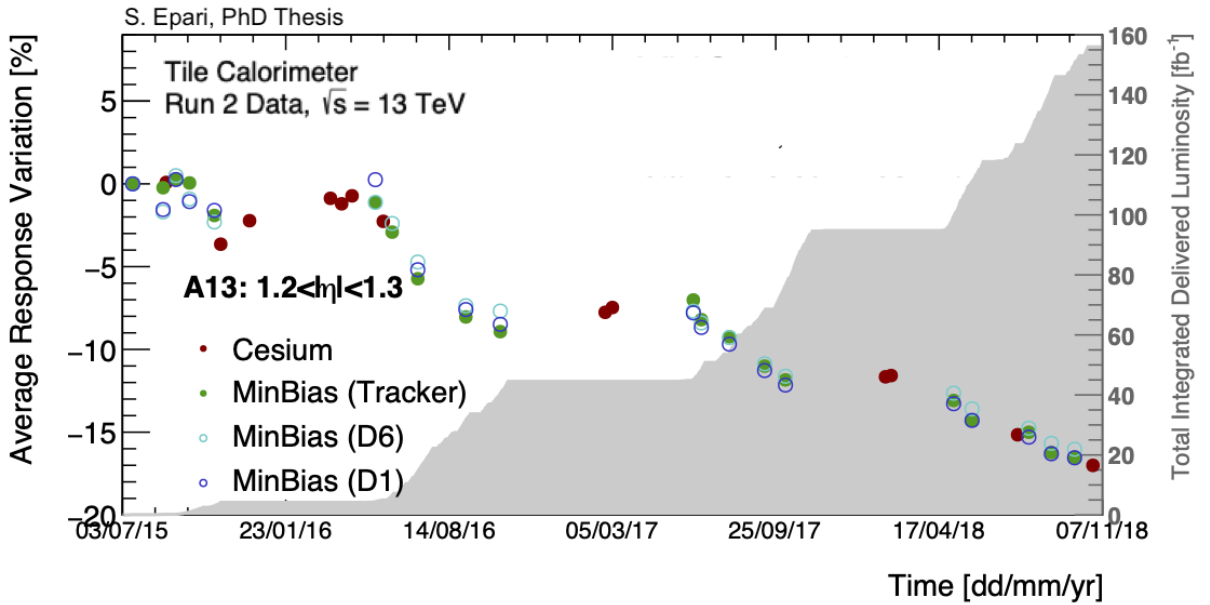


Figure 4.7: The variation of the average response to Cs and MinBias for the cell A13 as a function of time, for selected MinBias runs in the pp collision period of 2015-2018 (Run 2). The MinBias response is calculated with respect to three different references: the tracker luminosity, D1L (LBC) and D6R (EBC), with the aim of cross-checking results with the Cs runs. See text for more details.

While the MinBias estimates from the three references show good overall agreement, estimates from cell D1 suffer from lower statistics in 2015 affecting agreement in the beginning of the data-taking period, while the effect of scintillator ageing in cell D6 possibly introduces differences towards the end of the period. The first MinBias run of 2017 has a response about 0.5% lower than that estimated using the D-cells; this points to possible issues with the tracker estimate during that run. Further, the discrepancies between Cs and MinBias data for the remaining periods remains on changing the MinBias reference. One possible explanation for this effect can be the difference in methodology employed by the two analyses and its precision and deserves further scrutiny, not explored in this thesis.

4.3.2 Response variation of E-cells

The analysis was repeated for the gap/crack scintillators (E1, E2, E3, E4) and the results are shown in Figure 4.8. The cells in the gap/crack region of the TileCal are not calibrated by the Cs system, so only the response variation to Laser and MinBias is shown on these figures. The difference of the calorimeter response to the Laser versus MinBias is about 10% for cell E1, 12% for cell E2, 20% for cell E3 and 30% for cell E4. Figure 4.9 shows the variation of response of the E-cells to the MinBias system over the full Run 2 data-taking period.

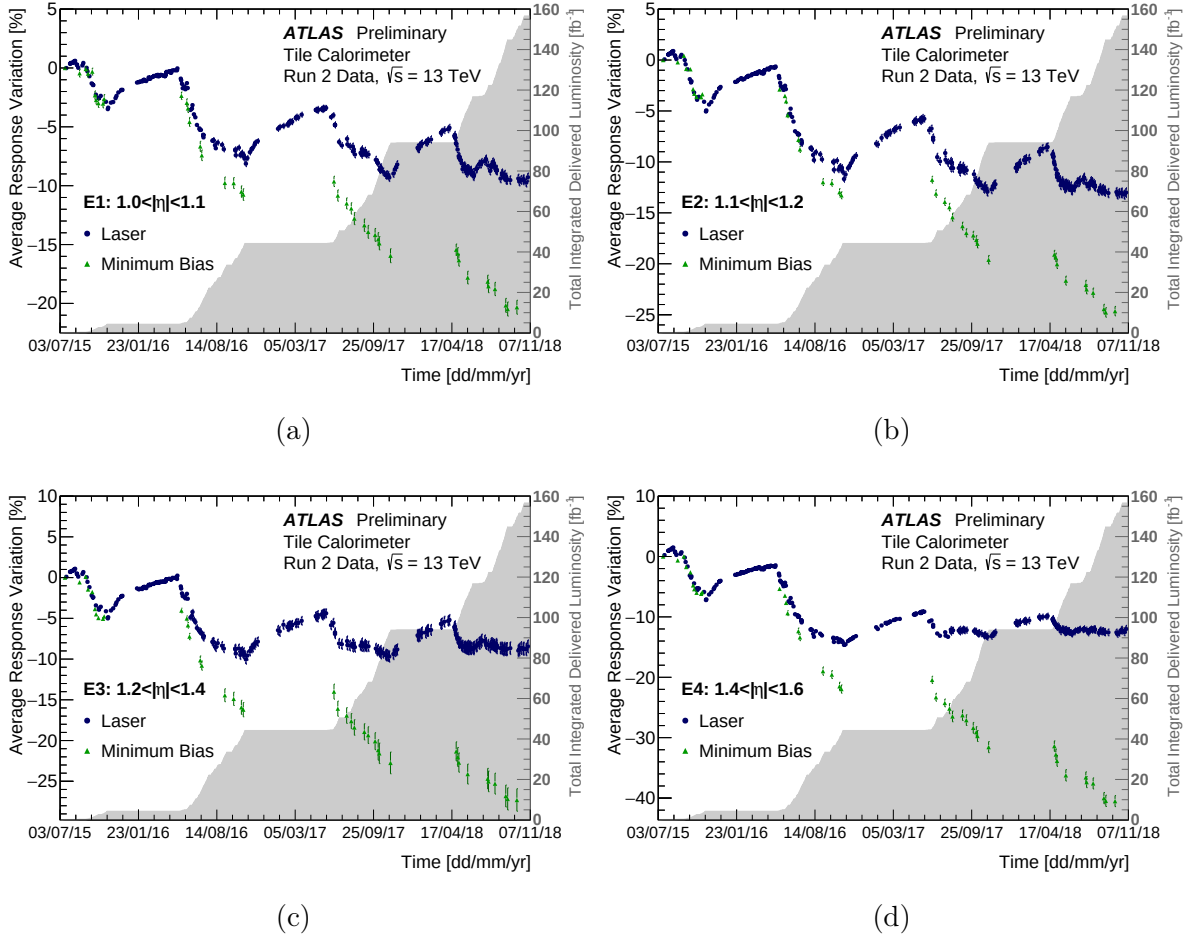


Figure 4.8: The variation of the average response to Laser and Minimum Bias for the E-cells in the gap/crack region of the Extended Barrel, as a function of time, for the pp collision period of 2015-2018 (Run 2). Figures taken from Ref. [63]. See text for more details.

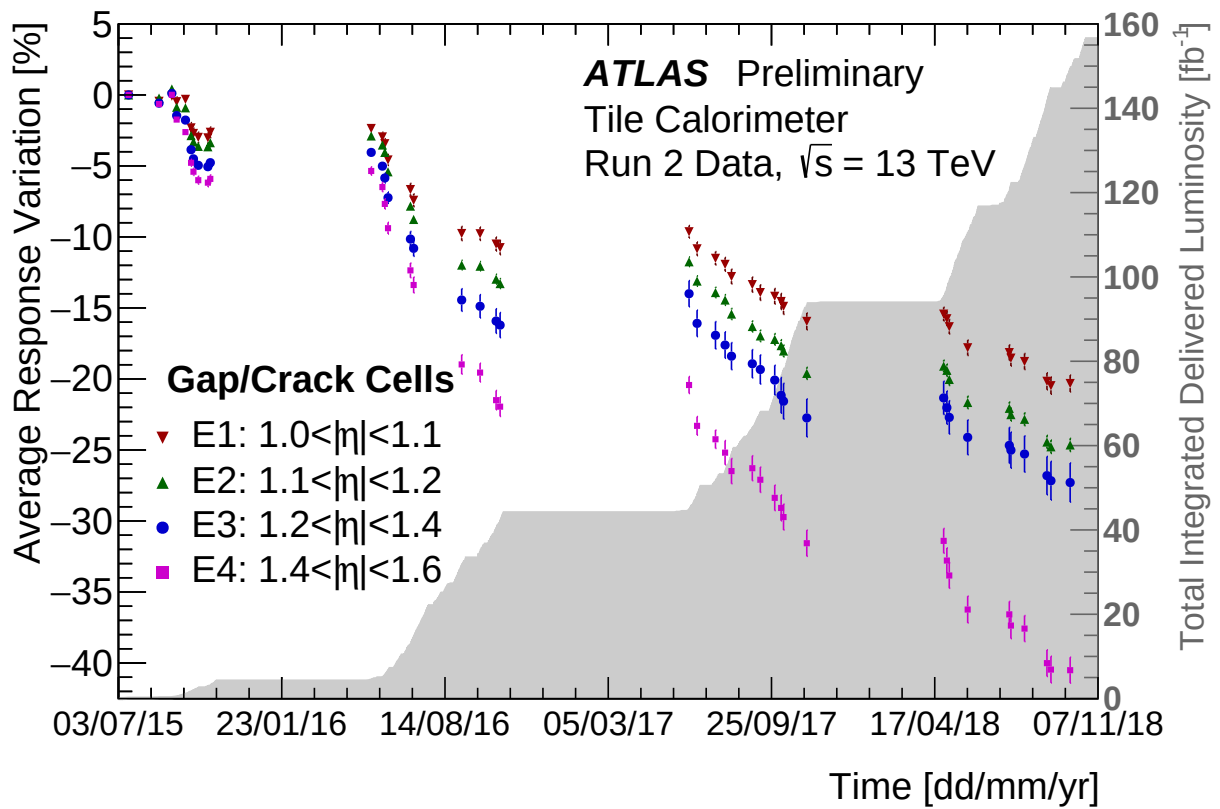


Figure 4.9: The variation of the average response to MinBias for the cells in the gap/crack region of the Extended Barrel as a function of time, for the pp collision period of 2015-2018 (Run 2). Figure taken from Ref. [63]. See text for more details.

4.4 Conclusions

This chapter presented the first study on TileCal scintillator ageing in Run 2 (2015-2018) using the MinBias data collected during this period. Compared to previous studies [60], track-counting luminosity was used as a reference to have a stable measurement over a large period of time. The study estimated the effect of damage and ageing of the scintillators and wavelength shifting fibres in cell A13 at about 10%. Similarly, for the gap/crack scintillators, the effect of ageing was estimated to be between 10% to 30% depending on the location of the cell from the interaction point. The results produced in this work are included in the Run 2 Tile Performance paper [64] and have provided valuable feedback to the Tile Phase-II upgrade plans. In particular, the E-cells were replaced during the Long Shutdown 2, before the start of Run 3.

Tile Calorimeter luminosity

This chapter emphasises the role of TileCal in the ATLAS luminosity measurement and the subtleties that go into providing a reliable and precise estimate of the luminosity and its uncertainty for use in every ATLAS analysis using the dataset. The focus is on the measurement in 2022 and 2023 (Run 3), using data collected by the MinBias readout of the TileCal.

5.1 Introduction

The instantaneous luminosity (L) is a measure of the number of pp collisions in the collider per second. Physically, the instantaneous luminosity dictates the measured number of events of a certain process ($N_{pp \rightarrow X}$) per unit time, given the theoretical production cross-section of the process ($\sigma_{pp \rightarrow X}$) via Equation 5.1.

$$\frac{dN_{pp \rightarrow X}}{dt} = \sigma_{pp \rightarrow X} \times L. \quad (5.1)$$

Thus, the *systematic* uncertainty in the luminosity measurement directly affects the measured number of events of a certain process. This uncertainty can be a limiting factor in precision analyses measuring physics cross-sections. On the other hand, most searches for BSM particles are typically statistically limited and this uncertainty has a negligible impact in these searches. Further, a precise determination of luminosity and its uncertainty is also important for setting trigger pre-scales and machine optimisation. The ATLAS experiment has several detectors suitable (i.e. sensitive to, linear and stable) to measure luminosity, shown in Figure 5.1, that provide either a real-time *online* or *offline* luminosity measurement for ATLAS.

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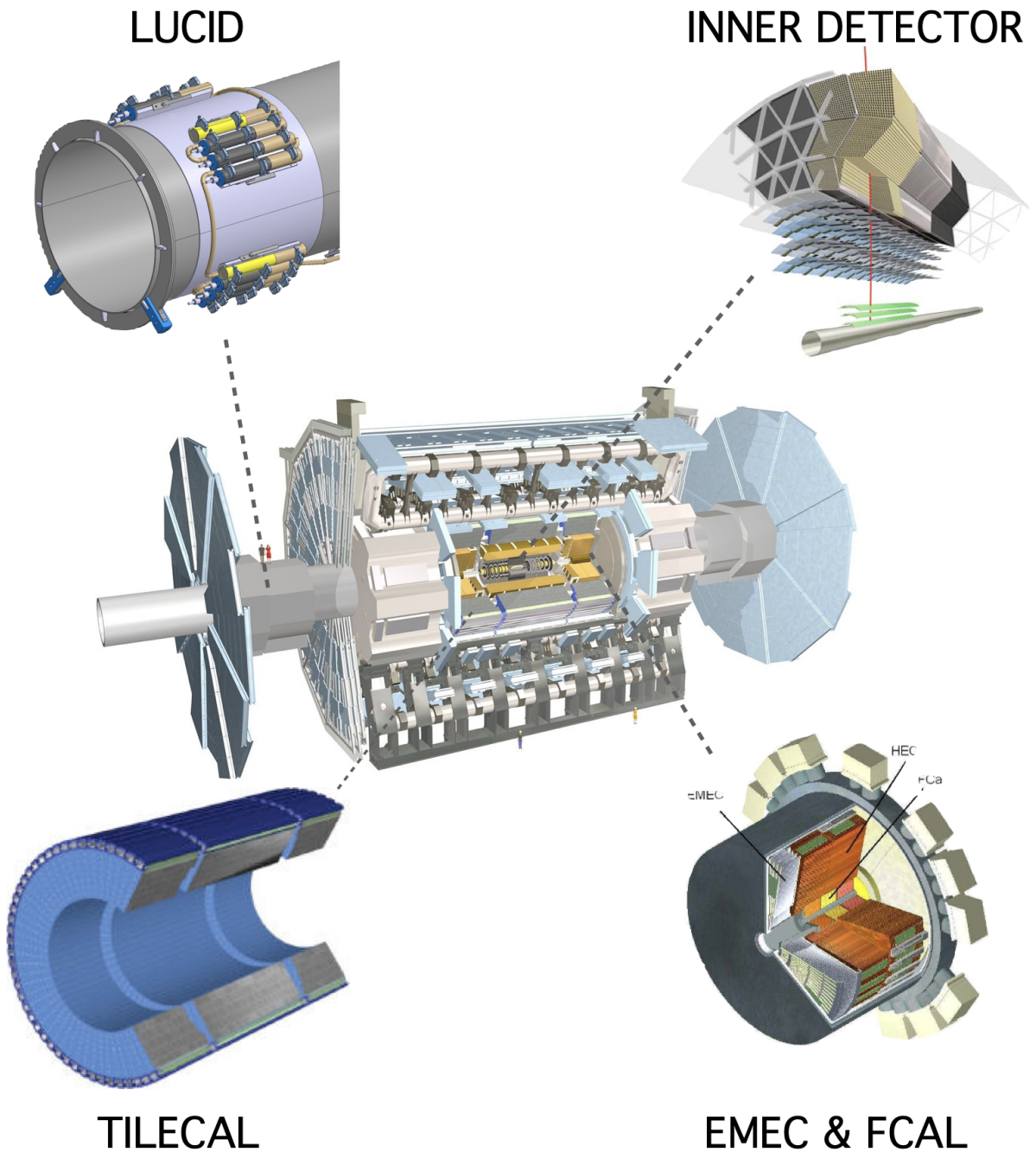


Figure 5.1: Illustrative sketch of the luminosity detectors in ATLAS. The primary luminometer for ATLAS in Run 2 and Run 3 is the LUCID detector. The other luminometers are used to correct pileup dependence of the LUCID measurement, monitor its long-term stability and estimate uncertainties in the luminosity measurement.

These *luminometers* measure a fraction of all inelastic interactions per bunch-crossing:

$$\mathcal{L}_b = f_{\text{LHC}} \frac{\mu_{\text{vis}}}{\sigma_{\text{vis}}}, \quad (5.2)$$

where, $\mathcal{L}_b$ is the luminosity of a colliding bunch, μ_{vis} is the *visible interaction rate* or the average number of pp collisions per bunch-crossing measured by the luminometer and σ_{vis} is the *visible cross-section*, a constant determined specifically for each luminometer. f_{LHC} denotes the bunch revolution frequency in the collider, set to 11.245 kHz.

The primary luminometer of ATLAS in Run 2 and Run 3 is the LUCID detector, described in Section 3.2.5. It provides per-bunch luminosity estimate based on signals recorded by PMT arrays as particles traverse the detector's gas-filled aluminium tubes and produce Cherenkov light. This detector is calibrated in special scans called *van der Meer* (vdM) scans [65,66] where the beams are separated and scanned in x and y planes to determine the *beam overlap integral* in the respective planes (Σ_x, Σ_y). vdM scans use beams with a roughly Gaussian-like profile, high β^* , ensuring a larger beam spot at the interaction point and higher beam emittance, ensuring a larger spread between particles in the beam ultimately also leading to a larger beam size. In addition, the beams are produced to have low bunch density with *isolated* proton bunches to avoid collisions between incoming and outgoing bunches at the interaction point and minimize beam-beam effects. As hinted at already in the scan conditions, the vdM method assumes that proton densities can be *factorised* into independent horizontal and vertical components. Using this assumption, the bunch luminosity can be re-written in terms of the number of protons per bunch (n_1, n_2) as:

$$\mathcal{L}_b = f_{\text{LHC}} \frac{n_1 n_2}{\Sigma_x \Sigma_y}. \quad (5.3)$$

The uncertainty coming from this assumption is termed *non-factorisation uncertainty* and typically has the largest contribution to uncertainties related to the vdM scan. Examples of beam overlap integral measurements performed with data from the first vdM session in 2023 (Run 3) are shown in Figure 5.2 [67]. The preferred LUCID luminosity measurement algorithm in Run 3 was the *LUCID Bi2HitOR* algorithm [67]. The scan curves in Figure 5.2 are used to determine each of the beam overlap integrals (Σ_x, Σ_y) according to Equation 5.4.

$$\Sigma_x = \frac{1}{\sqrt{2\pi}} \frac{\int R(\Delta x) d(\Delta x)}{R(\Delta x^{\text{max}})}. \quad (5.4)$$

where, $R(\Delta x)$ is the luminosity in arbitrary units measured when the horizontal or vertical beam separation is Δx and $R(\Delta x^{\text{max}})$ is the peak of the scan curve. The beam overlap

integral in the y direction, Σ_y , is determined similarly. Following this measurement, Equation 5.2 is related to Equation 5.3 to determine σ_{vis} . Other luminometers of ATLAS are then calibrated to the LUCID luminosity measured in the vdM run. The calibration of LUCID is then extrapolated to high pileup *physics* conditions using a procedure called *Calibration Transfer* using measurements from track-counting and TileCal. Further, the *long-term stability* of the LUCID or track-counting measurements is monitored by comparing their response to that of the calorimeters of ATLAS (TileCal, EMEC, FCAL). Due to a large number of cells in the TileCal, spread over large pseudorapidities and at varying distances from the interaction point, this calorimeter is sensitive to a wide range of luminosities and it plays an important role in the above procedures in the ATLAS luminosity measurement. The next subsections briefly describe the different uncertainties the ATLAS luminosity measurement, emphasizing the role of TileCal.

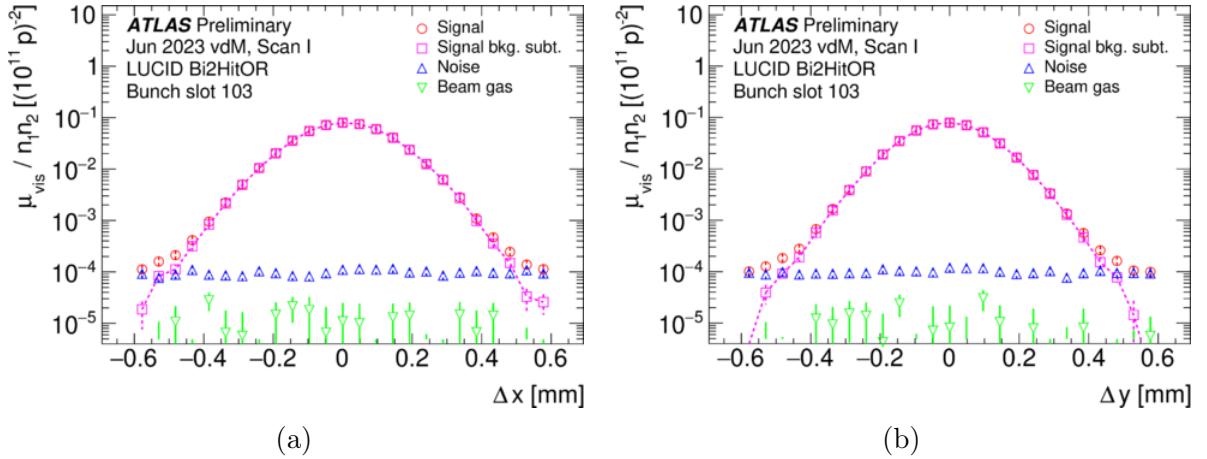


Figure 5.2: Beam separation scans during a vdM scan session in 2023 (Run 3) [67]. The beam separation in (a) x - and (b) y - planes is depicted as a function of the visible interaction rate per unit bunch population. The signal measured using the LUCID Bi2HitOR algorithm is shown in red circles. The estimated background from noise and afterglow are shown with blue upward triangles and that from beam–gas interactions with green downward triangles. The background subtracted signal is shown in pink squares. Only statistical errors are shown in all measurements.

Calibration transfer uncertainty

LUCID measurements are known suffer from non-linearity of $\mathcal{O}(10\%)$ [68] with increasing pileup due to the nature of the detector: with increasing number of collisions in the collider, the number of secondary particles with the potential to generate a small signal in the

PMT increase. When multiple such secondary particles hit the PMTs simultaneously, the combined signal may be over threshold, overestimating the LUCID measurement. Thus, vdM conditions are used to calibrate the response of LUCID and then extrapolated to physics conditions in a procedure called *Calibration Transfer* (CT), where the LUCID luminosity measurement is corrected to the track-counting measurement in a long physics run with gradually decreasing pileup. This run is called the *Calibration Transfer run* and is usually chosen to be close in time to the vdM scan to avoid additional effects from changing detector and data taking conditions.

The ratio of the track-counting luminosity to the LUCID measurement is parametrised by a first order polynomial shown in Equation 5.5, and the fitted parameters used to correct the LUCID measurement in all other runs.

$$\langle\mu_{\text{corr}}\rangle = p_0\langle\mu_{\text{uncorr}}\rangle + p_1(\langle\mu_{\text{uncorr}}\rangle)^2, \quad (5.5)$$

where μ_{uncorr} and μ_{corr} are the uncorrected and corrected LUCID measurement respectively and the parameter p_1 encodes any possible non-linearity in the track-counting measurement. The uncertainty in the CT extrapolation is estimated by evaluating the maximum shift between the track-counting and TileCal measurement from cells E3/E4 and A13/A14, in a set of runs with gradually increasing number of simultaneous interactions, number of bunches, and moving from isolated bunches to bunch trains. Prior to this, the response of TileCal for each cell of interest is equalised to that of the track-counting luminosity in a high-luminosity reference run close to the vdM scan known as the *anchoring run*. Further, TileCal currents are corrected for PMT response variation during and in-between fills. These corrections are estimated from dedicated calibration runs and ensure a robust and reliable TileCal measurement during data taking. The derivation of calibration transfer uncertainty for the 2022 and 2023 data taking periods in Run 3 are discussed in Sections 5.2.1 and 5.3.1 respectively.

Long-term stability

It is important to monitor the long-term drifts of LUCID or track-counting to ensure a good calibration throughout the entire data taking period. This is accomplished by comparing the pileup corrected LUCID measurements to those from TileCal D-cells (which are well shielded from radiation damage), EMEC and FCAL over the data taking period. Measurements from a set of ten runs around the vdM scan are used to anchor the calorimeter

measurements to the track-counting luminosity. The *calibration anchoring* uncertainty is derived by calculating the largest RMS in difference of measurements across the different calorimeter subsystems in these runs. The *long-term stability uncertainty* is derived by considering a stability band which encloses the bulk of the differences between LUCID and any of the other luminosity measurements during the data taking period. The derivation of long-term stability uncertainty for the 2022 and 2023 data taking periods in Run 3 are discussed in Sections 5.2.2 and 5.3.2 respectively.

Activation signal in the TileCal

Interaction of primary or secondary collision particles with the detector material surrounding the TileCal can produce radioactive isotopes with lifetimes ranging from minutes to days. The decay of these isotopes can produce additional signal in the TileCal scintillators and needs to be estimated and accounted for while measuring TileCal luminosity with MinBias integrators. For a short pulse of real instantaneous luminosity $L_{\text{inst}}^{\text{ref}}$ of duration δt at time $t = 0$, the resulting apparent instantaneous luminosity $L_{\text{inst}}^{\text{act}}$ from activation at a later time t is given by:

$$L_{\text{inst}}^{\text{act}} = \delta t L_{\text{inst}}^{\text{ref}} \frac{f e^{-t/\tau}}{\tau}, \quad (5.6)$$

where f characterises the strength of the activation-induced luminosity signal with respect to the source and τ is the half-life of the isotope. Estimating the activation signal involves fitting the values of f and τ from data, for several isotopes.

These fits are usually performed by minimising the χ^2 built from track and TileCal luminosity in the low- μ , 5- σ separation and high- μ parts of the CT and validated in the post beam-dump period. The χ^2 is defined using Equation 5.5 as:

$$\chi^2 = \sum \left(\frac{(L_{\text{int}}^{\text{calo}} - L_{\text{int}}^{\text{act}} - P - L_{\text{int}}^{\text{trk}}(p_0 + \langle \mu \rangle p_1))^2}{(\sigma_{L_{\text{int}}^{\text{calo}}})^2 + (\sigma_{L_{\text{int}}^{\text{trk}}})^2} \right). \quad (5.7)$$

where, $L_{\text{int}}^{\text{calo}}$ is the uncorrected TileCal measurement, P is a pedestal correction to the instantaneous luminosity and $(\sigma_{L_{\text{int}}^{\text{calo}}})$ and $(\sigma_{L_{\text{int}}^{\text{trk}}})$ represent the per-LB uncertainties in the luminosity measurements. An example of fitting and validation periods are indicated for the vdM run in 2022 (run 455702) in Figure 5.3. Effects from activation can be up to 0.5% depending on the cell family [68].

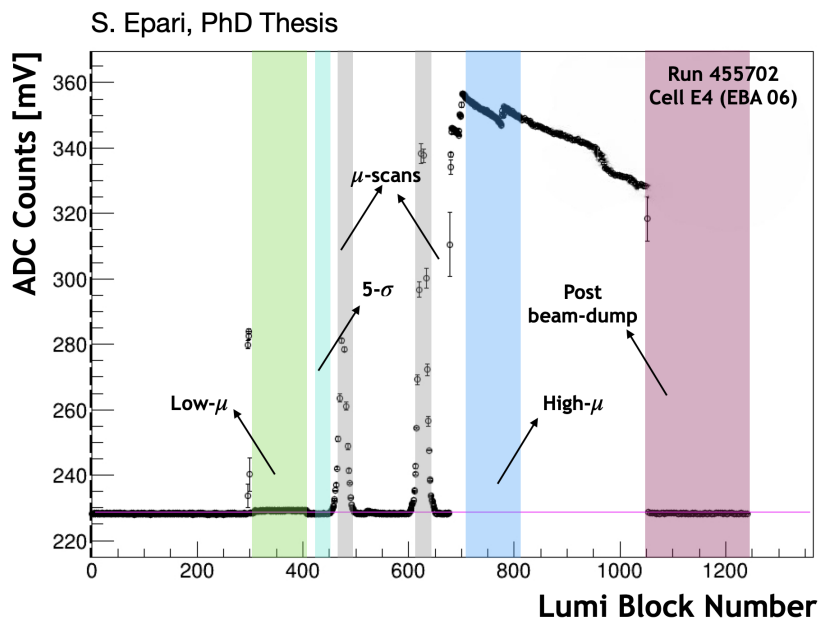


Figure 5.3: ADC counts as a function of LB number for run 455702, measured by cell E4 (Module 06) in the extended barrel A. The grey shaded area are the μ -scans, excluded in the TileCal activation fit. The green and blue shaded areas are the low- μ and high- μ parts respectively, showing only periods with good track-counting data. The 5- σ separation period, when the separation between the beams is the maximum, is shown in cyan. The post beam-dump period is highlighted in purple.

Additional uncertainties in the luminosity measurement

In addition to the systematic uncertainties associated with calibration transfer and the long-term stability, the offline luminosity measurement is also affected by uncertainties in the vdM calibration. These are estimated using dedicated prescriptions and some of the important contributions to this uncertainty are highlighted below [67]:

- *After-glow*, caused by photons produced from nuclear de-excitation when pp collision products initiate hadronic cascades.
- *Beam-halo interactions*, which are a combination of beam-gas interactions and halo particles recorded by LUCID, in-time with the main beam.
- Uncertainties from the vdM scan, including *beam-beam effects*, *length-scale calibration* measuring the beam-spot position and *non-factorisation effects*.
- Consistency of calibration between different scans and different bunches, determined from comparing measurements between the two vdM scans typically done per year.

Typically, the uncertainty from non-factorisation effects dominates this category.

5.2 The ATLAS luminosity measurement in 2022

This section discusses the uncertainty measurement in the ATLAS luminosity measurement for the 2022 data taking period in Run 3, with emphasis on the derivation of calibration transfer and long-term stability uncertainties. The section concludes with a brief discussion of the latest 2022 public ATLAS luminosity uncertainty recommendation.

The pileup (μ) dependence of the LUCID response with respect to that from track-counting was checked in fill 8146, taken on 20th August 2022, 10:28 CEST with 2400 isolated bunches. The luminosity profile of this fill together with the ratio of track-counting luminosity to LUCID response is shown in Figure 5.4. A linear fit to the ratio of track-counting luminosity to LUCID response shows a slope of about -0.14% per unit of μ .

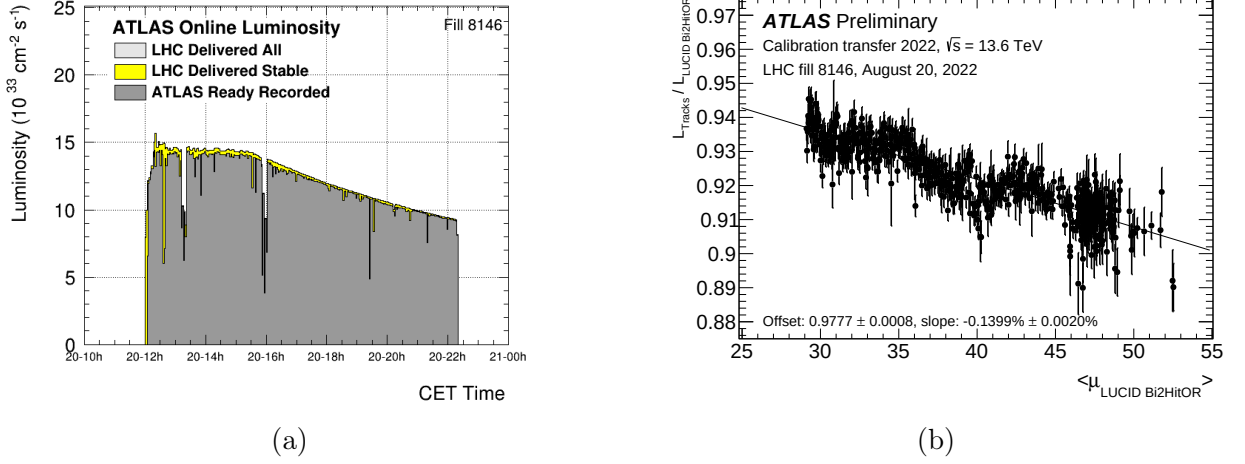


Figure 5.4: (a) Luminosity profile of the μ -correction fill, used for the calibration of LUCID to track-counting for physics data taking. (b) Ratio of bunch-averaged track-counting luminosity to the LUCID luminosity using the LUCID Bi2HitOR algorithm before any pileup correction, as a function of bunch-averaged pileup parameter (measured using LUCID Bi2HitOR algorithm) during LHC fill 8146 in 2022 [69].

5.2.1 Calibration transfer uncertainty

The CT uncertainty in 2022 was evaluated by selecting a set of eight runs around the vdM scan spanning September–November 2022, shown in Tables 5.1- 5.3. The CT run for 2022 was taken on 29th September 2022 (run 435678), with modules from cells E3 and E4 divided into one of two gain families: *low*, set to $0.2 \text{ M}\Omega$ and *high*, set to approximately $30 \text{ M}\Omega$. This arrangement was adopted to have sensitivity to the entire luminosity range explored in the run. Due to relatively smaller signals in cells A13 and A14, such a configuration was not adopted for these cells. Shortly after the CT run, a four week long, unexpected LHC stop occurred due to a cooling leak in one of the sectors. The vdM scan (run 439428) for the year was performed after recovery of the machine, on 9th November 2022. To avoid effects from scintillator ageing or activation signal from surrounding material during the LHC down-time, dedicated anchoring runs were used for the periods before and after the LHC stop. The first set of runs, summarised in Table 5.1 and 5.2, were chosen to be anchored in run 435816. All runs in this dataset, except the anchoring run, were collected without the ATLAS toroid field due to additional operational complications. The second set of runs, summarised in Table 5.3, were anchored to run 439519. In all cases, the pedestal was estimated as the mean of ADC counts in LBs before collision.

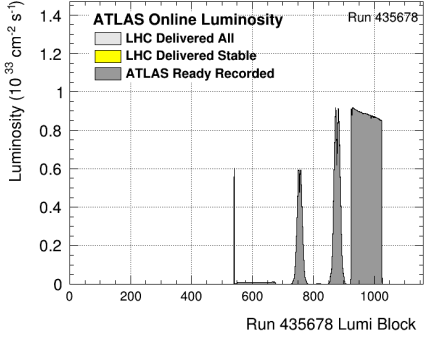
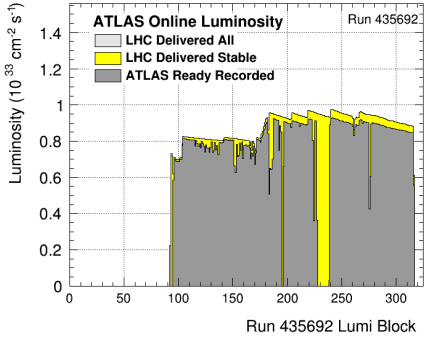
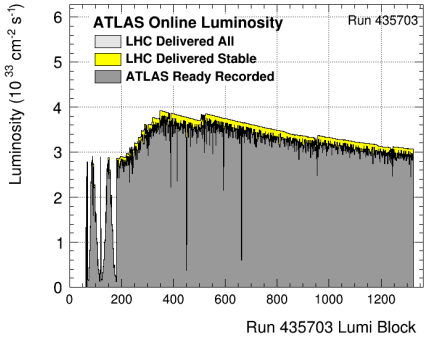
Run Luminosity Profile	Run Summary	Remarks
	• Start: Sep 29, 07:27 CEST • End: Sep 30, 01:23 CEST • β^*: 60 cm - 30 cm • Bunches Colliding: 140 • Toroid: OFF	CT fill
	• Start: Sep 30, 01:52 CEST • End: Sep 30, 05:30 CEST • β^*: 60 cm - 30 cm • Bunches Colliding: 146 • Toroid: OFF	-
	• Start: Sep 30, 06:34 CEST • End: Sep 30, 11:03 CEST • β^*: 60 cm - 30 cm • Bunches Colliding: 578 • Toroid: OFF	-

Table 5.1: Part of the dataset collected for estimating the calibration transfer uncertainty in 2022. These runs were taken without the toroid field due to operational issues. The CT fill, run 435678, had modules from cells E3 and E4 were divided in to one of two gain families (*low*, set to 0.2 M Ω and *high*, set to approximately 30 M Ω) to have sensitivity to the entire luminosity range explored in the run. Due to relatively smaller signals in cells A13 and A14, such a configuration was not adopted. The highest luminosity run, run 435816 shown in Table 5.2, is used for anchoring in the September 2022 period.

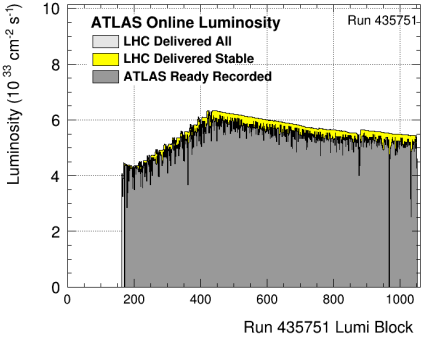
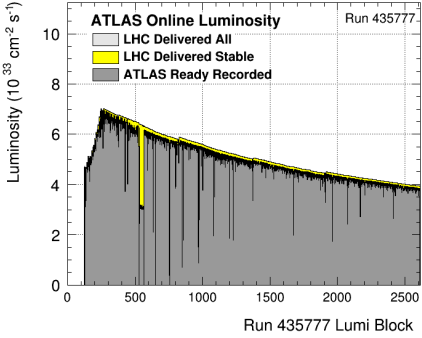
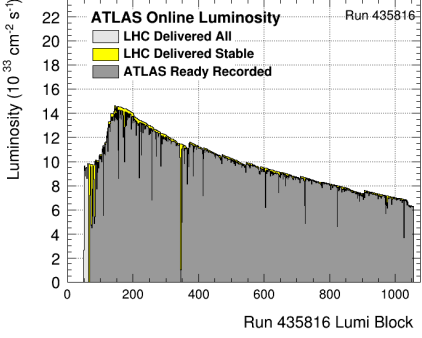
Run Luminosity Profile	Run Summary	Remarks
 Run 435751	• Start: Sep 30, 14:11 CEST • End: Sep 30, 19:40 CEST • β^*: 60 cm - 30 cm • Bunches Colliding: 1154 • Toroid: OFF	-
 Run 435777	• Start: Sep 30, 21:00 CEST • End: Oct 01, 06:58 CEST • Bunches Colliding: 1154 • β^*: 60 cm - 30 cm • Toroid: OFF	-
 Run 435816	• Start: Oct 01, 12:03 CEST • End: Oct 02, 01:32 CEST • β^*: 60 cm - 30 cm • Bunches Colliding: 2448 • Toroid: ON	-

Table 5.2: Part of the dataset collected for estimating the calibration transfer uncertainty in 2022. These runs were taken without the toroid field due to operational issues. The highest luminosity run, run 435816, is used for anchoring in the September 2022 period.

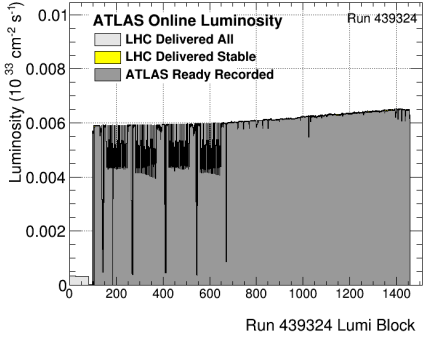
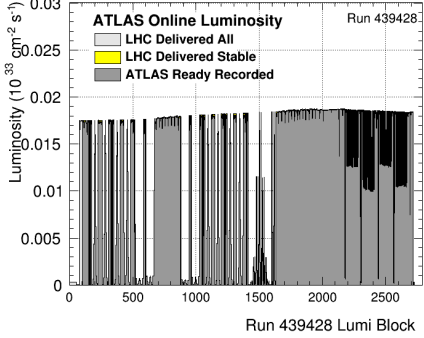
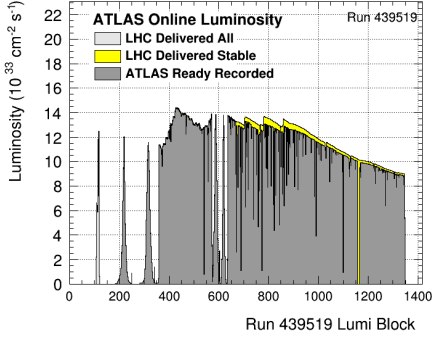
Run Luminosity Profile	Run Summary	Remarks
 Run 439324 Lumi Block	• Start: Nov 09, 23:26 CEST • End: Nov 10, 18:40 CEST • β^*: 19.2 m • Bunches Colliding: 58 • Toroid: ON	-
 Run 439428 Lumi Block	• Start: Nov 10, 18:53 CEST • End: Nov 11, 21:12 CEST • β^*: 19.2 m • Bunches Colliding: 144 • Toroid: ON	vdM fill
 Run 439519 Lumi Block	• Start: Nov 12, 02:11 CEST • End: Nov 12, 17:09 CEST • β^*: 60 cm - 30 cm • Bunches Colliding: 1802 • Toroid: ON	Anchor

Table 5.3: Part of the dataset collected for estimating the calibration transfer uncertainty in 2022. The vdM run is indicated in the table. The highest luminosity run, run 439519 is used for anchoring in the November 2022 period.

The removal of *bad* modules was done for cells E3, E4, A13 and A14 separately following the procedures established in Section 4.2. This accounts to about 15% or less of the total modules for each PMT. In the anchoring run, a calibration constant per *good* module was calculated as the ratio of the Tile current to the track-counting luminosity in the run and used to rescale the Tile currents in all other runs. For run 435816, anchoring constants were calculated in the LB range 400–600, while for 439519, the LB range 360–390 was used. These ranges were chosen to contain only LBs where both the track-counting data and TileCal currents were collected without operational issues. Finally, the ratios of TileCal to track luminosity ratios were derived as the measurement from all good modules average over the LBs. In the case of A-cells, the average of the measurement from the two PMTs is used. The results are shown in Figure 5.5.

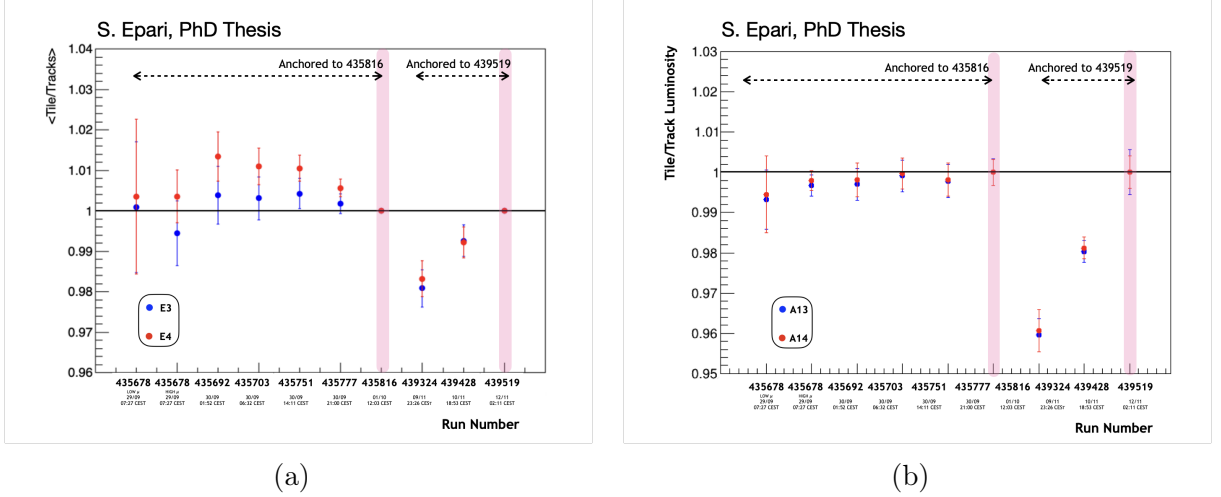


Figure 5.5: Ratio of TileCal to track-counting luminosity for cells (a) E3 and E4, and (b) A13 and A14 for runs considered to estimate the calibration transfer uncertainty in 2022. Activation is not accounted for in these figures and can be up to 1% additional signal in the PMTs [68].

The TileCal to track-counting luminosity ratios for modules with sensitivity to the low-luminosity periods of the CT fill show much larger deviation from the mean largely due to larger statistical fluctuations in the period. The ratios show good compatibility with unity in the September dataset and up to 4% deviation from the anchoring run in the November dataset. These deviations can be well accounted for by accounting for PMT response variations and TileCal activation (not shown in the plots). While publishing the preliminary uncertainty estimate, the laser data was not available to provide corrections to PMT response variation. The effect of these missing corrections was estimated to be around

0.5% from previous analyses [68] and added linearly to the TileCal estimates. The range of shifts in the ratio of TileCal to track-counting luminosity measurement over the used TileCal families was checked over the different runs of the dataset, going from the vdM regime (low- μ , low number of bunches, isolated bunches) to the data taking conditions of physics running (high- μ , large number of bunches, bunch trains), summarised in Table 5.4. The first extrapolation considers the variation in Tile/Track ratios of A-cells, between the CT conditions ($\mu = 0.5$, 140b, isolated bunches in run 435678) and physics conditions ($\mu = 40$, 1154b, trains in run 435751 or 435777) and put an upper limit at 0.8%. This is a more conservative estimate than those derived from E-cells, which show slightly lower variation in ratios for the same period. The second extrapolation involves two steps: first, the maximum variation in ratios between the CT fill ($\mu = 0.5$, 140b, isolated bunches in run 435678) and vdM conditions ($\mu = 45$, 144b, isolated bunches in run 439428) is checked, taking into account activation; second, the extrapolation to physics conditions is considered ($\mu = 40$, 1154b, trains in run 435751 or 435777). The upper limit on this extrapolation stands at about 1% taking into account both TileCal cell families, and added linearly with the expected effects from laser corrections, gives the CT uncertainty to be 1.5%.

Extrapolation of luminosity calibration	Used cell families	Range of shifts across used cell families
1-step extrapolation		
$(\mu \approx 0.5, 140\text{b, isolated}) \rightarrow (\mu \approx 40, 1154\text{b, trains})$	A13, A14	$[-0.1, 0.8]\%$
Alternative: 2-step extrapolation		
$(\mu \approx 0.5, 140\text{b, isolated}) \rightarrow (\mu \approx 45, 144\text{b, trains})$	A13, A14, E3, E4	$[0.1, 0.7]\%$
$(\mu \approx 45, 144\text{b, trains}) \rightarrow (\mu \approx 40, 1154\text{b, trains}) (*)$	A13, A14	$[0.0, 0.4]\%$
Combined 2-step extrapolation		$[0.1, 1.1]\%$
Upper limit on extrapolation impact (rounded)		$< 1\%$
Effect of missing laser corrections (linearly added)	A14	0.5%
Upper limit on total extrapolation impact		$< 1.5\%$

Table 5.4: Range of shifts in the ratios of the Tile-calorimeter luminosity and the track-counting luminosity in the CT dataset in 2022 [69]. The selected runs are shown in Tables 5.1, 5.2 and 5.3 and are taken with varying number of simultaneous interactions, number of bunches, and moving from isolated bunches to bunch trains, to extrapolate the calibration of LUCID from vdM to physics conditions. The Tile data has been corrected for residual ambient activation, except for one extrapolation step indicated with (*), where at high μ -values the bias from the activation is considered small. The rounded maximum shifts are used as an upper limit on the impact of the extrapolation on the luminosity calibration. This is added linearly with the potential effect from missing laser corrections, which trace gain changes in the Tile readout photomultiplier tubes (PMTs). The upper limit on the total impact of the extrapolation from the vdM to the regime of physics data taking is symmetrized and considered as calibration transfer uncertainty.

5.2.2 Long-term stability uncertainty

The long-term stability uncertainty was estimated using runs passing the Good Run List (GRL) in 2022, using measurements from track-counting, EMEC and FCAL. TileCal measurements from D-cells were not processed at the time of publication. Figure 5.6 shows fractional differences between the run-integrated luminosity measured from EMEC and FCAL with respect to either the baseline LUCID or track-counting algorithms. All luminosity estimates were normalised in ten runs close to the vdM scan. Estimates from EMEC and FCAL show good compatibility in this region and are used to estimate the calibration anchoring uncertainty to be 0.53%.

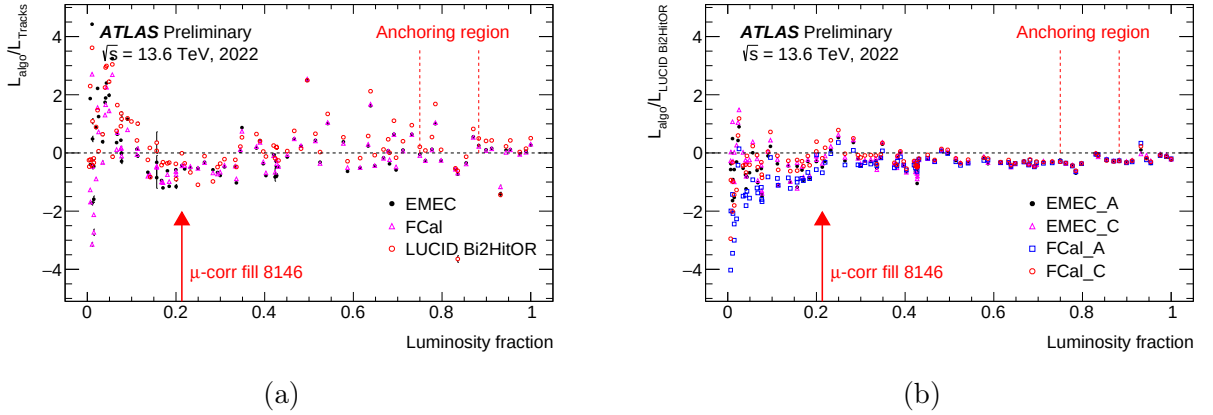


Figure 5.6: Fractional differences in fill-integrated luminosity between (a) the EMEC, FCAL (averages of the respective A- and C-side algorithms), LUCID Bi2HitOR luminosity and the track-counting luminosity algorithm and (b) the EMEC and FCAL luminosity measurements (A- and C-sides separately) and the baseline LUCID Bi2HitOR luminosity algorithm, as a function of the fractional cumulative integrated luminosity in 2022 [69]. The μ -correction fill corresponds to the dataset used for the calibration of LUCID to track-counting for physics data taking, the anchoring region marks the range of ten fills around the vdM fill used for normalising the calorimeter measurements to track-counting. The selection of fills is restricted to those passing standard data-quality requirements.

Next, the variation between the algorithms from the respective subdetectors is checked in the μ -correction fill and the long-term stability uncertainty is evaluated conservatively by considering the largest mean deviation across the calorimeter subsystems and track counting sets. These results are shown in Figure 5.7. For the 2022 dataset, this uncertainty is estimated to be 0.41%, from the FCAL (side A).

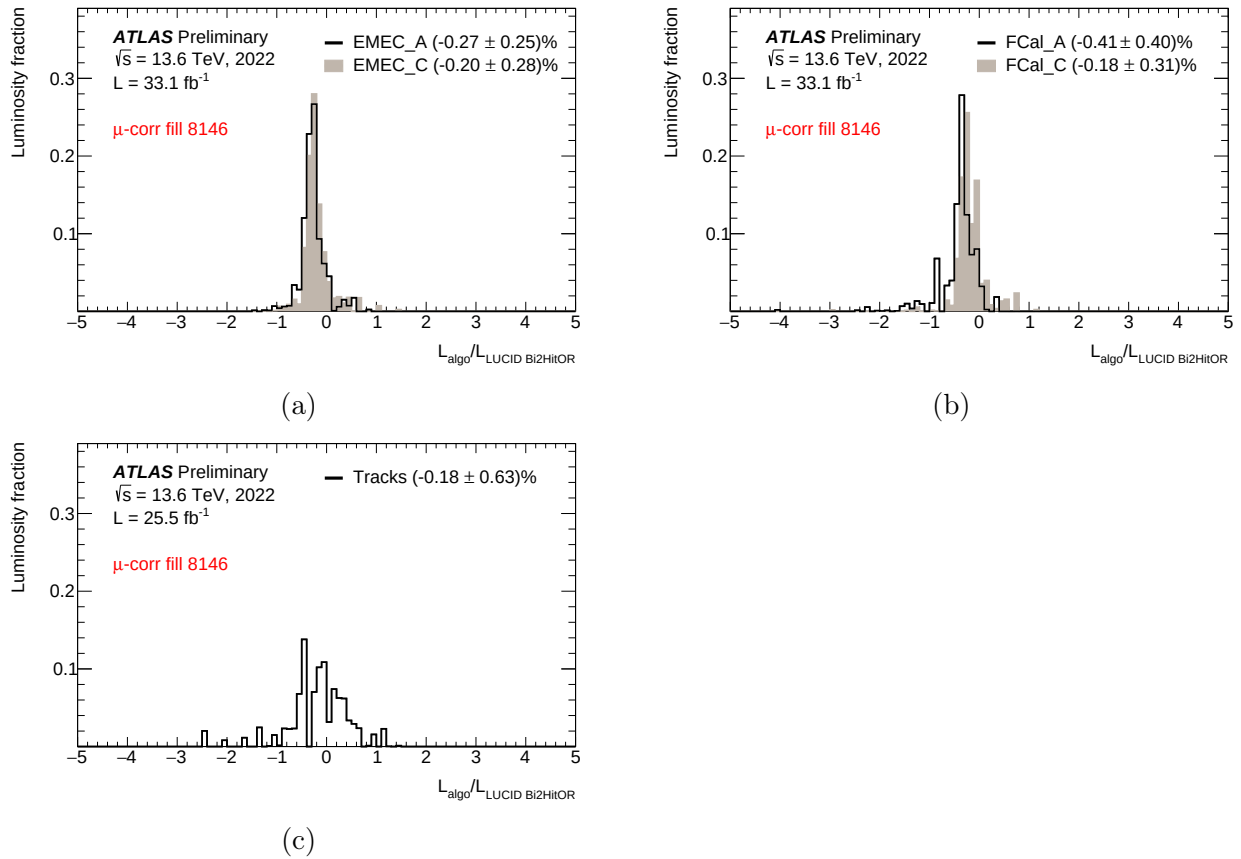


Figure 5.7: Distributions of relative differences in fill-integrated luminosity between the baseline LUCID Bi2HitOR luminosity measurement (weighted by the integrated luminosity) and (a) the EMEC luminosity measurements (A-side and C-side separately), (b) FCal luminosity measurements (A-side and C-side separately), (c) track-counting luminosity measurements in the μ -correction fill for 2022 [69]. The selection of fills is restricted to those passing standard data-quality requirements; in the case of track-counting, requirements are tightened to reject fills suffering from known Inner-Detector operational issues that affect the track-counting luminosity measurement. The quoted integrated luminosity is the one delivered by the LHC, not corrected for ATLAS detector and trigger readiness. The mean and RMS values for each algorithm are indicated in the legend. The largest mean deviation across the calorimeter subsystems and track counting sets the long-term stability uncertainty.

5.2.3 Results

The final uncertainty in the luminosity measurement was derived taking into account multiple effects described in the earlier section, summarised in Table 5.5. The vdM calibration is dominated by non-factorisation effects ($\sim 1\%$). The calibration transfer uncertainty (1.5%) has the leading contribution to the total uncertainty (2.19%).

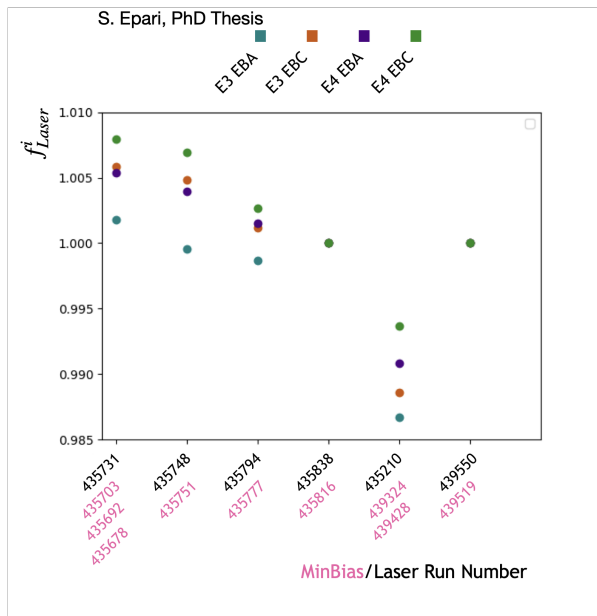
Data sample	2022
Integrated luminosity (fb^{-1})	31.40
Total uncertainty (fb^{-1})	0.7
Uncertainty contributions (%):	
vdM calibration	1.45
Calibration transfer	1.50
Calibration anchoring	0.53
Long-term stability	0.41
Total uncertainty (%)	2.19

Table 5.5: Systematic uncertainties associated with the preliminary luminosity calibration of the 2022 pp data sample at $\sqrt{s} = 13.6$ TeV. The fractional systematic uncertainty is broken down into four main contributions: absolute vdM calibration, the calibration transfer from the vdM to the physics regime, calibration anchoring of the calorimeters for physics runs, and long-term stability of the luminometer response. Table modified from Ref. [69].

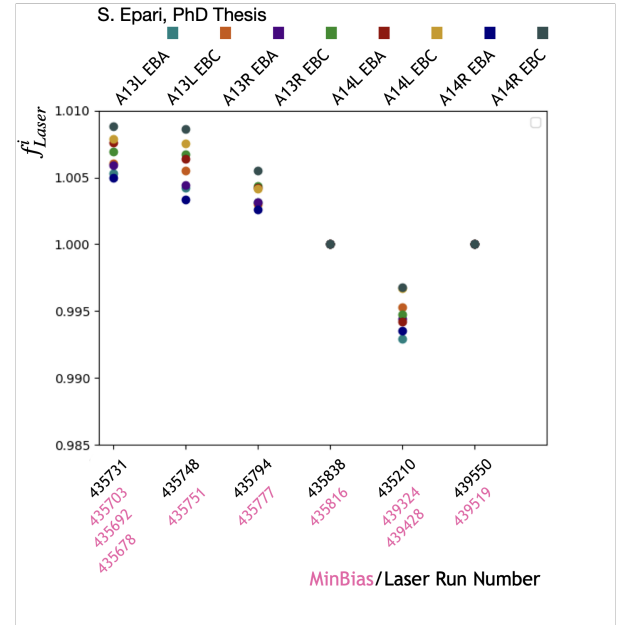
5.2.4 Data reprocessing and outlook

Following the publication of the preliminary luminosity measurement for 2022, a reprocessing of the data from all detector subsystems is on-going to improve the overall uncertainty estimate. In particular, TileCal data provided for calibration transfer has been updated with corrections to account for PMT response variation between and during the runs, namely inter-run and in-gap laser corrections respectively. The inter-run laser corrections for E3/E4 and A13/A14 are shown in Figure 5.8. The average value of the correction is about 1% for each of the PMTs. In-gap laser corrections derived from the 2018 dataset, shown in Figure 4.5, are used.

The updated ratios of TileCal to track-counting luminosity are shown in Figure 5.9 for E3/E4 and Figure 5.10 for A13/A14 respectively. For E3/E4, the application of laser corrections progressively improves the agreement of the ratio with unity. A similar trend is observed for A13/A14. The impact of the corrections will be fully assessed after the



(a)



(b)

Figure 5.8: Average value of inter-run laser corrections for (a) E3 and E4 cells and (b) A13 and A14 cells. The corrections are derived from laser calibration runs marked in black and the MinBias run(s) to which they are applied is marked in pink. These corrections are applied per module for each PMT. An average of ten laser runs close to the anchoring run in September and November were chosen to normalise the data for laser runs used in the analysis.

activation analysis is repeated on the dataset but preliminary estimates show that the CT error would reduce by a few percent.

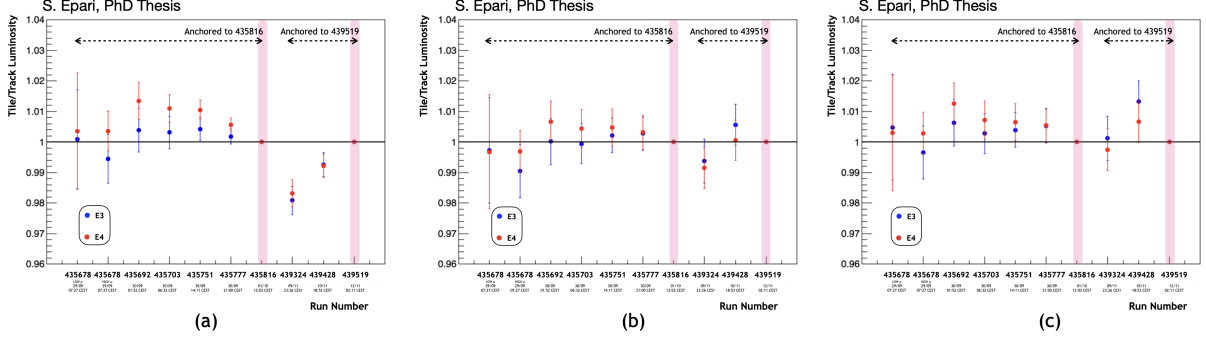


Figure 5.9: Ratio of TileCal to the track-counting luminosity for cells E3 and E4 for runs considered to estimate the calibration transfer uncertainty in 2022 (a) before any laser corrections are applied, (b) after run-to-run laser corrections and (c) after in-gap laser corrections are applied. Activation is not accounted for in these figures and can be up to 1% additional signal in the PMTs [68].

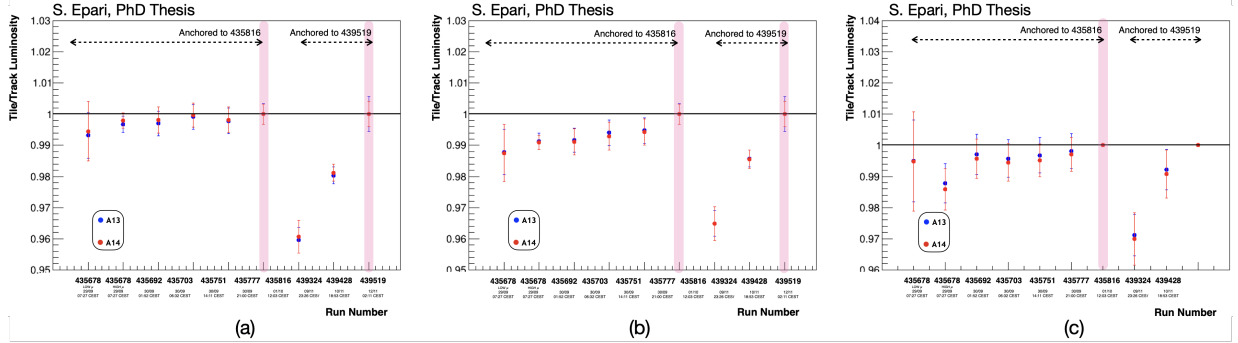


Figure 5.10: Ratio of TileCal to the track-counting luminosity for cells A13 and A14 for runs considered to estimate the calibration transfer uncertainty in 2022 (a) before any laser corrections are applied, (b) after run-to-run laser corrections and (c) after in-gap laser corrections are applied. Activation is not accounted for in these figures and can be up to 1% additional signal in the PMTs [68].

TileCal data from cell D6 was also processed after the preliminary study. Figure 5.11 shows fractional differences between the run-integrated luminosity measured from EMEC, FCAL and the cell D6 with respect to either the baseline LUCID algorithm. The TileCal measurement agrees well with that from the other calorimeters (also reprocessed) in the anchoring region.

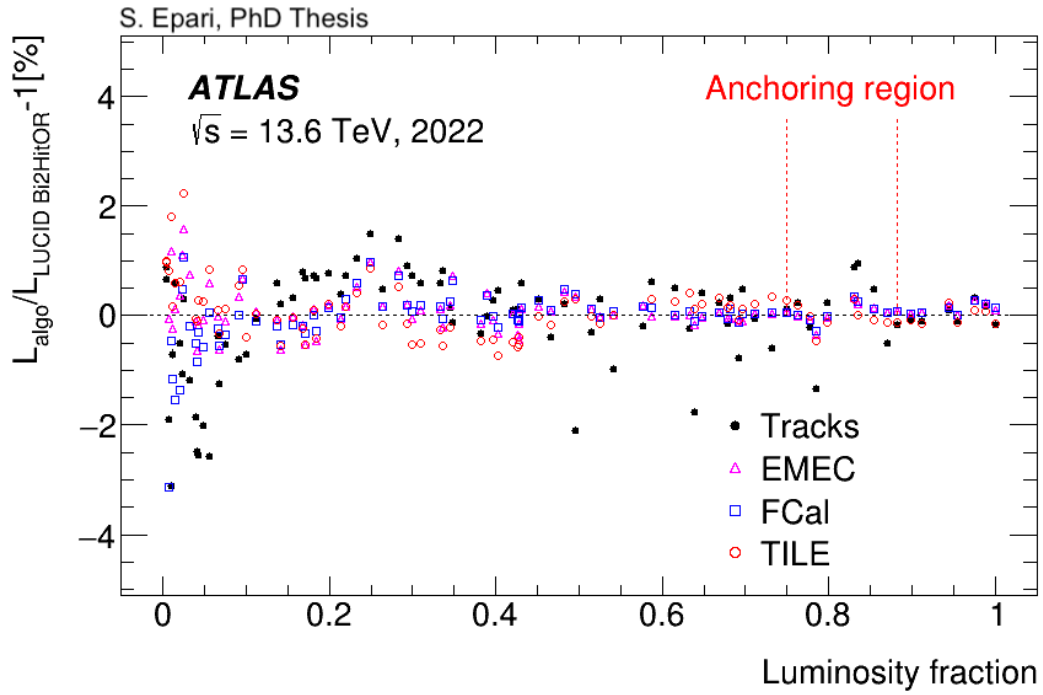


Figure 5.11: Fractional differences in fill-integrated luminosity between the baseline LUCID Bi2HitOR luminosity measurement (weighted by the integrated luminosity) and calorimeter and track-counting luminosity measurements as a function of the fractional cumulative integrated luminosity in 2022. For EMEC and FCal, the measurements are re-processed relative to the preliminary result in Figure 5.6 and averaged over the A- and C- sides. The TileCal luminosity from cell D6 is quoted, averaged over the two PMTs from the two extended barrels.

The variation between the algorithms from the calorimeters was checked in the μ -correction fill, shown in Figure 5.12. The reprocessed EMEC uncertainty presents the largest mean deviation across the calorimeter subsystems and track counting sets and will be taken as the long-term stability uncertainty, reducing the preliminary estimate by more than half. Thus, the combined uncertainty from the calibration transfer and long-term stability are estimated to reduce by a few percent each, improving the overall luminosity uncertainty estimation. The reprocessed results are expected to be made public by the end of the year and is currently outside the scope of this thesis.

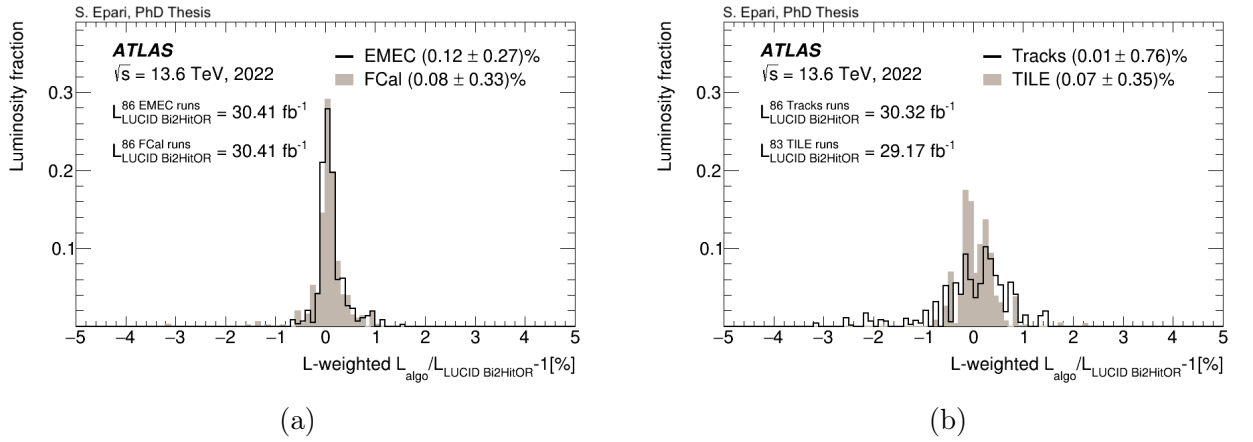


Figure 5.12: Distributions of relative differences in fill-integrated luminosity between (a) the baseline LUCID Bi2HitOR luminosity measurement (weighted by the integrated luminosity) and (b) the EMEC and FCAL luminosity measurements (averaged for A-side and C-side). The track-counting and TileCal luminosity measurements in the μ -correction fill for 2022. The selection of fills is restricted to those passing standard data-quality requirements; in the case of track-counting, requirements are tightened to reject fills suffering from known Inner-Detector operational issues that affect the track-counting luminosity measurement. The quoted integrated luminosity is the one delivered by the LHC, not corrected for ATLAS detector and trigger readiness. The mean and RMS values for each algorithm are indicated in the legend. The largest mean deviation across the calorimeter subsystems and track counting sets the long-term stability uncertainty.

5.3 The ATLAS luminosity measurement in 2023

This section discusses the uncertainty measurement for ATLAS luminosity for the 2023 data taking period in Run 3 with emphasis on the role of TileCal in the derivation of the calibration transfer and long-term stability uncertainty. The section concludes with a brief discussion of the latest 2023 public ATLAS luminosity uncertainty recommendation.

The μ -dependence of the LUCID response to track-counting luminosity was checked using the average of ten runs around the vdM fills in 2023. The ratio of track-counting luminosity to LUCID response is shown in Figure 5.13. A linear fit to the ratio of track-counting luminosity to LUCID response shows a slope of about -0.14% per unit of μ .

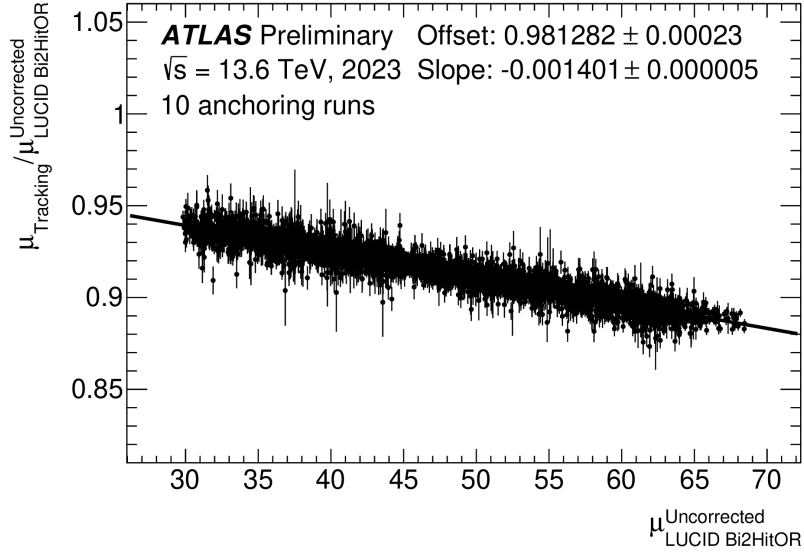


Figure 5.13: Ratio of the bunch-averaged pileup parameter reported by the track-counting luminosity algorithm to that measured by LUCID Bi2HitOR before any pileup correction, as a function of the bunch-averaged pileup parameter (measured using LUCID Bi2HitOR algorithm) using data from ten runs around the vdM fill [67]. The ratio is fit to a straight line and the slope of the line estimates the amount of correction to LUCID per unit pileup (approximately -0.14%).

5.3.1 Calibration transfer uncertainty

The CT uncertainty in 2023 was evaluated by selecting a set of eight runs around the vdM scan spanning June–July 2023. Two vdM fills, run 455889 and run 455623, were taken during the period because the beam was lost during the vdM scan in the first run. Runs with less than 140 bunches were taken without the toroid field due to operational issues with the ATLAS toroid magnet. Two CT fills were taken, run 455837 with isolated proton bunches and run 455899 with proton bunches in trains. Both fills had modules from cells E3 and E4 were divided in to one of two gain families (*low*, set to $0.2\text{ M}\Omega$ and *high*, set to approximately $30\text{ M}\Omega$) to have sensitivity to the entire luminosity range explored in the run. Due to relatively smaller signals in cells A13 and A14, such a configuration was not adopted. The entire set of runs is shown in Tables 5.6–5.8. Run 455924 was chosen as the anchoring run for the entire period. In all cases, the pedestal was estimated as the mean of ADC counts in LBs before collision. In run 455870, only data from the EBA was available due to a power-cycle of module 64 in LB 370, leading to loss of MinBias data in the following LBs.

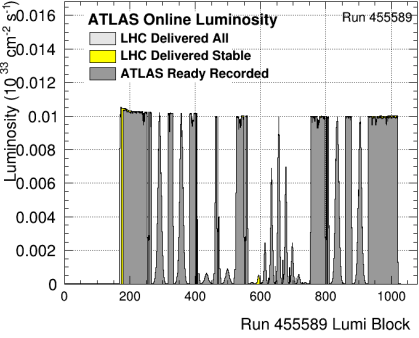
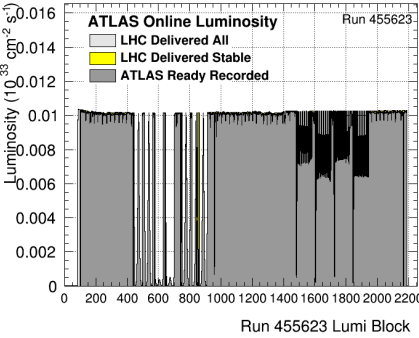
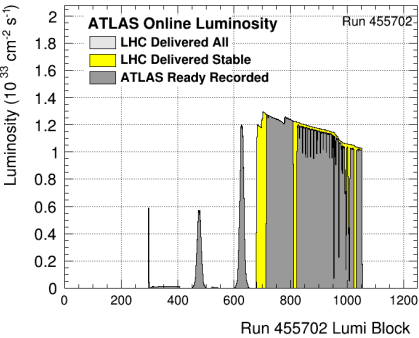
Run Luminosity Profile	Run Summary	Remarks
 Run 455589 Lumi Block	• Start: Jun 28, 09:38 CEST • End: Jun 28, 20:14 CEST • β^*: 19.2 m • Bunches Colliding: 136 • Toroid: OFF	vdM fill
 Run 455623 Lumi Block	• Start: Jun 28, 20:42 CEST • End: Jun 28, 23:24 CEST • β^*: 19.2 m • Bunches Colliding: 136 • Toroid: OFF	vdM fill
 Run 455702 Lumi Block	• Start: Sep 30, 06:34 CEST • End: Sep 30, 11:03 CEST • β^*: 60 cm - 30 cm • Bunches Colliding: 578 • Toroid: OFF	-

Table 5.6: Part of the dataset collected for estimating the calibration transfer uncertainty in 2023. These runs were taken without the toroid field due to operational issues. Two vdM fills, run 455889 and run 455623, were taken during the period because the beam was lost during the vdM scan in the first run. The highest luminosity run, run 455924 shown in Table 5.8, was used for anchoring the dataset

Run Luminosity Profile	Run Summary	Remarks
	• Start: Jun 30, 08:16 CEST • End: Jun 30, 23:17 CEST • β^*: 1.2 m - 30 cm • Bunches Colliding: 898 • Toroid: OFF	CT (in-divs)
	• Start: Jul 02, 17:39 CEST • End: Jul 02, 23:31 CEST • β^*: 1.2m - 30 cm • Bunches Colliding: 1165 • Toroid: ON	-
	• Start: Jul 03, 01:11 CEST • End: Jul 03, 06:27 CEST • β^*: 60 cm - 30 cm • Bunches Colliding: 1873 • Toroid: ON	-

Table 5.7: Part of the dataset collected for estimating the calibration transfer uncertainty in 2023. In the CT fill with isolated proton bunches, run 455837, modules from cells E3 and E4 were divided in to one of two gain families (*low*, set to 0.2 M Ω and *high*, set to approximately 30 M Ω) to have sensitivity to the entire luminosity range explored in the run. Due to relatively smaller signals in cells A13 and A14, such a configuration was not adopted. The highest luminosity run, run 455924 shown in Table 5.8, was used for anchoring the dataset.

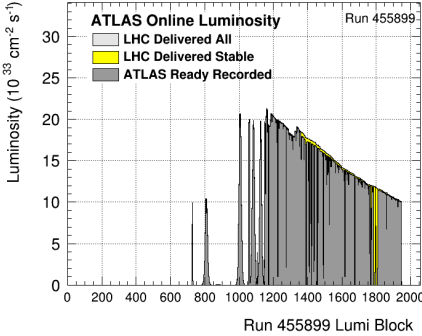
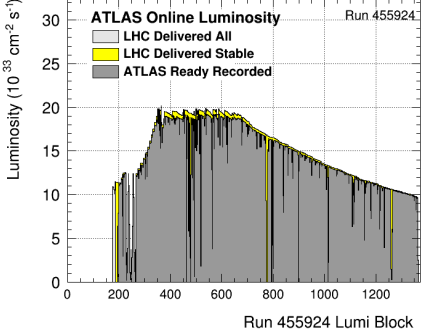
Run Luminosity Profile	Run Summary	Remarks
 Run 455899 Lumi Block	• Start: Jul 03, 18:06 CEST • End: Jul 04, 16:02 CEST • β^*: 1.2 m - 30 cm • Bunches Colliding: 2345 • Toroid: ON	CT (trains)
 Run 455924 Lumi Block	• Start: Jul 04, 17:32 CEST • End: Jul 05, 08:18 CEST • β^*: 1.2 m - 30 cm • Bunches Colliding: 2345 • Toroid: ON	Anchor

Table 5.8: Part of the dataset collected for estimating the calibration transfer uncertainty in 2023. In the CT fill with proton bunches in trains, run 455899, modules from cells E3 and E4 were divided in to one of two gain families (*low*, set to $0.2\text{ M}\Omega$ and *high*, set to approximately $30\text{ M}\Omega$) to have sensitivity to the entire luminosity range explored in the run. Due to relatively smaller signals in cells A13 and A14, such a configuration was not adopted. The highest luminosity run, run 455924, was used for anchoring the dataset.

The removal of *bad* modules was done for cells E3, E4, A13 and A14 separately following the procedures established in Section 4.2. This accounts to about 15% or less of the total modules for each PMT. In the anchoring run, a calibration constant per *good* module was calculated as the ratio of the Tile current to the track-counting luminosity in the run and used to rescale the Tile currents in all other runs. Anchoring constants were calculated in the LB range 700–1200, choosing only LBs where both the track-counting data and TileCal currents were collected without operational issues. Finally, the ratios of TileCal to track luminosity ratios were derived as the measurement from all good modules average over the LBs. Dedicated run-to-run laser corrections were derived from laser calibrations taken around the runs in the dataset and applied using the procedure outlined in Section 4.2. A summary of the average run-to-run laser corrections for E3/E4 and A13/A14 is shown in Figure 5.14.

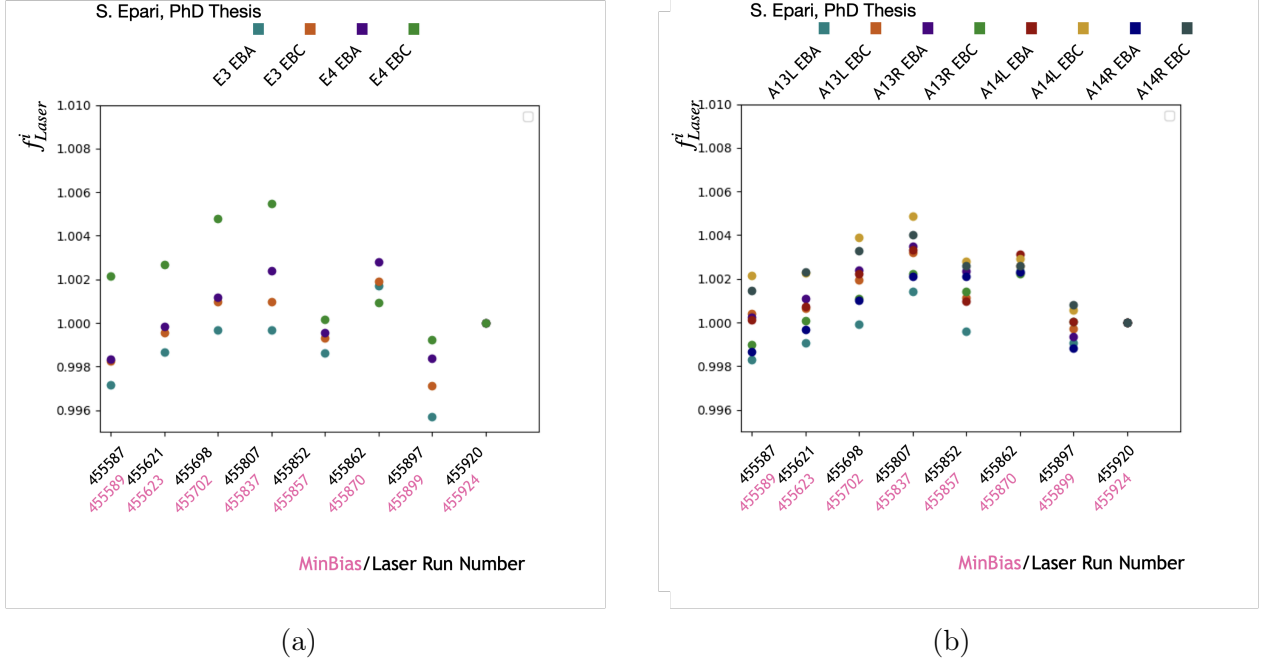


Figure 5.14: Average value of inter-run laser corrections for (a) E3 and E4 cells and (b) A13 and A14 cells. The corrections are derived from laser calibration runs marked in black and the MinBias run(s) to which they are applied is marked in pink. These corrections are applied per module for each PMT. An average of ten laser runs close to the anchoring run was chosen to normalise the data for laser runs used in the analysis.

The ratio of TileCal to track-counting luminosity, with and without run-to-run laser corrections, is shown for cells E3 and E4 in Figure 5.15. For cells A13/A14, shown in Figure 5.16, the average of the measurement from the two PMTs for each cell is used.

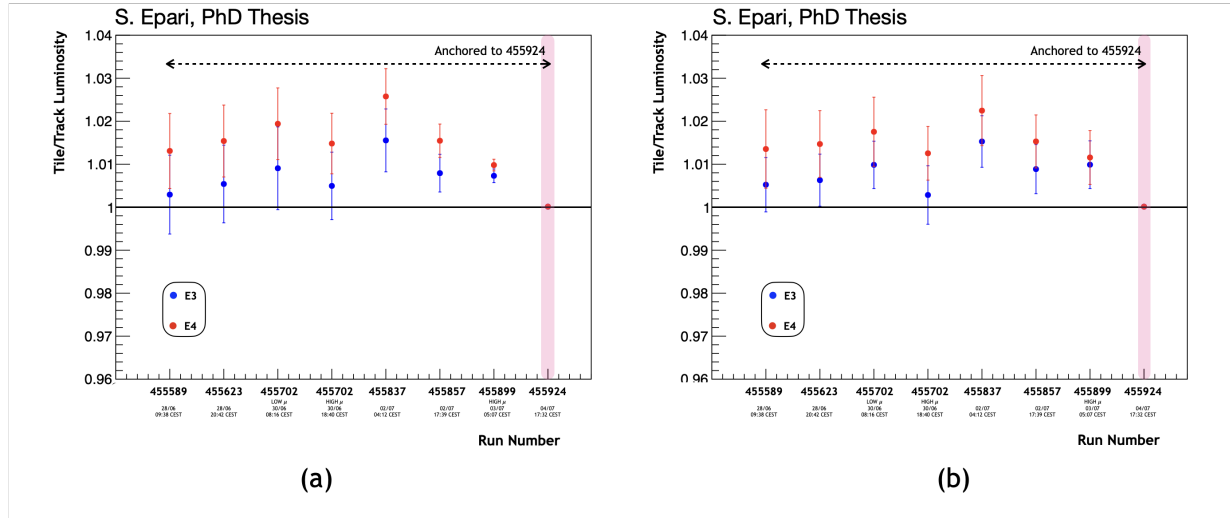


Figure 5.15: Ratio of TileCal to track-counting luminosity for cells E3 and E4 for runs considered to estimate the calibration transfer uncertainty in 2022 (a) before any laser corrections and (b) after run-to-run laser corrections. All instances show improvement on the application of laser corrections. Activation is not accounted for in these figures and can be up to 1% additional signal in the PMTs [68].

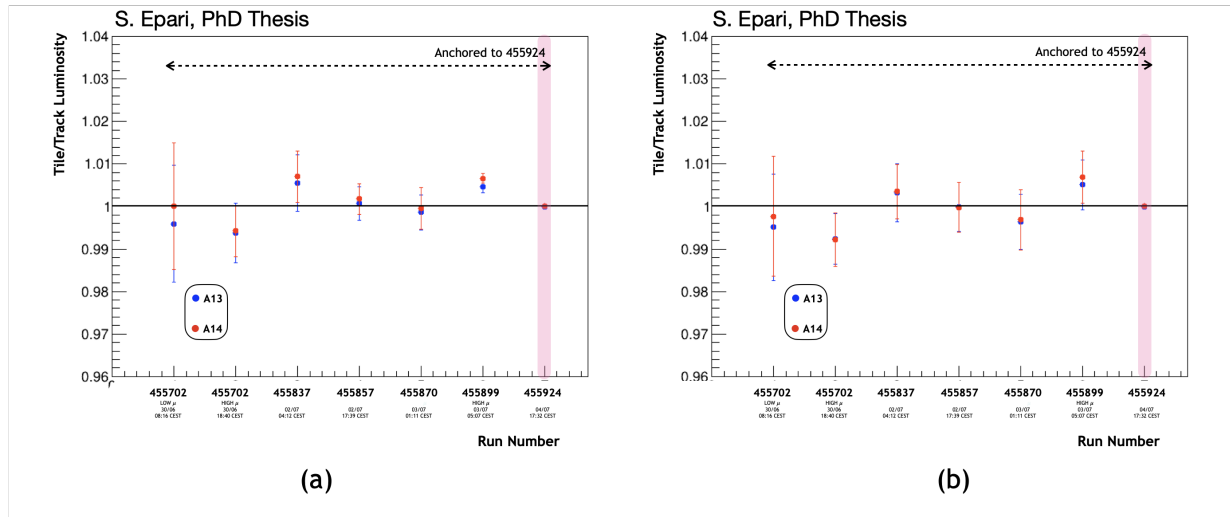


Figure 5.16: Ratio of TileCal to track-counting luminosity for cells A13 and A14 for runs considered to estimate the calibration transfer uncertainty in 2022 (a) before any laser corrections and (b) after run-to-run laser corrections. For each cell, the average of the measurement from the two PMTs is used. All instances show improvement on the application of laser corrections. Activation is not accounted for in these figures and can be up to 1% additional signal in the PMTs [68].

The ratio of TileCal to track-counting luminosity shows great stability and compatibility with unity and improves on the application of laser corrections. The slight increase in standard deviation between the mean measurements of the modules results from the propagation of errors from laser corrections. Activation in Tile cells from the surrounding material is not accounted for in the above plots and can be up to 1% additional signal [68]. At the time of writing this thesis, laser in-gap corrections were not available and have thus not been accounted for in the work. However, no more than 0.3% effect is expected from this correction [68].

The range of shifts in the ratio of TileCal to track-counting luminosity measurement over the used TileCal families was checked over the different runs of the dataset, going from the vdM regime (low- μ , low number of bunches, isolated bunches) to the data taking conditions of physics running (high- μ , large number of bunches, bunch trains), summarised in Table 5.9. The first extrapolation is considers the variation in Tile/Track ratios of A-cells and E-cells, between the CT conditions ($\mu = 0.5$, 140b, isolated bunches in runs 455589 and 455623) and physics conditions ($\mu = 40$, 898b, trains in run 455837) and put an upper limit at 1.1%. The second extrapolation is two step: first, the maximum variation in ratios between the CT fill ($\mu = 0.5$, 140b, isolated bunches in runs 455589 and 455623) and vdM conditions ($\mu = 60$, 140b, isolated bunches in run 455702) is checked, taking into account activation. Second, the extrapolation to physics conditions is considered ($\mu = 40$, 898b, trains in run 455837). The upper limit on this extrapolation stands at about 1.3% taking into account both TileCal cell families. The CT uncertainty is estimated as the maximum upper bound from two extrapolation steps to be 1.1%.

Extrapolation of luminosity calibration	Used cell families	Range of shifts across used cell families
1-step extrapolation		
$(\mu \approx 0.5, 140\text{b, isolated}) \rightarrow (\mu \approx 40, 898\text{b, trains})$	E3, E4, A13, A14	[0.5, 1.1]%
Alternative: 2-step extrapolation		
$(\mu \approx 0.5, 140\text{b, isolated}) \rightarrow (\mu \approx 60, 140\text{b, isolated})$	E3, E4, A13, A14	[-0.7, -0.3]%
$(\mu \approx 60, 140\text{b, isolated}) \rightarrow (\mu \approx 40, 898\text{b, trains})$ (*)	E3, E4, A13, A14	[0.7, 1.3]%
Combined 2-step extrapolation		[0.0, 1.0]%
Upper limit on total extrapolation impact		< 1.1%

Table 5.9: Range of shifts in the ratios of the Tile-calorimeter luminosity and the track-counting luminosity in the CT dataset in 2023 [67]. The selected runs are shown in Tables 5.6, 5.7 and 5.8 and are taken with varying number of simultaneous interactions, number of bunches, and moving from isolated bunches to bunch trains, to extrapolate the calibration of LUCID from vdM to physics conditions. The Tile data has been corrected for residual ambient activation, except for one extrapolation step indicated with (*), where at high μ -values the bias from the activation is considered small. The rounded maximum shifts are used as an upper limit on the impact of the extrapolation on the luminosity calibration. The upper limit on the total impact of the extrapolation from the vdM to the regime of physics data taking is symmetrized and considered as calibration transfer uncertainty.

5.3.2 Long-term stability uncertainty

The long-term stability uncertainty was estimated using runs passing the GRL in 2023 using measurements from EMEC, FCAL and TileCal (D6). Figure 5.17 shows fractional differences between the run-integrated luminosity measured from track-counting and the calorimeters with respect to the baseline LUCID algorithm. All luminosity estimates were normalised in ten runs close to the vdM scan and, as before, the calibration anchoring uncertainty is estimated to be 0.16%.

Next, the variation between the algorithms from the respective subdetectors is checked in the average measurements from this fill and the long-term stability uncertainty is evaluated considering the largest mean deviation across the calorimeter subsystems and track-counting measurements. The results are shown in Figure 5.18. For the 2023 dataset, this uncertainty is estimated to be 0.1%, from the FCAL.

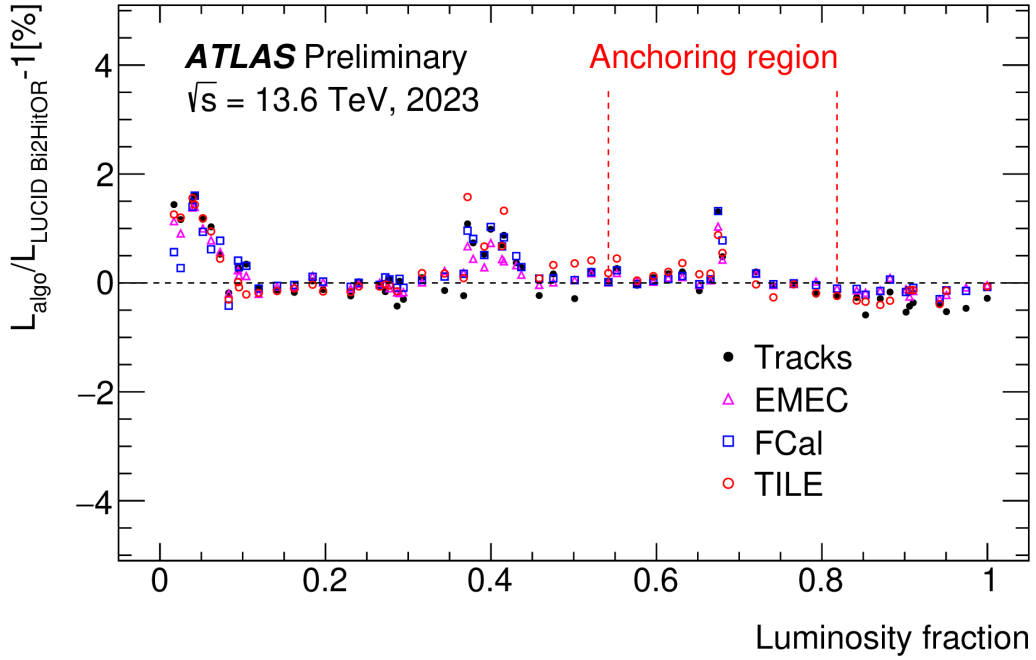


Figure 5.17: Fractional differences in fill-integrated luminosity between the LUCID Bi2HitOR luminosity measurements and the calorimeters and track-counting luminosity algorithm, as a function of the fractional cumulative integrated luminosity in 2023 [67]. The EMEC, the FCAL and the TileCal D6-cells measurements are averages of the respective A-side and C-side algorithms. The anchoring region marks the range of ten fills around the vdM fill used to normalise the calorimeter measurements to track-counting and to evaluate the μ -correction parameters used for the calibration of LUCID to track-counting during physics data taking. The selection of fills is restricted to those passing standard data-quality requirements.

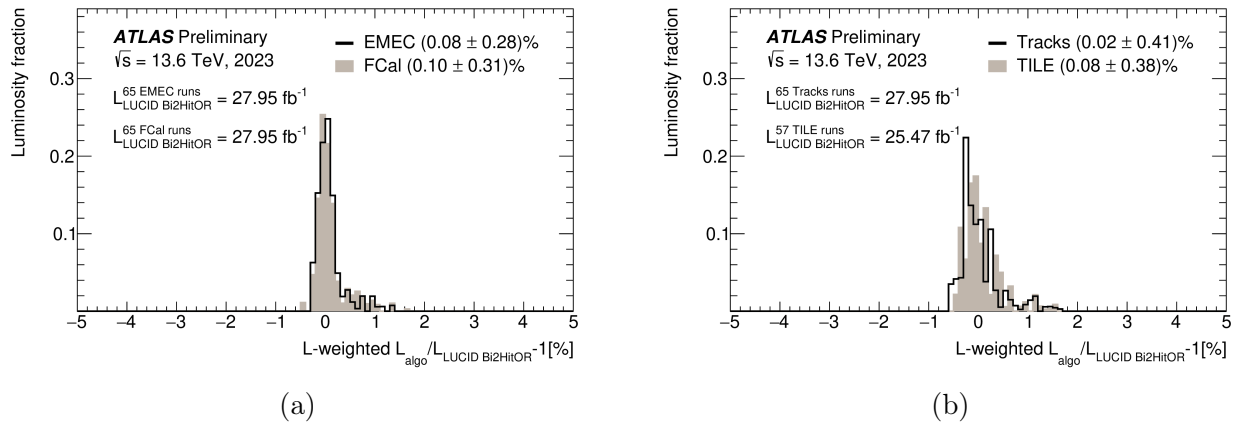


Figure 5.18: Distributions of relative differences in fill-integrated luminosity between the baseline LUCID Bi2HitOR luminosity measurement (weighted by the integrated luminosity in each fill) and (a) EMEC and (b) FCal luminosity measurements (A-side and C-side averages), for 2023 [67]. The selection of fills is restricted to those passing standard data-quality requirements; the quoted integrated luminosity is the one delivered by the LHC, not corrected for ATLAS detector and trigger readiness. The mean and RMS values for each algorithm are indicated in the legend. The largest mean deviation across the calorimeter subsystems and track counting sets the long-term stability uncertainty.

5.3.3 Results

The final uncertainty in luminosity was derived taking into account multiple effects described in the earlier sections, summarised in Table 5.10. The vdM calibration is dominated by non-factorisation effects ($\sim 1.4\%$). The calibration transfer uncertainty (1.1%) has the leading contribution to the total uncertainty (2.04%).

Data sample	2023
Integrated luminosity (fb^{-1})	27.58
Total uncertainty (fb^{-1})	0.55
Uncertainty contributions (%):	
vdM calibration	1.71
Calibration transfer	1.1
Calibration anchoring	0.16
Long-term stability	0.1
Total uncertainty (%)	2.04

Table 5.10: Systematic uncertainties associated with the preliminary luminosity calibration of the 2023 pp data sample at $\sqrt{s} = 13.6$ TeV. The fractional systematic uncertainty is broken down into four main contributions: absolute vdM calibration, the calibration transfer from the vdM to the physics regime, calibration anchoring of the calorimeters for physics runs, and long-term stability of the luminometer response. Table modified from Ref [67].

5.4 Conclusions

This chapter emphasized the role of TileCal in the ATLAS luminosity measurement and presented results of this calibration for the 2022 and 2023 dataset. These results are very crucial because they are necessary in every ATLAS measurement using these datasets. The overall uncertainty in the luminosity determination in 2022 was estimated to be 2.19% (calibration transfer: 1.5% and long-term stability: 0.41%) [69]. The overall uncertainty in the luminosity determination in 2023 was estimated to be 2.04% (calibration transfer: 1.1% and long-term stability: 0.1%) [67]. The 2022 dataset has been reprocessed by all detector subsystems and an update estimate is on the way.

Event simulation

Collisions between proton bunches at the LHC can be rather spectacular and intricate because of the composite structure of the proton. The simulation of pp collisions and interactions of the resulting particles with the detector material serve as a bridge between predictions from theoretical models and experimental observations. They are important in decisions for detector design, choosing trigger menus and offline selections to optimise strategies for maximal signal acceptance. They are also needed to optimize signal-to-background discrimination and for the physics interpretation of the data.

Simulation of pp collisions is a joint effort involving theoretical, experimental and Monte Carlo (MC) based methods. The steps involved in such a simulation is described in this chapter, together with the MC generators used in the analyses in this thesis.

6.1 Simulation of pp collisions

Figure 6.1 illustrates the many processes that happen in a pp collision: the event of interest usually results from inelastic scattering between partons, with its products subjected to the laws of QCD, producing showers of quarks and gluons called a *parton shower*. Low energy quarks and gluons eventually recombine to form colorless states in a process called *hadronisation*. Initial partons involved in the hard scattering can radiate gluons (*initial state radiation*) and so can the products of the hard scatter (*final state radiation*). Partons not involved in the hard scattering can interact and produce additional particles in a process referred to as the *underlying event*. Engines based on pseudo-random numbers, called *Monte Carlo (MC) generators*, are used to simulate individual events and reproduce the predicted kinematics of parton showers, hadronisation and the underlying event. The output is fed to

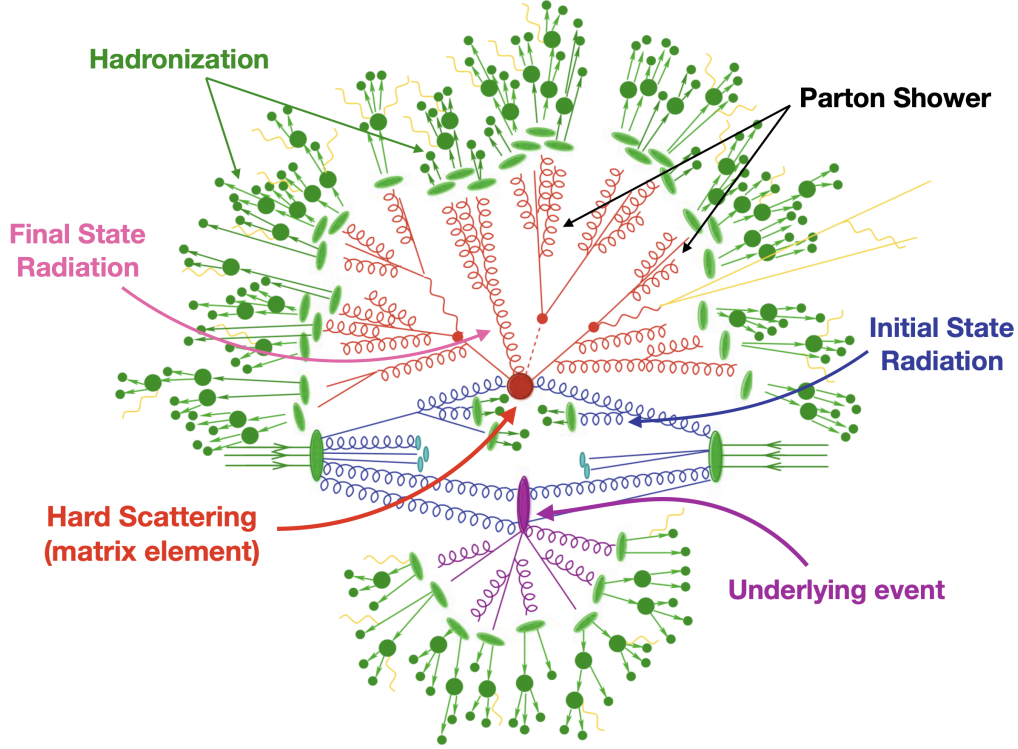


Figure 6.1: Schematic of the processes that take place in a pp collision.

a GEANT [70]-based simulation of the ATLAS detector to mimic experimental signatures seen at the detector.

6.1.1 Parton distribution functions

The factorisation theorem [71] allows the cross-section of a process to be factorised into short and long distance effects at an arbitrary scale called the *factorisation scale* (μ_F). This is shown in Equation 6.1:

$$\sigma_{pp \rightarrow X} = \sum_{a,b} \int dx_a dx_b \text{PDF}(x_a, \mu_F^2) \text{PDF}(x_b, \mu_F^2) \times \hat{\sigma}_{ab \rightarrow X}. \quad (6.1)$$

Here, the sum runs over all parton types that can initiate the process. The *parton density function* (PDF) encodes the probability of finding a parton of type i inside the proton, carrying a fraction x_i of the proton's momentum. PDFs are universal, scale-dependent functions and determined from deep-inelastic scattering and collider experiments. The evolution of PDFs as a function of the energy scale μ is determined by the *Altarelli-Parisi*

equations (DGLAP) [72]:

$$\frac{\partial q_i(x, \mu^2)}{\partial \ln \mu^2} = \frac{\alpha_s(\mu)}{2\pi} \int_x^1 \frac{dz}{z} \left[P_{qq}(z) q_i\left(\frac{x}{z}\right) + P_{qg}(z) g\left(\frac{x}{z}\right) \right], \quad (6.2)$$

$$\frac{\partial g(x, \mu^2)}{\partial \ln \mu^2} = \frac{\alpha_s(\mu)}{2\pi} \int_x^1 \frac{dz}{z} \left[P_{gq}(z) \sum_{i=1}^{n_f} q_i\left(\frac{x}{z}\right) + P_{gg}(z) g\left(\frac{x}{z}\right) \right], \quad (6.3)$$

where q_i and g are the the quark and gluon PDFs respectively and x corresponds to the momentum fraction of the parton. The function P_{ij} are called *splitting functions*, used to describe the probability of an outgoing parton j to be emitted by an initial parton i . The splitting functions are given by:

$$P_{qq}(z) = C_F \left(\frac{1+z^2}{1-z} \right)_+,$$

$$P_{qg}(z) = \frac{1}{2} (z^2 + (1-z)^2),$$

$$P_{gq}(z) = C_F \left(\frac{1+(1-z)^2}{z} \right),$$

$$P_{gg}(z) = 2N_c \left(\frac{z}{(1-z)_+} + \frac{1-z}{z} + z(1-z) \right) + \frac{11N_c - 4(0.5)n_f}{6} \delta(1-z),$$

where n_f is the number of active quark flavors, and for a $SU(N_c)$ theory, the following definition is used:

$$C_F = \frac{N_c^2 - 1}{2N_c},$$

and the $+$ distribution is defined as

$$\int_0^1 dz \frac{f(z)}{(1-z)_+} = \int_0^1 dz \frac{f(z) - f(1)}{1-z}.$$

A leading collaboration that measures PDFs is the NNPDF Collaboration [73]. PDFs determined by this collaboration are widely used in physics analysis, shown in Figure 6.2.

In Equation 6.1, the parameter $\hat{\sigma}_{ab \rightarrow X}$ is the partonic cross-section at a centre-of-mass energy $\sqrt{\hat{s}} = \sqrt{s} \sqrt{x_a x_b}$, where $\sqrt{s}$ is the centre-of-mass energy of the pp collision. This factor is dependent on μ_F and an additional scale, the *renormalisation scale* (μ_R),

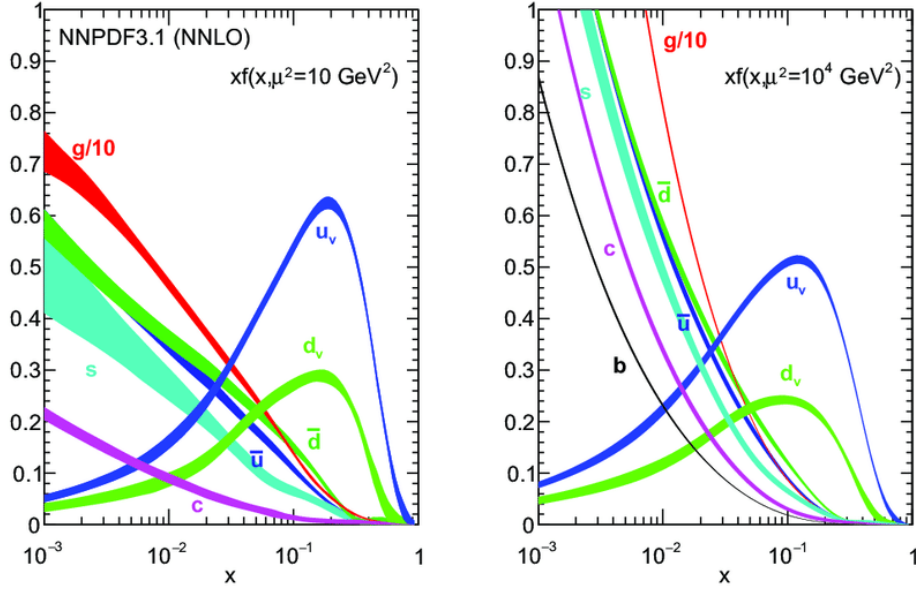


Figure 6.2: PDFs as determined by the NNPDF Collaboration for $Q^2 = 10 \text{ GeV}^2$ (left) and $Q^2 = 10^4 \text{ GeV}^2$ (right). Figure taken from Ref. [73].

which is introduced to resolve logarithmic divergences that appear while computing loop diagrams representing the amplitude. The dependence on μ_F vanishes once the calculation is performed at all orders in perturbation theory.

6.1.2 Matrix-element calculation

The partonic cross-section, $\hat{\sigma}_{ab \rightarrow X}$, is calculated using the *Matrix-element*, which describes the transition from an initial to a final state in a parton interaction, shown in Equation 6.4.

$$\sigma_{ab \rightarrow X} \sim \sum_k \int d\Phi_{X+k} \left| \sum_l \mathcal{M}_{X+k}^l \right|^2 \quad (6.4)$$

Here, $d\Phi_{X+k}$ represents the phase space of the configuration with k real emissions. The sum over k corresponds to the sum of the additional real emissions that can occur and the sum over l is the sum over the number of virtual loops. The matrix-element, $\mathcal{M}_{X+k}$, is computed as the sum of the Feynman diagrams resulting in a final state with k real emissions and l virtual loop corrections.

Various fixed order calculations in perturbative QCD use different values of k and l :

- A leading order (LO) calculation for the production of X corresponds to $k = l = 0$.
- A leading order (LO) calculation for the production of X with n jets corresponds to $k = n, l = 0$.
- Setting $k + l \leq n$ gives the calculation at $N^n\text{LO}$ for X , including $N^{n-1}\text{LO}$ for $X+1$ jet, $N^{n-2}\text{LO}$ for $X+2$ jets and so on up to LO for $X + n$ jets.

For a fixed-order calculation, the integral is modified to be restricted to the energy scale μ_R . The remaining part of the phase space is used in the next stage: the *Parton Shower*.

6.1.3 Parton shower

A *Parton Shower* (PS) is described as the iterative emission of quarks and gluons from partons in the initial or final state, forming collimated sprays of strongly interacting particles. Theoretically, the differential cross-section of the production of an additional parton ($d\sigma_{n+1}$) is related to the n -parton differential cross-section ($d\sigma_n$) by Equation 6.5.

$$d\sigma_{n+1} \approx d\sigma_n \frac{\alpha_s}{2\pi} \frac{d\mu^2}{\mu^2} dz P_{ij}(z), \quad (6.5)$$

where α_s is the strong coupling constant and P_{ij} are the splitting functions. This approximation assumes an almost collinear splitting of the initial partons in to two, called the *soft and collinear regime*.

In MC simulation, the parton shower is implemented by repeatedly applying the *Sudakov form factors*, which represent the probability that a parton evolves from an initial scale q_1 to a lower scale q_2 without splitting, shown in Equation 6.6.

$$\Delta_i(q_1^2, q_2^2) = \exp\left(-\sum_j \int_{q_2^2}^{q_1^2} \int_{z_{min}}^{z_{max}} dP_i(z, q^2)\right). \quad (6.6)$$

For final state showers, the procedure stops when the energy scale drops below the hadronisation scale (~ 1 GeV). For initial state showers, the procedure is evolved backwards, starting at the correct parton momentum for the hard scatter. Overlap between the ME and PS part of the simulation are addressed with dedicated ME-PS matching algorithms. Two widely used algorithms for this are the Catani-Krauss-Kuhn-Webber (CKKW [74]) and the Michelangelo L. Mangano (MLM [75]) algorithms. The CKKW algorithm clusters

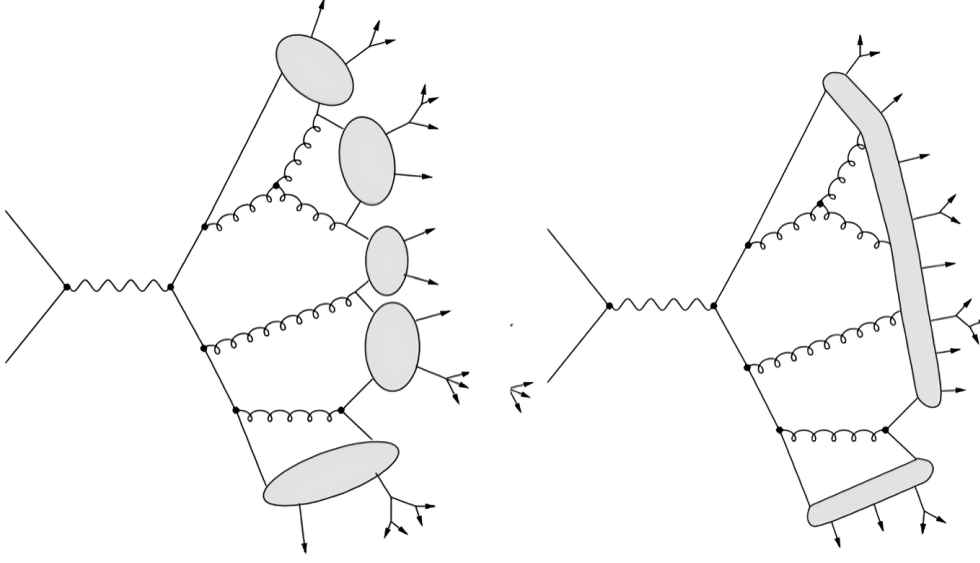


Figure 6.3: Illustrative sketch of the (a) Lund String fragmentation and (b) Cluster hadronisation models. Figure taken from Ref. [78].

partons into jets using a jet algorithm followed by reclustering of jets by merging parton shower emissions that are not already included in the fixed-order ME calculation. The ME and PS components are finally weighted and merged to obtain a coherent description of multi-jet final states. The MLM algorithm, on the other hand, focuses on reducing the double counting of emissions by rejecting parton shower emissions that are already described by the matrix-element calculation. It also starts with clustering of partons into jets using a jet algorithm. Then, it rejects parton shower emissions already covered by the matrix-element calculation, thus reweighing and merging the ME and PS components. This algorithm has reduced dependence on tuning parameters.

6.1.4 Hadronisation

Hadronisation is the formation of bound states of quarks and gluons when their energy drops below the hadronisation scale (~ 1 GeV). These dynamics follow non-perturbative QCD. Two commonly used hadronisation models are the *Lund String Fragmentation model* [76] and the *Cluster Hadronisation model* [77], illustrated in Figure 6.3.

The Lund String Fragmentation model is based on the concept of color confinement, where quarks and antiquarks are connected by color flux tubes or *strings* as they move apart. As the strings stretch and the energy increases, they can break to produce additional quark-antiquark pairs leading to the fragmentation of partons into hadrons. Hadronisation

occurs through the fragmentation of these strings into color-neutral hadrons. The fragmentation process is governed by the *Lund string fragmentation function*, which describes the probability distribution of hadron production along the string.

In the Cluster Hadronisation Model, also known as the *Webber Cluster Model*, partons produced in high-energy collisions are clustered into color-singlet clusters through the emission of soft gluons. These clusters represent the color-neutral hadronising objects that subsequently decay into observed hadrons. The model emphasizes the role of soft gluon interference effects in the hadronisation process. These interference effects influence the angular and momentum distributions of the emitted partons and play a crucial role in determining the final state hadron spectra.

6.1.5 Underlying event, multiple parton interactions and pileup

Soft interactions between spectator partons in the hard collision form the *underlying event*. They are usually seen as soft jets in the beam direction and estimated using experimental data [79]. If multiple hard scattering occur in the same bunch crossing, this is referred to as *Multiple Partons Interactions* (MPIs) and signature of these processes are back-to-back jets with little total transverse momentum. The fraction of such processes is typically small and computed in the perturbative regime. Finally, interactions of multiple protons either in the same bunch crossing (*in-time*) or previous or subsequent bunch crossings (*out-of-time*) are referred to as *pileup*. Soft interactions arising due to in-time pileup are modelled with similar techniques to those used for the underlying event while for out-of-time pileup, additional elements are incorporated in the computation to account for the detector response and signal processing.

6.2 Monte Carlo generators

Dedicated software tools based on Monte Carlo methods, called *Monte Carlo generators*, are used for the simulation of either part or the entirety of the chain described in Section 6.1.

General-purpose MC generators simulate the entire collision chain, starting from the matrix-element computation to the hadronisation process. They can either be used stand-alone or interfaced to dedicated generators for improved accuracy in parts of the simulation chain.

The following general-purpose MC generators are used in the analyses presented in this thesis:

- PYTHIA [80] is a general-purpose event generator for simulating the full event evolution including initial and final state radiation, multiple parton interactions, hadronization and underlying event activity. matrix-element calculation for $2 \rightarrow n (n \leq 3)$ processes is performed with LO precision and hadronisation is carried out following the Lund String model.
- HERWIG [81] is another general-purpose event generator that performs LO matrix-element calculation for $2 \rightarrow 2$ processes. The hadronisation and underlying event activity is modelled following the cluster model. Additionally, the parton shower simulation includes full spin correlation for all partons, which leads to more accurate computation than PYTHIA, since it includes gluon splitting asymmetries in the collinear approximation. It is often used alongside PYTHIA to cross-check results and explore different modeling approaches.
- SHERPA [82] computes matrix-elements for the process $F + k$ at NLO precision for $k \leq 2$ and at LO precision for $k \leq 4$. It includes its own parton shower based on the Catani-Seymour dipole formalism [83] and ME-PS matching using an improved version of the CKKW algorithm.

Matrix-element (ME) generators are specialised for providing accurate ME calculations. Some of the common ME generators are:

- POWHEG-BOX [84] is used to generate events with matrix-element computations at NLO accuracy and provides a systematic approach for matching NLO calculations with parton shower simulations. It can thus be interfaced to general purpose MC generators like PYTHIA or HERWIG to model the parton shower, hadronisation and underlying event.
- MADGRAPH5_AMC@NLO [85] is an alternative generator for matrix-element computation at NLO accuracy and matching them to parton shower simulations using the MLM algorithm. It is also interfaced to general purpose MC generators like PYTHIA or HERWIG to model the parton shower, hadronisation and underlying event.

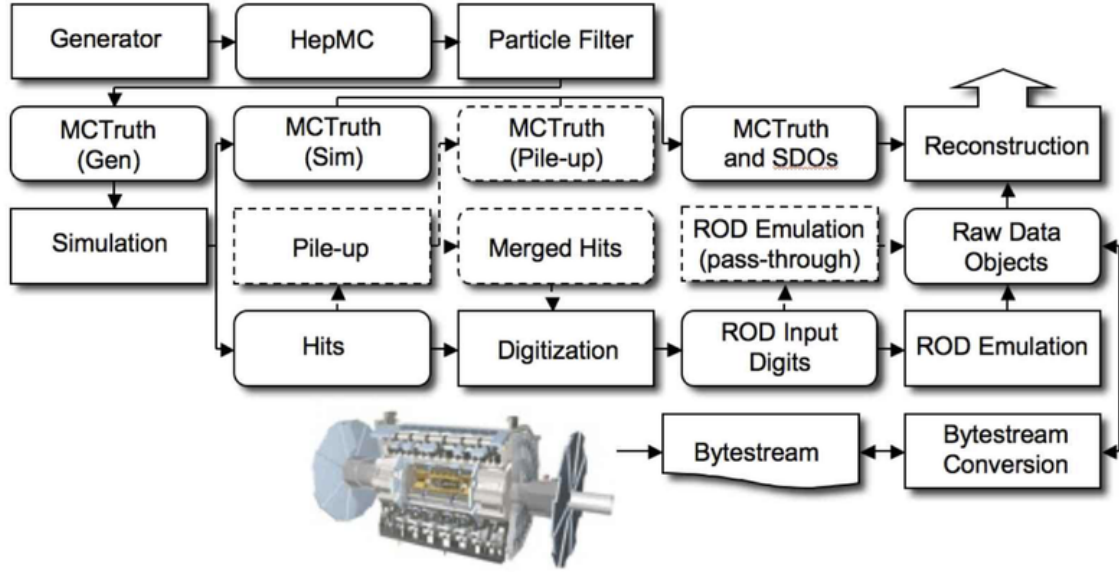


Figure 6.4: Schematic of ATLAS simulation software, from event generation to reconstruction. Figure taken from Ref. [89].

Special purpose generators may be used in addition to the above to improve modelling in specific stages of event generation. Some examples of such generators are:

- EVTGEN [86] is a MC generator that includes dedicated algorithms for modelling semi-leptonic and CP-violating decays. It is often interfaced with PYTHIA and HERWIG after the PS and hadronisation to describe decay chains of B and D mesons.
- MADSPIN [87] is used for modelling heavy resonance decays, taking in to account spin correlations among the decay products and off-shell corrections. It is used after the ME of the processes is estimated by MADGRAPH.

6.3 Simulation of the ATLAS detector

The output of MC generators is a four-momenta for all stable particles in the event, encoded in a format called HEPMC [88]. Events at this level cannot be compared to real data collected by the ATLAS detector but can be used to study kinematics of specific processes. For comparing these to real data, a simulation of the ATLAS detector is carried out by means of the GEANT4 [70] package which can efficiently reproduce effects arising from interactions with matter. This process is shown in Figure 6.4.

Stable particles from MC generators are interfaced to GEANT4 to reproduce interactions with all detector sub-systems and recorded as detector hits. The hits are digitised to emulate the response of the read-out detector electronics. All Level-1 algorithms configured in the trigger menu are simulated based on the digitised signals with an accept decision for each. The output object, called a *Raw Data Object*, is used to compute decisions of the High Level Trigger and as input for object reconstruction (Chapter 7).

Simulation of the ATLAS detector can be performed including a full description of all particles with matter called ATLAS Full Simulation (FullSim)[89] or with a simplified detector response, called ATLFAST-II (AFII) [90], for a computationally cheaper alternative. AFII reproduces the behaviour of calorimeters using a fast calorimeter simulation (FastCaloSim) where the calorimeter response is replaced by a detailed parameterization of the shower shapes, while using the full GEANT4 simulation for the trackers. A version of AFII called ATLFAST-IIF [91] uses a simplified version of the trackers through fast ATLAS tracking simulation (FATRAS).

Samples produced at this stage are called Monte Carlo samples, usually normalised to the highest-order available theoretical cross-section. Due to the different pileup conditions for each data-taking year, the MC samples are generated in three campaigns: *mc16a*, which reproduces the pileup conditions of the data taking periods 2015 and 2016, *mc16d* for the year 2017 and *mc16e* for 2018. Additional weights are applied to correct MC to the recorded luminosity. Further, in some cases, the parton level distributions may be used to derive further reweighting factors to match existing higher-order differential cross-section predictions. An example of this is described for the nominal and alternate $t\bar{t}$ MC in Chapter 10. Finally, residual effects from inaccuracies in reconstruction and identification of physics objects are corrected to data using dedicated scale factors.

Reconstruction and identification of physics objects

Particles produced in collisions traverse the various subdetectors of ATLAS and leave distinct signatures such as hits and energy deposits, detected as raw signals by the readout systems. This chapter describes techniques used to translate raw signals to physics objects used in the analyses described in this dissertation. The reconstruction of tracks and pp interaction vertices is covered in Section 7.1. Section 7.2 describes light lepton reconstruction, Section 7.4 describes jet reconstruction, calibration and tagging algorithms and Section 7.5 describes the reconstruction of hadronically decaying τ -leptons. Finally, Section 7.6 describes the estimation of missing transverse energy in an event.

7.1 Track and vertex reconstruction

The inner detector (ID) is immersed in a solenoid magnetic field of 2 T, as described in Section 3.2. Charged particles follow a helical trajectory in the ID, leaving hits in the Insertable B-Layer (IBL), the silicon detectors, and the Transition Radiation Tracker (TRT). These hits allow for reconstruction of the particle's path known as a *track* while curvature of the particle's trajectory provides information about its charge and transverse momentum (p_T). The ID is capable of reconstructing charged particles with $p_T > 500$ MeV within $|\eta| < 2.5$.

A particle track is characterized with respect to a reference point, usually taken as the average position of pp interactions in the detector. A track is defined in terms of five parameters with respect to the reference point, as depicted in Figure 7.1:

- d_0 : *transverse impact parameter*, defined as the closest point in the transverse plane to the reference point.
- z_0 : *longitudinal impact parameter*, defined as the closest point in the longitudinal plane to the reference point.
- ϕ, θ : azimuthal and polar angles respectively.
- q/p : ratio of the reconstructed track charge (q) to momentum (p).

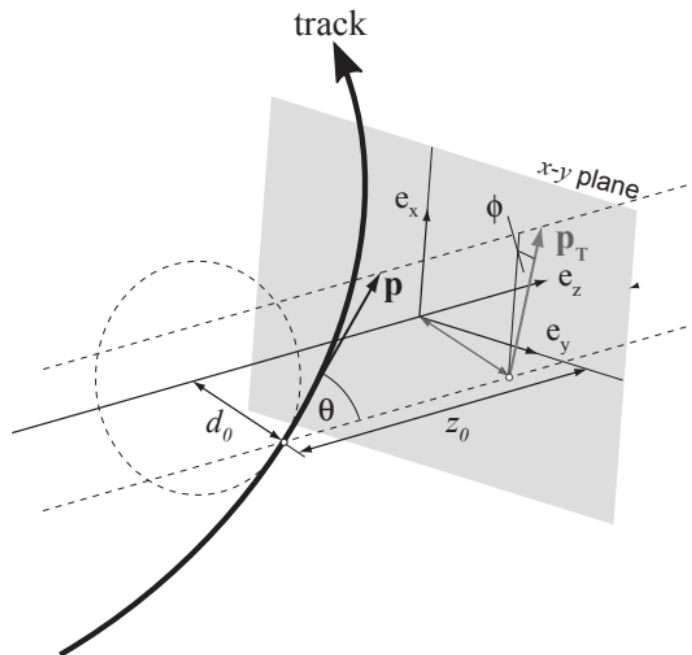


Figure 7.1: Illustration of global parameters of a particle track. The reference point is taken as the average position of pp interactions in the detector. Figure taken from Ref. [92].

The first hit is typically registered in the IBL, closest to the beam pipe. Tracking begins with combining signals from adjacent channels in the silicon detectors into clusters called as *hits*. These clusters are converted into three-dimensional space-points with position uncertainties determined by the detector geometry and sensor pitch. There are two main techniques to reconstruct tracks in ATLAS: the *inside-out* approach, where tracks are

seeded in the silicon detectors and grown outwards to the TRT, and the *outside-in* approach where TRT segments are used as the starting point.

Inside-out tracking algorithm

ATLAS Primary Tracking

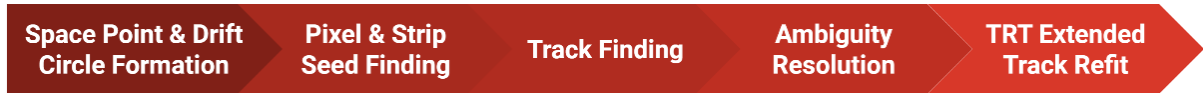


Figure 7.2: Sequential stages of the inside-out tracking algorithm which initiates track reconstruction from seed points within the silicon subdetectors. Figure taken from Ref. [92].

The *inside-out* approach [93], depicted in Figure 7.2, begins by generating track seeds using triplets of space-points from either of the silicon subdetectors followed by a preliminary estimation of the track parameters. Subsequently, the track seed undergoes extension via a window search employing a combinatorial Kalman filter. Seeds that fail initial track finding are checked for compatibility with the calorimeter. If a seed falls within a defined *Region of Interest (RoI)* in the calorimeter, the track finding process is repeated to accommodate an additional kink in the track. This is valuable for recovering electrons that have undergone Bremsstrahlung radiation. Track candidates identified at this stage are subjected to an ambiguity solver to resolve overlaps between track candidates and discard erroneous combinations of clusters. A limited number of shared hits is allowed to maintain optimal performance in dense topologies, such as the core of high-energy jets. Finally, a χ -squared global fit is executed for the track candidates to obtain a refined, high-precision estimate of the track parameters. In the concluding phase of this algorithm, an extension to the TRT is attempted using a Kalman filter and if successful, the global χ -squared fit is reiterated. Tracks with silicon-only hits are retained if the addition of TRT hits deteriorates the fit quality.

Outside-in tracking algorithm

The *outside-in* approach [92], illustrated in Figure 7.3, is used to enhance the acceptance of particles originating farther from the beam pipe, such as electrons resulting from photon conversions. TRT segments compatible with a RoI in the calorimeter serve as seeds for this algorithm. Segments are extended using two space-points from the silicon subdetector

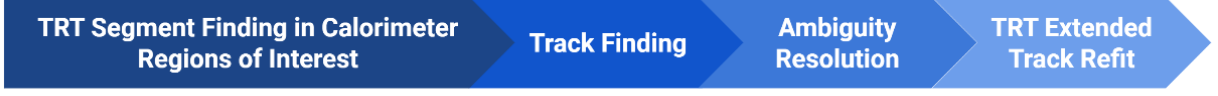
ATLAS Back-Tracking

Figure 7.3: Sequential stages of the outside-in tracking algorithm. This approach is seeded from leftover TRT hits within electromagnetic calorimeter RoIs. Figure taken from Ref. [92].

layers nearest to the TRT and developed into track candidates through the application of the Kalman filter, followed by an ambiguity resolution step, and ultimately a global chi-square fit.

Special tracking algorithms

In addition to the previously discussed tracking approaches, ATLAS employs two specialized algorithms tailored for specific scenarios, utilizing leftover hits from the primary tracking processes [94]. The first algorithm focuses on pixel-only short *tracklets* which are particularly adept at reconstructing muons in the forward region and short-lived decaying charged particles. The second algorithm, known as *large radius tracking*, is specifically designed to reconstruct tracks with extremely large transverse impact parameters. This capability is particularly relevant for searches involving long-lived particles and has been integrated into the default ATLAS track reconstruction framework for Run 3.

Reconstructed tracks are separated into two sets depending on the quality criteria satisfied by them. These two sets of tracks are called the *Loose* and *Tight Primary* tracks. *Loose* are required to have $p_T > 400$ MeV, $|\eta| < 2.5$, at least 7 hits in the silicon tracking layers, no more than one shared module between the hits and less than or equal to two (one) missing hits in the silicon (pixel) detectors. *Tight Primary* tracks are required to satisfy the requirements for *Loose* tracks, in addition to no missing hits in the pixel layers, at least one hit in the inner most pixel layers, and at least 9 (11) hits in the silicon layers if the track lies within $\eta \leq 1.65$ ($\eta \geq 1.65$). The efficiency of the track reconstruction algorithms is measured separately in simulated minimum bias events for both sets of tracks, as a function of the truth track p_T and η , given by:

$$\text{Eff}(p_T, \eta) = \frac{N_{\text{reco}}^{\text{matched}}(p_T, \eta)}{N_{\text{gen}}(p_T, \eta)}, \quad (7.1)$$

where $N_{\text{reco}}^{\text{matched}}(p_T, \eta)$ is the number of reconstructed tracks matched to truth charged particles and $N_{\text{gen}}(p_T, \eta)$ is the number of truth charged particles in that range. The

tracking efficiency is shown in Figure 7.4. Lower track reconstruction efficiency $|\eta| > 1$ is due to increasing amount of material traversed by the particle in these regions, leading to multiple scattering and energy loss. For $|\eta| > 2$, the efficiency increases due to an increase in the number of sensitive silicon layers. Above $p_T > 500$ GeV, the efficiency plateaus at about 90% (85%) for the *Loose* (*Tight Primary*) selections.

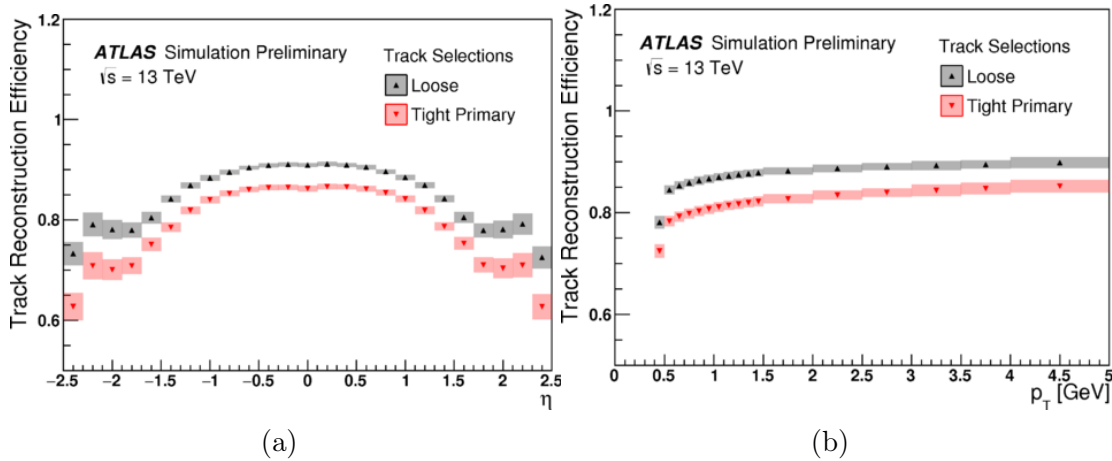


Figure 7.4: Track reconstruction efficiency for *Loose* and *Tight Primary* track selections as a function of truth (a) η and (b) p_T of the track, measured using minimum bias simulated events. Figures taken from Ref. [95].

Vertex reconstruction

After all track candidates have been identified, the location of pp interaction vertices are determined to identify the interaction with the highest energy, known as the *hard scatter interaction*. This process involves two main steps: vertex finding and vertex fitting [96]. For vertex finding, initial vertex candidates are constructed by identifying global maxima in the z -distributions of track coordinates for tracks passing strict quality criteria. Subsequently, a weighted adaptive Kalman filter is used to fit sets of nearby tracks to each vertex candidate simultaneously. The output of this step is a list of three-dimensional vertex positions and covariance matrices. *Primary Vertices* are identified as vertex candidates with at least two associated tracks with $p_T > 500$ GeV that are consistent with originating from the beam collision region in the x - y plane. The hard-scatter interaction is determined as the vertex with the largest sum of squared transverse track momenta.

7.2 Electron reconstruction

Electrons travelling through the detector leave one or more tracks in the ID and develop electromagnetic showers in the electromagnetic calorimeter (ECAL). Energy clusters are identified from *topoclusters*, which are three-dimensional clusters of calorimeter cells formed using a nearest-neighbor algorithm. Topocluster *seeds* are identified as calorimeter cells with a readout signal (E) four times higher than the electronic and pileup noise (σ) [97]. Following this, adjacent cells with $E > 2\sigma$ are added to the seeds in an iterative manner. In a subsequent step, cells with $E > 0$ are included. This process is visually illustrated in Figure 7.5. Topoclusters with two or more local maxima with $E > 500$ MeV are expected to originate from the merging of decays of different particles close to the calorimeter and are thus split in three dimensions to form separate clusters.

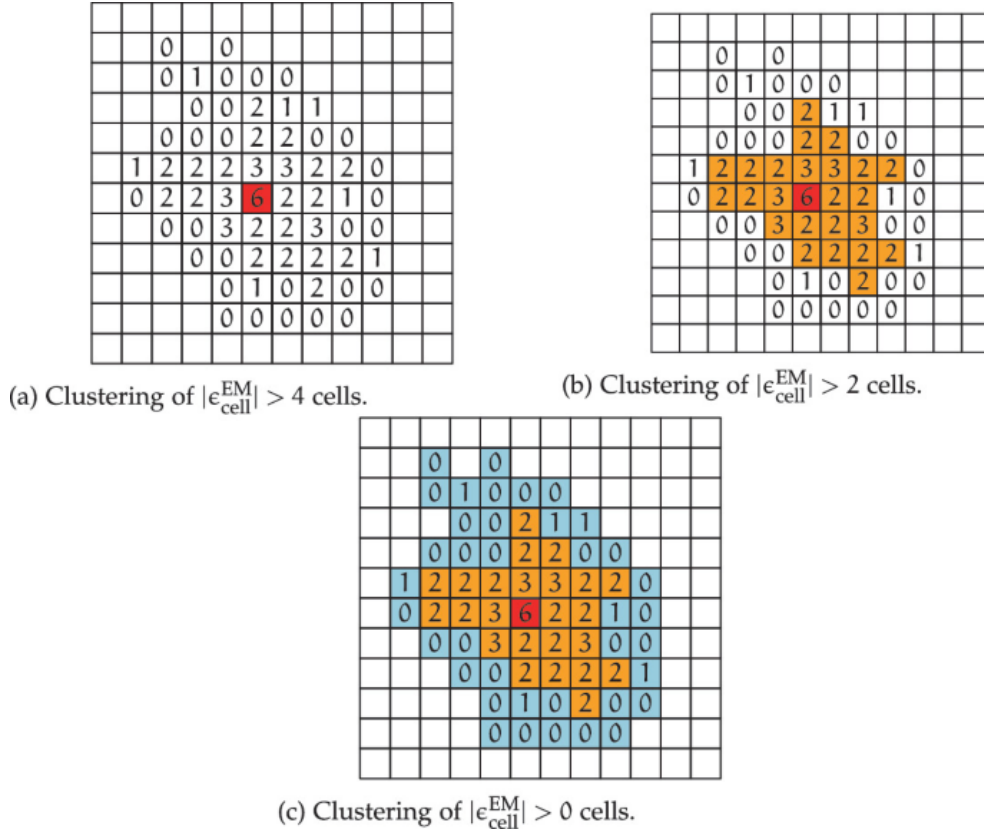


Figure 7.5: Schematic representation of topocluster formation. Figure taken from Ref. [98].

Topoclusters are initially calibrated to the electromagnetic (EM) scale to give the same response as for electromagnetic showers from electrons or photons. Electron *seeds* are identified as topoclusters with $E_T > 1$ GeV and a matched track in the ID consisting of at

least four hits in the silicon detectors. Next, satellites for electron seeds, by searching for energy deposits in a $\eta \times \phi = 0.075 \times 0.125$ window about the seed bary-centre. To recover electrons from photon conversions, a broader window of 0.125×0.300 is used. Seed clusters with their associated satellite clusters are called *superclusters* [99]. After the formation of superclusters, electron candidates are calibrated in a multi-step procedure.

Electron identification

Electron identification is performed using a likelihood (LH) discriminant built from information on the track quality, the longitudinal and lateral development of the electromagnetic shower and cluster-track matching. This discriminant is defined in Equation 7.2.

$$d = \frac{\mathcal{L}_S}{\mathcal{L}_S + \mathcal{L}_B} \quad \text{with} \quad \mathcal{L}(\vec{x}) = \prod_{i=1}^n P_i(x_i) \quad (7.2)$$

Here, $\mathcal{L}_S$ and $\mathcal{L}_B$ are the LH functions for the signal and background respectively defined using the respective PDFs ($P(x)$) and the sum runs over the set of variables used for the identification of electrons compared to the background.

Background PDFs are extracted from dijet samples for high-momentum electrons and from minimum bias events for low-momentum electrons. Signal PDFs are extracted in the same regimes from simulated $Z \rightarrow ee$ and $J/\psi \rightarrow ee$ events respectively.

Based on the minimum of the likelihood discriminant, three working points (WPs) called *Loose*, *Medium* and *TightLH* are defined, ordered according to increase in electron signal purity. The *Medium* and *TightLH* WPs are used in the analyses in this thesis. These WPs are optimized in bins of E_T and η with average electron efficiencies of 98%, 90% and 80%, respectively, shown in Figure 7.6.

Electron isolation

Electrons originating from prompt processes are expected to be more isolated from nearby activity compared to those from hadronic decays or photon conversions. The isolation of an electron is quantified by defining working points, using both calorimeter and track isolation based quantities. Calorimeter-based isolation defines the sum of energy clusters in the ECAL in a cone of $\Delta R = 0.2$ around a track-matched electron cluster. Track-based isolation defines the scalar sum of transverse momentum of tracks within a p_T -dependent cone of size $\Delta R = \min(0.2, 10\text{GeV}/E_T)$. The loosest isolation requirement, called *FCLoose*,

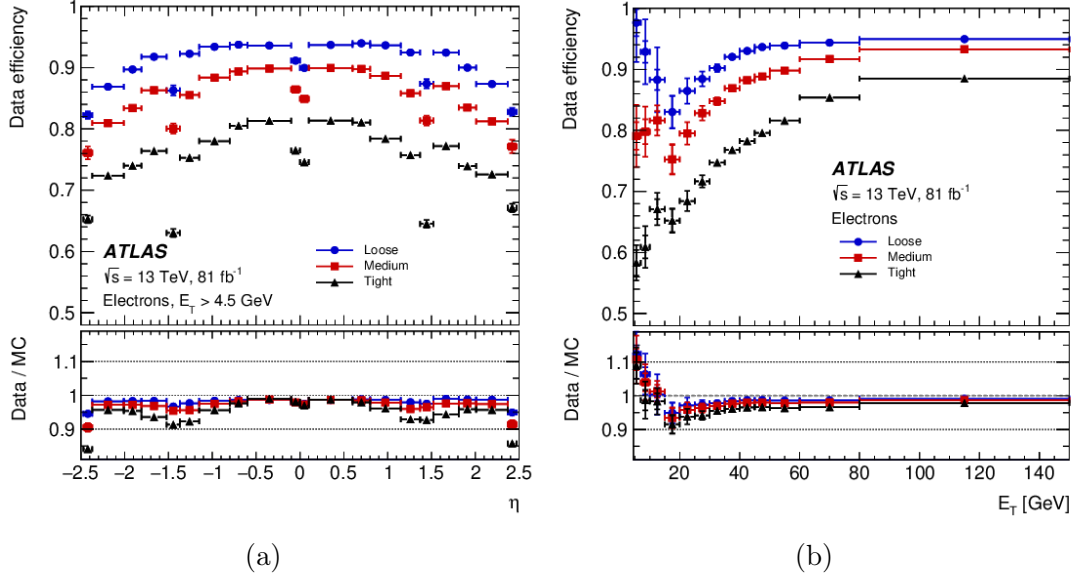


Figure 7.6: Electron identification efficiency for the *Loose*, *Medium* and *TightLH* working points as a function of (a). E_T and (b). η . Figures taken from Ref. [99].

has an efficiency of about 99% and is used in the analyses in this thesis. It corresponds to an E_T cone of less than 0.2 and p_T cone of less than 0.15.

The rejection of non-prompt leptons from semi-leptonic b - or c -decays is improved using a boosted decision tree (BDT) discriminant called the PromptLeptonImprovedVeto (PLIV) [100]. Such heavy flavor hadrons are usually embedded within jets, with decay vertices displaced from the primary vertex. Thus isolation cones described above might fail to collect high p_T tracks from such decays, and thus fail to identify the non-prompt lepton. This situation is shown schematically in Figure 7.7, where the high p_T track from the semi-leptonic decay is missed by the isolation cone. Also shown is an alternative scenario with a larger radius that collects the said track to be included in the analysis.

The PLIV BDT is trained with information on variables related to the track-jet that matches the selected lepton, isolation and p_T of the lepton candidate and variables related to the hadron lifetime. The complete list of variables used is shown in Table 7.1. Three separate BDTs are trained separately for identifying non-prompt muon, electrons in the central region and electrons in the forward region.

Three exclusive PLIV working points are introduced as a function of lepton p_T : *Tight*, *VeryTight* and *Tight-not-VeryTight*, allowing selection efficiencies of about 60% (60%/70%) for leptons with $p_T \approx 20$ GeV and plateauing at 95% (95%/90%) for leptons with $p_T \approx 40$ (40/65) GeV.

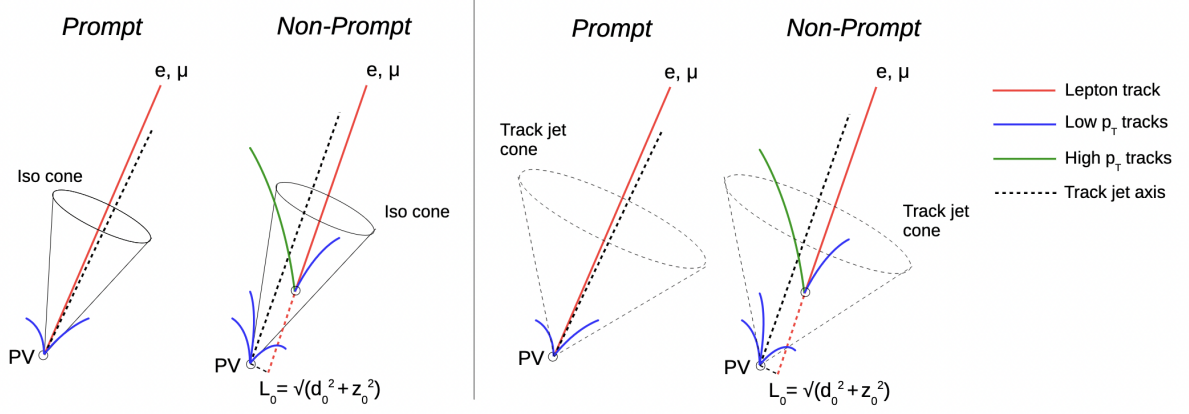


Figure 7.7: Schematic of non-prompt lepton candidates that pass basic impact parameter (d_0, z_0) and isolation cuts. L_0 corresponds to the secondary vertex decay length from the primary vertex (PV). Figure taken from Ref. [100].

Variable	Description	PLIV BDT (μ)	PLIV BDT (e)
PromptLepton RNN	RNN using track impact parameters and other variables related to track jet and lepton	Y	Y
$l_{SV \text{ to PV}}^{\text{longitudinal}}$	Secondary vertex longitudinal significance using tracks with $p_T > 500$ MeV	Y	Y
$p_T \text{ VarCone30}/p_T$	Lepton isolation using ID tracks within cone of $\Delta R < 0.3$	-	Y
$p_T \text{ Cone30TightTTVA500}/p_T$	In addition to $p_T \text{ VarCone30}/p_T$, cuts on track $p_T < 0.5$ GeV and pass loose vertex association requirement	Y	-
$E_T \text{ TopoCone30}/p_T$	Lepton isolation using topological clusters within cone of $\Delta R < 0.3$	Y	Y
$E_{\text{cluster}}^{\mu}/E_{\text{expected}}$	Relative muon calorimeter cluster energy	Y	-
$\sum_{\text{cluster}} dR < 0.15 E_T/p_T$	Sum of cluster energy divided by lepton p_T	-	Y
N_{track} in track jet	Number of tracks clustered by the track jet	-	Y
p_T^{rel}	Lepton p_T along the track jet axis: $p \cdot \sin(\langle \text{lepton, track jet} \rangle)$	-	Y
$p_T^{\text{lepton track}}/p_T^{\text{track jet}}$	Lepton track p_T divided by track jet p_T	Y	Y
$\Delta R(\text{lepton, track jet})$	ΔR between the lepton and the track jet axis	Y	Y
p_T^{lepton} bin number	Index of the bin of lepton p_T	Y	Y

Table 7.1: Variables used for training the PromptLeptonImprovedVeto BDTs, taken from Ref. [100].

Electron calibration

The total electron efficiency is a product of efficiencies of the electron reconstruction, identification and isolation. Electron reconstruction efficiency is defined as the fraction of the energy clusters in the ECAL matched to a track, compared to the total number of energy clusters, while the identification and isolation efficiencies are defined based on the fraction of tracks satisfying an identification or isolation requirement to the total number of tracks after reconstruction or identification. Dedicated scale factors (SFs) are derived to correct MC to data, as a function of the electron energy and η .

Calibrating the energy scale of the resulting electrons involves first correcting to data to reduce the impact of non-uniform calorimeter response. Corrections are applied to both data and MC to correct for any energy loss before the electrons reach the ECAL. Finally, an in-situ calibration derived from $Z \rightarrow ee$ events is used to correct any residual differences in MC to data. Energy scale calibration is applied to data while energy resolution calibration is applied to MC [101].

7.3 Muon reconstruction

Muon tracks are reconstructed independently in the Inner Detector (ID) and the Muon Spectrometer (MS) and combined to provide muons for physics analyses [102]. In the ID, the steps described in Section 7.1 are followed. In the MS, a combinatorial search is performed for track segments in each muon chamber. Tracks are built starting from the middle layer; at least two muon segments are required to form a track candidate except in the barrel-endcap transition region where a single high quality segment suffices. Tracks satisfying a global chi-squared fit criteria are then combined with ID tracks, resulting in four kinds of muon objects:

- *Combined muons* are formed by taking a global fit of all hits associated to muon tracks in the ID and MS.
- *Segment-tagged muons* are those with a muon track from the ID matched to at least one segment in the MS. These are particularly useful for reconstructing low- p_T muons or in regions with limited acceptance.
- *Calorimeter-tagged muons* are formed from a track in the ID matched to a calorimeter energy deposit compatible with the expected signature of muons. These are useful

to recover acceptance in regions where the MS is only partially instrumented due to cabling and services for other subdetectors.

- *Extrapolated muons* are constructed solely from MS information with a loose requirement on the compatibility with an origin on the pp interaction point. These extend muon reconstruction acceptance to the region not covered by the ID ($2.5 < |\eta| < 2.7$).

After reconstruction, muon objects are calibrated to improve momentum and resolution to per-mille and percent levels respectively. These corrections are derived using Combined muons, by performing a maximum-likelihood fit of the distribution of invariant mass of the di-muon system in $Z \rightarrow \mu\mu$ and $J/\psi \rightarrow \mu\mu$.

Muon identification

Muon identification is achieved by using a discriminant built from quality of the track fit, the number of holes in the candidate muon trajectory (defined as points compatible with the trajectory where no hit was recorded) and momentum compatibility between ID and MS measurements. Four working points (WPs) are defined in ATLAS, namely *Loose*, *Medium*, *Tight* and *High- p_T* , in order of increasing muon purity. The analyses in this thesis use the *Medium* WP. The *High- p_T* WP is used in analyses with a substantial number of muons with p_T above 800 GeV, to reduce muon p_T mis-modelling in simulation. The use of this WP was explored for the VLL $e\mu$ analysis in Chapter 10 but not used because no significant mis-modelling was observed in the analysis phase space and further, preliminary studies on the effect of this WP in the analysis suggested loss at sensitivity at high signal masses. The identification efficiencies of the first three WPs, estimated as a function of track p_T and η is shown in Figure 7.8.

Muon isolation

As in the case of electrons, to identify muons originating in the hard scatter, isolation working points are defined by comparing the sum of transverse energy of all tracks within a defined radius of the reconstructed muon to the measured energy of the muon. The loosest isolation requirement is called *FCLoose*, with an efficiency of about 99% over all energy and η range, corresponding to an $E_T^{\text{cone20}}/p_T < 0.3$ and $p_T^{\text{varcone30}}/p_T < 0.15$. Further, PLIV working points defined with the muon PLIV BDT described in Section 7.2 can be used for better suppression of non-prompt muons from semi-leptonic b -decays. In particular, the

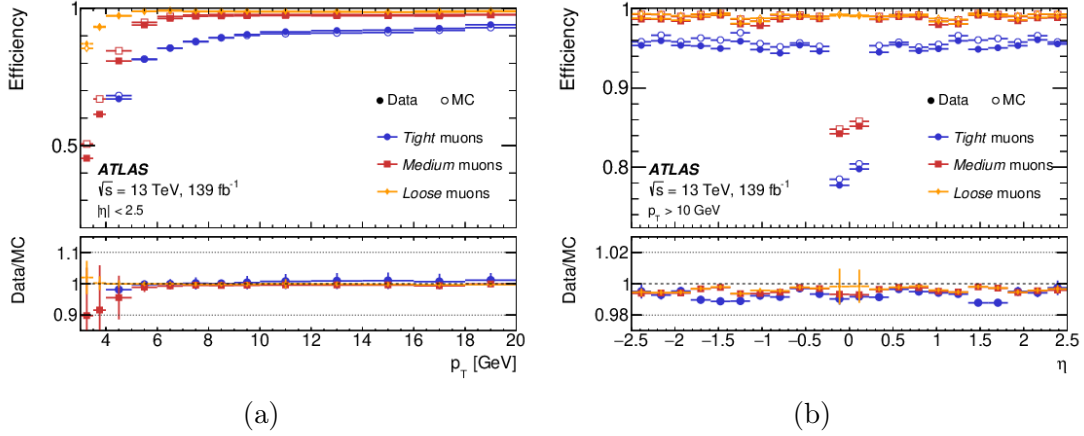


Figure 7.8: Muon identification efficiency for *Loose*, *Medium* and *Tight* working points as a function of muon (a) p_T and (b) η . Figures taken from Ref. [103].

PLImprovedTight and *PLImprovedVeryTight* OPs are used in the g2HDM and VLLe/ μ analyses.

Muon calibration

Muon efficiencies are estimated in a procedure similar to that established for electrons in Section 7.2. This efficiency is measured in data in events with $Z \rightarrow \mu\mu$ and $J/\psi \rightarrow \mu\mu$ events using a tag and probe method and a smearing is applied to the p_T distribution of the muon candidates from these events in the MC simulated samples to match the relative p_T resolution to data. Correction factors for muon energy scale and resolution are derived separately for ID and MS measurements.

7.4 Jet reconstruction

Jets are characterized as clusters of well-collimated particles originating from a radiative shower of strongly interacting particles. The jet reconstruction process in ATLAS starts with the formation of three-dimensional clusters of calorimeter cells termed *topoclusters*, described in Section 7.2. Subsequently, jets are constructed using a dedicated clustering algorithm relying solely on calorimeter information or incorporating tracking information prior to clustering. The resulting jets undergo calibration for energy and are categorized into different *flavors* based on their origin. To account for response to hadronic interactions, usually lower than the EM scale, hadronic topoclusters are calibrated to the correct scale

using a *local cluster (LC) weighting scheme* [97].

Particle Flow jets

Prior to the end of Run 2, topoclusters corrected to the position of the primary vertex were used as input to the jet clustering algorithm, with subsequent incorporation of tracking information to identify pileup objects and calibrate the jets. Run 2 commissioned an alternative approach to jet reconstruction known as the *Particle Flow (pFlow) algorithm* [104] which enhances the measurement of jet parameters by integrating calorimeter and tracking information prior to jet clustering. The energy of low-momentum charged hadrons that reach the calorimeter are measured with better resolution by the tracker, so those topoclusters are removed and replaced by the associated tracks. At sufficiently high p_T , the calorimeter is more precise than the tracker, and the topoclusters are used instead. For neutral hadrons, only the calorimeter is used. The steps of the ATLAS pFlow algorithm are illustrated in Figure 7.9.

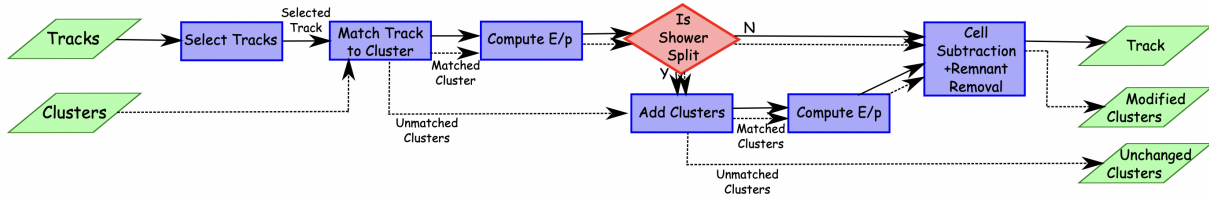


Figure 7.9: Flow chart of the steps of the Particle Flow (pFlow) algorithm [104]. Identification of tracks matched to a topocluster is followed by removing the energy of the track from the topocluster. The output of the algorithm are charged particles, unmodified topoclusters and remnants of topoclusters which have had part of their energy removed.

The inputs to the algorithm consist of topoclusters and *Tight* ID tracks defined as having at least 9 hits in the ID with no missing pixel hits, $|\eta| < 2.5$ and $p_T > 500$ MeV. Tight tracks with momentum p are matched to topoclusters with energy E , requiring $E/p > 0.1$ and $\Delta R' < 1.64$, defined as:

$$\Delta R' = \sqrt{\left(\frac{\Delta\phi}{\sigma_\phi}\right)^2 + \left(\frac{\Delta\eta}{\sigma_\eta}\right)^2}, \quad (7.3)$$

where, σ_η and σ_ϕ represent the angular widths of the topoclusters calculated as the standard deviation of the displacements of the topocluster's cells in η and ϕ with respect to its barycenter. The energy associated with reconstructed charged particles is subtracted from

the corresponding matched topocluster to identify any possible neutral particles merged with a charged object. Finally, the dispersion of estimated energy deposition is employed to determine whether the topocluster originated from a single object or not. If so, the residual energy is removed; otherwise it is retained. Following this sequence, two sets of Particle Flow Objects (PFOs) are generated, serving as inputs to the anti- k_t clustering algorithm for jet reconstruction:

- *Neutral* PFOs consist of topoclusters not linked to any track or calorimeter signals that persist after the subtraction process.
- *Charged* PFOs consist of isolated tracks or tracks and topoclusters matched by the pFlow algorithm.

The performance of pFlow jets versus the older topocluster-only jets (calibrated to the hadronic scale) is illustrated in Figure 7.10.

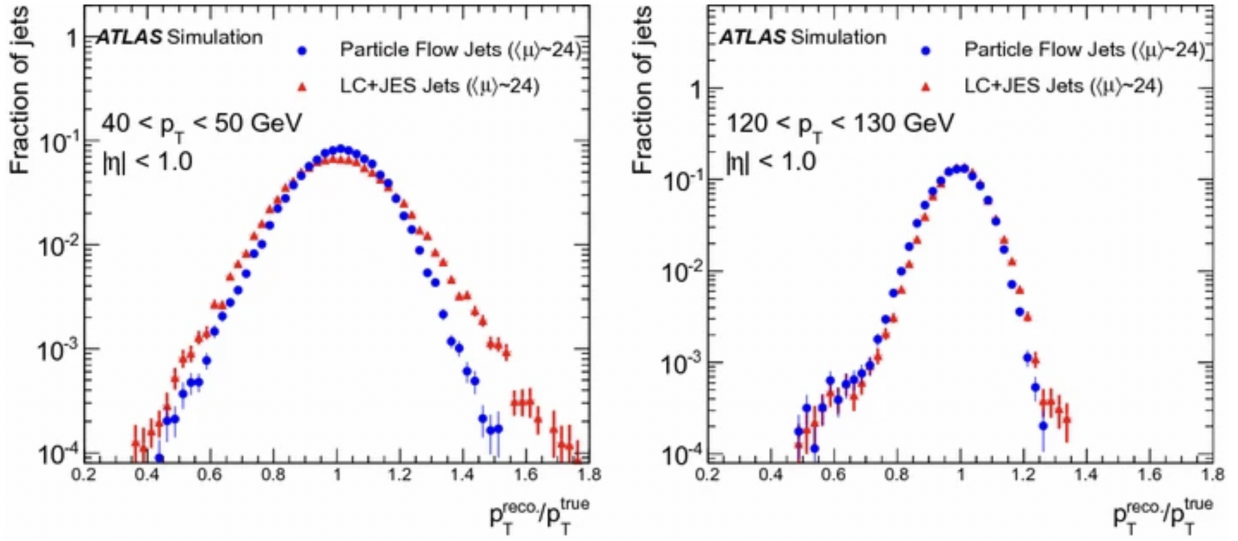


Figure 7.10: Distributions of jet transverse momentum response in dijet MC events for calorimeter jets and particle flow jets, shown separately for jets in $40 < p_T < 50$ GeV and $120 < p_T < 130$ GeV. Pileup conditions were simulated to be similar to the data-taking in 2012. Figures taken from Ref. [104].

The anti- k_T algorithm

The anti- k_T algorithm [105] belongs to a group of jet clustering algorithms built on defining a distance parameter d_{ij} between two particles i and j as:

$$d_{ij} = \min(p_{T,i}^{2n}, p_{T,j}^{2n}) \frac{\Delta R_{ij}^2}{R^2}; \quad d_{iB} = p_{T,i}^{2n}, \quad (7.4)$$

where d_{iB} is defined between particle i and the beam and the parameter R is the jet radius in $\eta - \phi$ coordinates. The algorithm proceeds in the following steps:

- For each particle i , a database is built collecting distances of the particle from other particles j and the beam B .
- If there is any object j closer to input i than its distance to the beam axis, $d_{ij} < d_{iB}$, then objects i, j are merged together in a single object.
- If there is no object j closer to i than the beam axis, then i is defined to be a jet and removed from the pool of inputs.
- This procedure is repeated until no more particles are left in the database.

The anti- k_T algorithm, defined with $n = -1$, is employed for reconstructing jets in the analyses presented in this thesis. The minima term in the anti- k_T equation collects all soft radiations into the jet cone and makes the algorithm infrared and collinear (IRC) safe. Other algorithms like the Cambridge-Aachen ($n = 0$) and k_T ($n = 1$) algorithm use different values of n . All three algorithms are illustrated in Figure 7.11a. In ATLAS, jets with $R = 0.4$ are called *small- R* jets, while those with $R = 1.0$ are called *large- R* jets. Large- R jets are important to reconstruct boosted particles decaying into jets and recognised by looking at the jet substructure.

7.4.1 Jet calibration

The calibration of jets formed at this stage is essential to account for detector effects such as the detector response, dead material, pileup, punch-through and energy deposits below the noise threshold [50]. The calibration of pFlow jets is performed through the series of steps illustrated in Figure 7.12.

Pileup subtraction is the first step in the chain and is performed to remove excess energy due to additional pp interactions within the same or nearby bunch crossings. It is

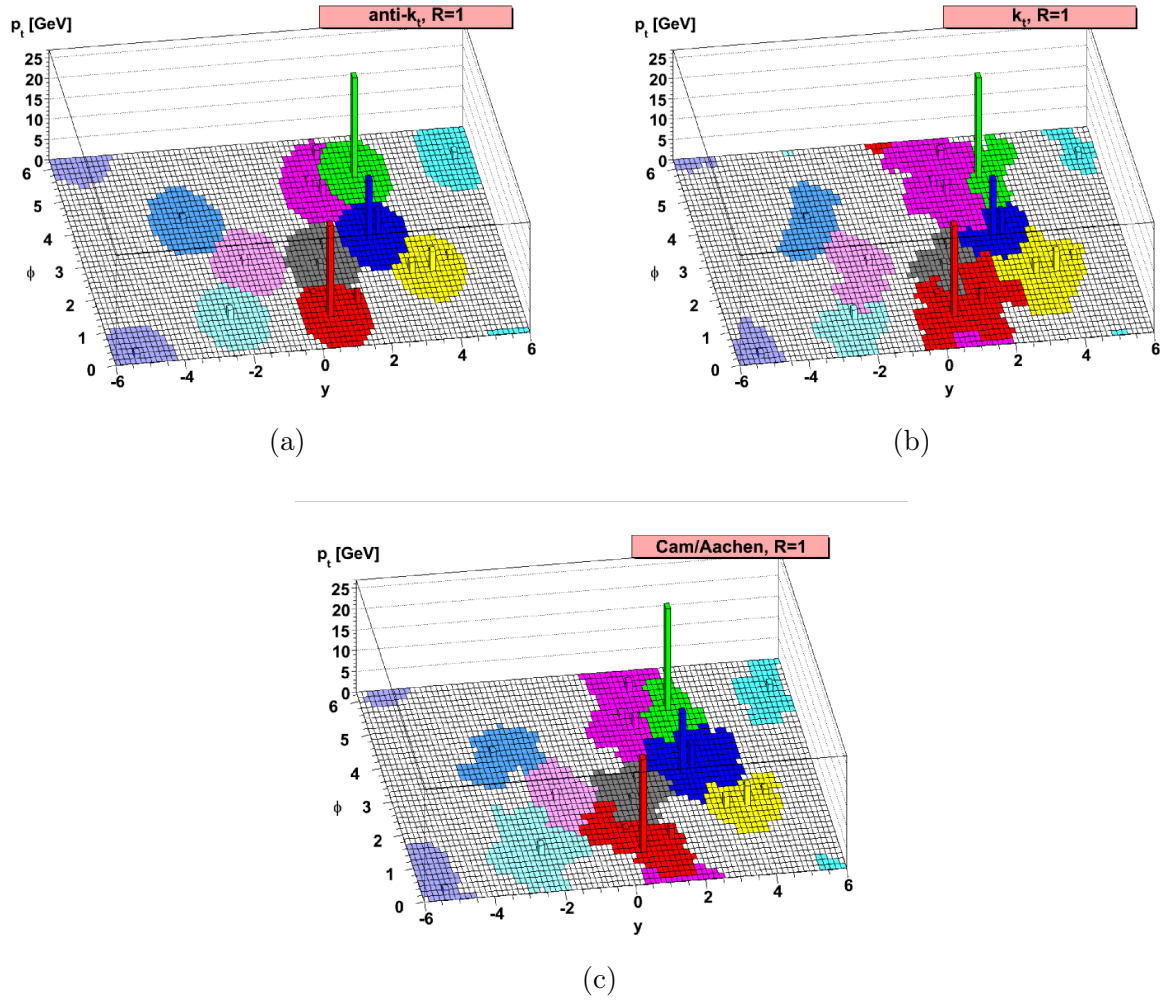


Figure 7.11: Jet clustering algorithms (a) anti- k_T ($n = -1$) (b) k_T ($n = 1$) and (c) Cambridge-Aachen ($n = 0$). Figure taken from Ref. [105].

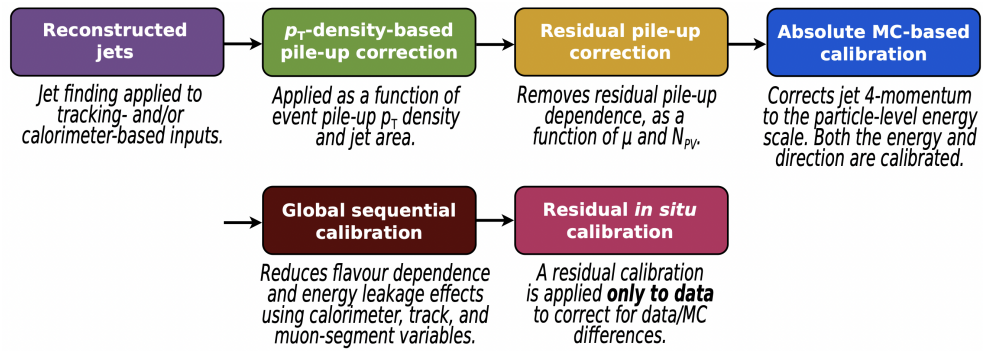


Figure 7.12: Stages of jet energy scale calibration Figure taken from Ref. [50].

accomplished in two steps: first, an area-based subtraction of the pileup contribution to the p_T of each jet is performed per event, followed by a residual correction derived from MC simulation, parameterized as a function of the number of reconstructed primary vertices and average number of interactions per bunch crossing. This is followed by a correction to the *Jet Energy Scale (JES)*, η and mass (only for large R jets), by comparing reconstructed jets to truth jets from dijet MC events. For small- R jets, the difference in the calorimeter response observed in different flavor jets is reduced by using information from the tracks associated with the jet, in a process called *Global Sequential Calibration (GSC)*. All these calibrations are applied to both data and MC simulation. The GSC calibration does not change the average JES of the sample, but improves the *Jet Energy Resolution (JER)*. The final step in the chain applies a residual in-situ calibration only to data to correct for remaining differences between data and MC simulation. This correction is derived using well-measured reference objects, including photons, Z bosons and calibrated jets: jet $|\eta|$ is calibrated in the forward region of the detector with well-measured central jets from QCD dijet events; jet p_T in central jets is calibrated against well-measured Z bosons or photons in Z/γ +jets events. For high- p_T central jets, the calibration is performed against low-momentum jets in QCD multijet events.

The full JES uncertainty prescription consists of about 125 individual terms [50], provided centrally by the ATLAS Collaboration. These uncertainties are derived from in situ measurements, pileup effects, flavor dependence and estimation of additional effects such as punch-through. For central jets ($|\eta| < 1.2$), they vary from about 5% for low p_T jets (20 GeV) to 1% for high- p_T jets ($250 < p_T < 400$ GeV), and 3.5% for very high- p_T jets ($p_T > 2.5$ TeV). An example of the magnitude of these uncertainties are shown in Figure 7.13. Jet energy resolution is measured in dijet MC events and the relative uncertainty ranges from $(24 \pm 1.5)\%$ at 20 GeV to $(6 \pm 0.5)\%$ at 300 GeV.

7.4.2 Jet vertex tagging

The jet vertex tagging (JVT) algorithm [106, 107] is used to identify jets arising from pileup. After the identification of the hard-scatter vertex (PV_0), the jet vertex fraction (JVF) is calculated as the ratio of the sum of transverse momentum of all tracks associated the jet and compatible with PV_0 , to the sum of transverse momentum of all tracks in the jet associated with other primary vertices in the event.

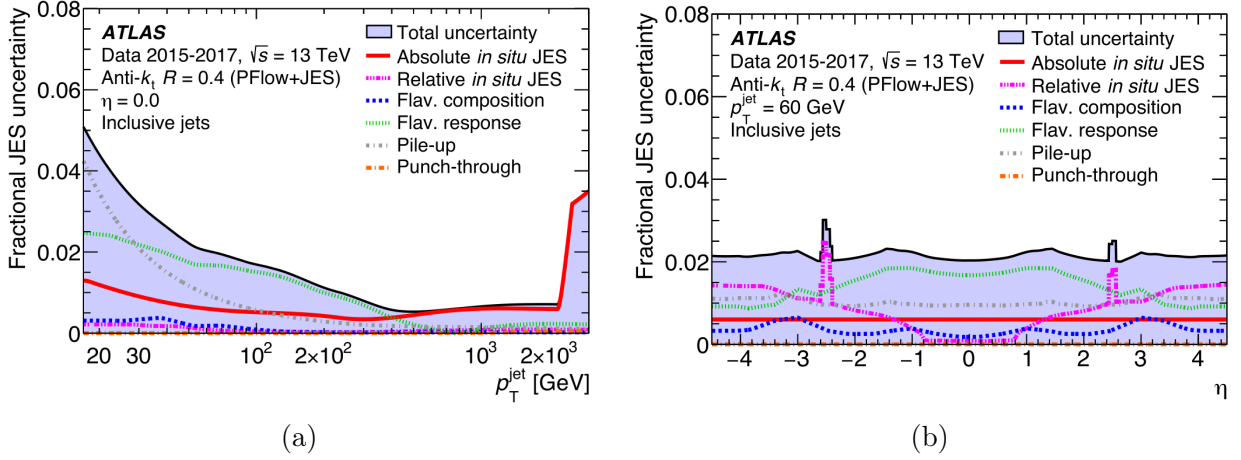


Figure 7.13: Fractional jet energy scale systematic uncertainty components for anti- k_T $R = 0.4$ jets reconstructed from pFlow objects as a function of (a) jet p_T at $\eta = 0$ and (b) η for jet $p_T = 60$ GeV. The total uncertainty is shown in the purple band, calculated as a quadratic sum of all components. Figures taken from Ref. [50].

The dependence on number of pileup tracks in the event, n_{trk} , is reduced by an additional term in the denominator of the ratio:

$$\text{JVT} = \frac{\sum_m p_{T,m}^{\text{trk}}(PV_0)}{\sum_l p_{T,l}^{\text{trk}}(PV_0) + \frac{\sum_{n \geq 1} \sum_l p_{T,l}^{\text{trk}}(PV_n)}{10^{-3} n_{\text{trk}}}}. \quad (7.5)$$

Another useful discriminant is ratio R_{p_T} , of the transverse momentum of the tracks associated to a jet compatible with PV_0 and that of the jet:

$$R_{p_T} = \frac{\sum_k p_{T,k}^{\text{trk}}(PV_0)}{p_T^{\text{jet}}}. \quad (7.6)$$

The JVT algorithm combines these variables in a multi-variate technique to compute the probability of a jet to have originated in pileup. It is optimised separately for central jets ($|\eta| < 2.5$) and the forward region ($|\eta| > 2.5$), where a dedicated forwardJVT (fJVT) algorithm [107] following a similar approach is used. A systematic uncertainty corresponding to the JVT selection is added in physics analyses.

7.4.3 Jet flavor tagging

The structure of a jet varies depending on the parton it originates from. Jets originating from gluons or a u - or d -quark are called light jets; those from b - and c -hadrons are called

b - and c -jets respectively. Tagging jets originating from b -hadrons, called *b-tagging*, is of particular interest to analyses in multilepton final states where semi-leptonic decays of b -hadrons is a major non-prompt background.

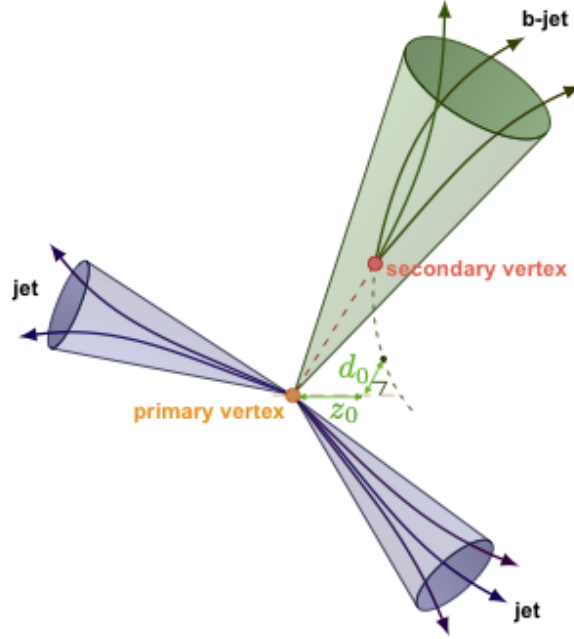


Figure 7.14: Topology of a b -jet.

The typical topology of an event with a jet from a b -hadron is shown in Figure 7.14. B -hadrons have a long lifetime (~ 1.5 ps) and travel distances up to 4.5 mm inside the detector before decaying, creating a *secondary vertex* in the event. Low level b -tagging algorithms exploit the long lifetime and displaced decays of b -hadrons to look for secondary vertices and displaced tracks. The commonly used low level b -tagging algorithms, illustrated in Figure 7.15, can be classified based on the variables they exploit:

- Impact Parameter (IP) algorithms exploit the large transverse and longitudinal impact parameters of b -jets to identify them. Two traditionally known algorithms of this type are IP2D and IP3D [108]. The former uses the signed significance of the transverse impact parameter (d_0/σ_{d_0}) as an input to the algorithm while the latter develops a two-dimensional template additionally including the significance of the longitudinal impact parameter ($z_0 \sin \theta / \sigma_{z_0}$). The most recent of IP algorithm is called RNNIP[109], which also takes into account track-to-track correlations using a recurrent neural network.

- Secondary vertex finding algorithms identify b -jets by searching for a single secondary vertex compatible with that from a b -hadron decay. The most popular algorithm of this type is called SV1 [110]. It uses a likelihood discriminant to identify all two track vertex candidates from sources other than b -decays, like kaons, photon conversions and material interactions and uses the remaining tracks for b -jet identification.
- Multi-vertex finding algorithms are used to identify jets with more than one secondary vertices. JetFitter [111] is a popular algorithm of this type that uses a modified Kalman filter to reconstruct the full decay chain of b -hadron.

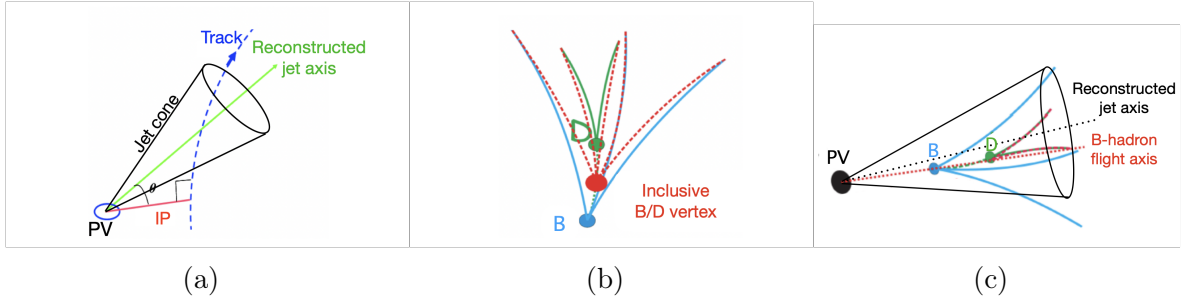


Figure 7.15: Illustration of the low-level b -tagging algorithms: (a) Impact Parameter (IP) algorithms which identify b -jets by exploiting their large impact parameters, (b) Secondary vertex finding algorithms which determine a singlet inclusive weak b -hadron decay vertex and (c) Multi-vertex finding algorithms that look for b -hadron decay chains for a detailed determination of decay vertex topology.

The outputs of low-level impact parameter taggers and vertexing algorithms are combined in a high-level tagger that uses a multi-class deep neural network called *DL1*. The *DL1* algorithm used in this thesis is called *DL1r* [112], which integrates the output discriminants of low-level tagging algorithms to output the probability of a jet to be identified as a light, b - or c -jet (denoted by p_l , p_b and p_c respectively):

$$D_{DL1r} = \ln \frac{p_b}{f_c p_c + (1 - f_c) p_l}, \quad (7.7)$$

where f_c denotes the effective c -jet fraction in the background hypothesis and is set to 0.018 for *DL1r*. The distributions of the outputs of the *DL1r* b -tagging algorithm for b -jets, c -jets and light-flavour jets in $t\bar{t}$ simulated events is shown in Figure 7.16.

Different single-cut operating working points (OP) are defined using the output score of *DL1r*, corresponding to b -jet tagging efficiency (T_f) of 60%, 70%, 77% and 85%, derived for the nominal $t\bar{t}$ sample:

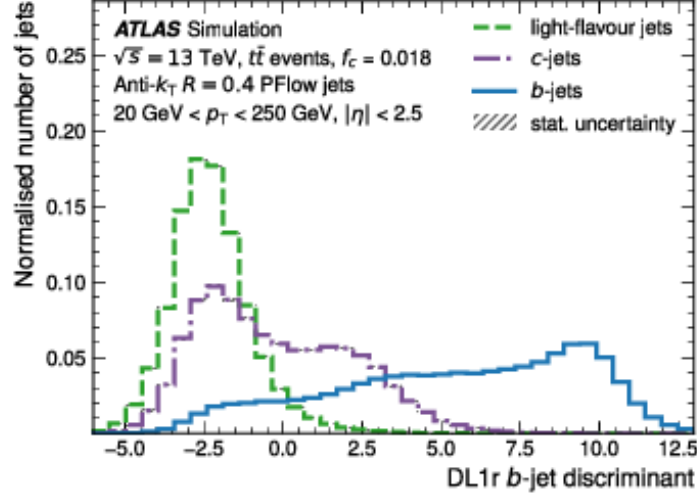


Figure 7.16: Distributions of the outputs of the DL1r b -tagging algorithm for b -jets, c -jets and light-flavour jets in $t\bar{t}$ simulated events. Figure taken from Ref. [113].

$$\epsilon_{\text{flav}} = \frac{N_{\text{pass}}^{\text{flav}}(D_{\text{DL1r}} > T_f)}{N_{\text{total}}^{\text{flav}}}. \quad (7.8)$$

The b -tagging efficiency and c - and *light*-flavor mistag rates of the DL1r algorithm as a function of jet p_T for the different OPs for the POWHEG+PYTHIA8 $t\bar{t}$ sample is shown in Figure 7.17. Using the edges of the OP cuts on the DL1r score, pseudo continuous b -tagging working points can be defined. This is useful for defining regions of varying b -jet purity in the analyses. These intervals correspond to b -jet tagging efficiencies of [100,85]% (most light jets fall in this bin), [85,77]%, [77,70]%, [70,60]%, [60,0]% (most b -jets are enriched in this bin).

Mis-modelling of the DL1r output score in MC simulation may result in difference in tagging rates between data and MC. To address this, data-MC efficiency *scale factors* (SFs), evaluated as a function of jet p_T , are provided centrally in ATLAS, separately for b -, c - and *light*-flavor jets. The calibration of b -jets is derived from $t\bar{t}$ samples with two opposite-sign leptons in the final state. For jets with $20 < p_T < 600$ GeV, a combinatorial likelihood approach is used to derived the SFs, and extrapolated to jets with $p_T > 600$ GeV. These SFs are shown for the different b -tagging OPs in Figure 7.18 with total uncertainties that range from 1% to 8% at high and low jet p_T respectively.

The c -jet mistag rate is estimated from semi-leptonic $t\bar{t}$ events using a likelihood approach [114]. The derived c -tag mistag rate SFs at the 70% DL1r efficiency OP are shown

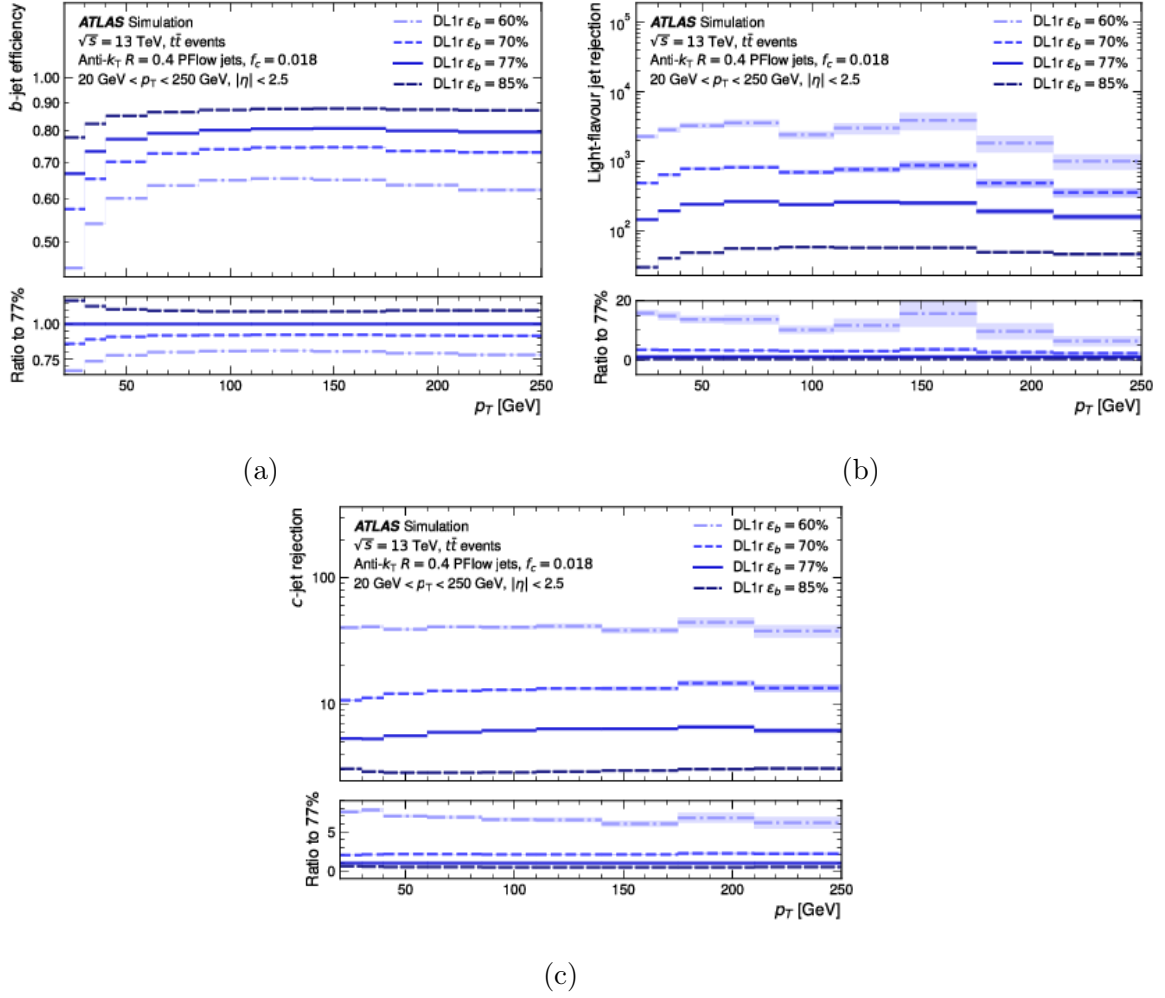


Figure 7.17: (a) b -tagging efficiency, (b) c -mistag rates and (c) $light$ -flavor mistag rates of the DL1r algorithm as a function of jet p_T for the different OPs for the POWHEG+PYTHIA8 $t\bar{t}$ sample. Figure taken from Ref. [113].

in Figure 7.19. The associated uncertainties range from 3% to 17% at high and low jet p_T respectively. The mistag rates of light-jet events is measured from multijet events with two methods: the *negative-tag* and the *adjusted MC* method [115]. The former method is based on the assumption that the signed IP distribution of light-jets should be more symmetrical around zero compared to the one from b -jets. In the latter method, MC simulated events are modified to match the tracking performance in data and the mistag rate SFs are given as the ratio of efficiency in the MC-adjusted samples to the initial MC-samples. Figure 7.19 shows the light-jet mistag rate SFs at the 70% DL1r efficiency OP using the negative-tag method. The associated uncertainties range from 18% to 39% at high and low jet p_T

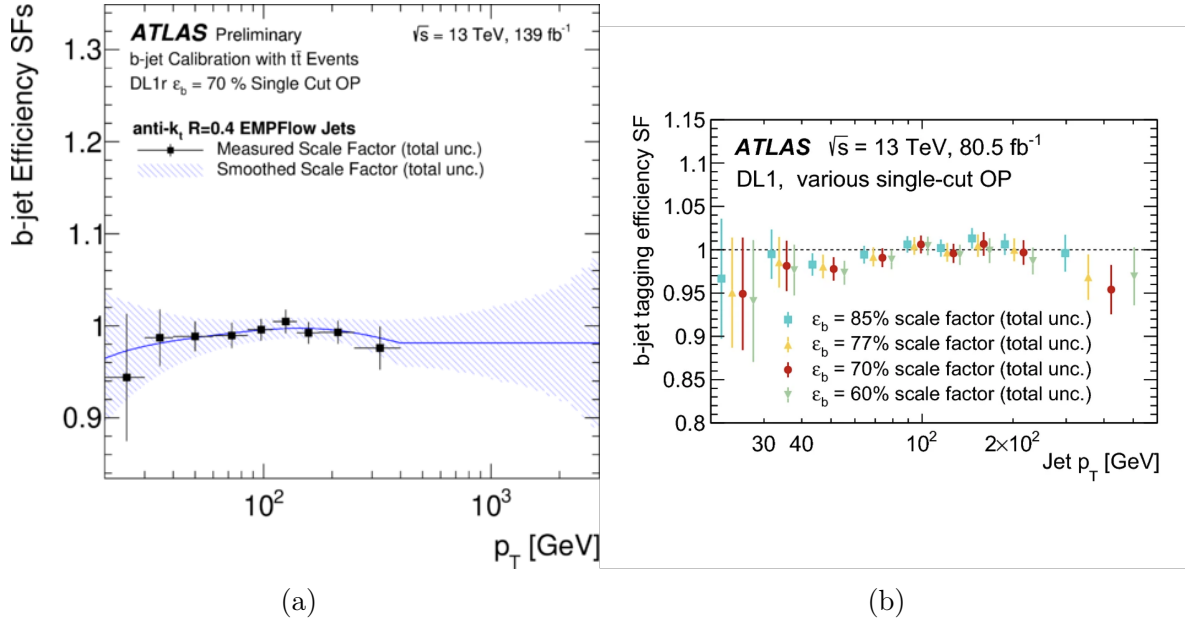


Figure 7.18: (a) b -jet efficiency scale factors for the 70% DL1r OP and (b) b -tagging efficiency scale factors for various OPs, as a function of the jet p_T . Figures taken from Ref. [113].

respectively.

Overall, a total of 60 systematic uncertainties, corresponding to b -tagging (20), c -jets mistag rates (20) and light-jet mistag rates (20), collectively called *FTAG* uncertainties, are taken into account in all the analyses in this dissertation.

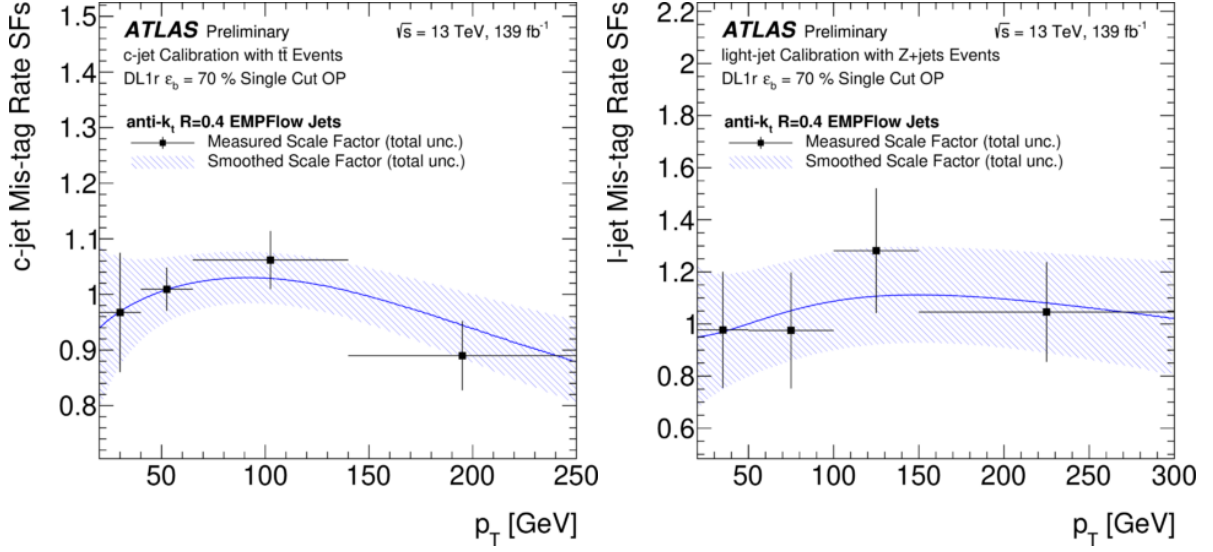


Figure 7.19: Efficiency scale factors for (a) c -jet mistag rates and (b) light-jet mistag rates (determined using the negative-tag method), for the 70% DL1r OP. Figures taken from Ref. [113].

7.5 Hadronically decaying τ -leptons

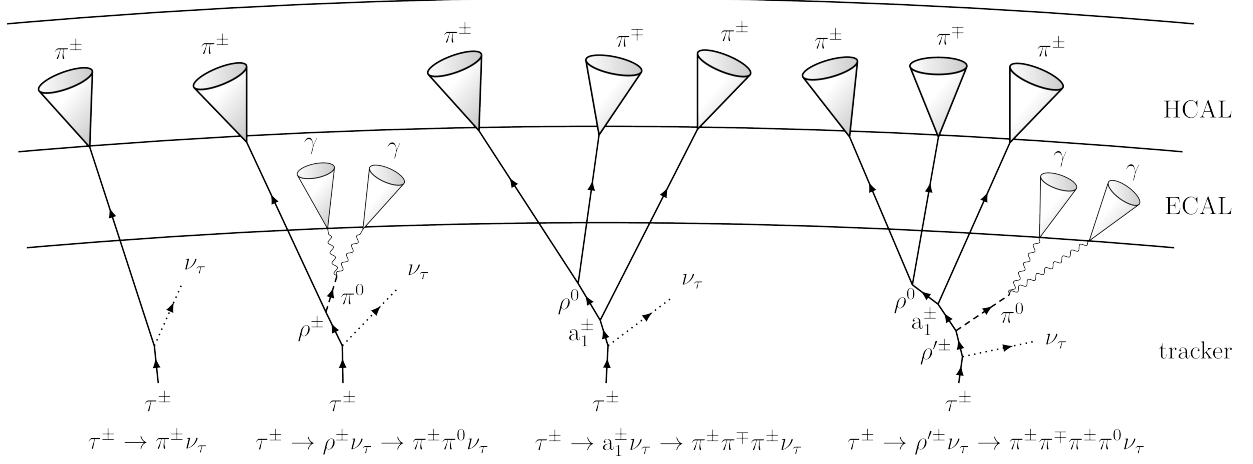
This section discusses the reconstruction, identification and calibration of hadronically decaying τ -leptons (τ_{had}).

7.5.1 Reconstruction of τ_{had}

τ -leptons can travel distances up to $87 \mu\text{m}$ before decaying. Typically, τ decays are initiated in the pixel detector and may be displaced from the primary vertex. τ -leptons may decay leptonically (35%) or hadronically (65%). Due to their larger branching ratio, hadronic τ decays (τ_{had}) are of greater interest in physics analysis. The hadronic decay modes of the τ -lepton are illustrated in Figure 7.20.

τ_{had} decays typically result in one or more charged pions, a neutrino and may be accompanied by a neutral pion. They can be classified into $1\text{-prong } \tau_{\text{had}}$, identified with a narrow jet with one associated track in the ID, or $3\text{-prong } \tau_{\text{had}}$, identified with three narrow jets and three associated track in the ID.

τ_{had} candidates are seeded by jets formed using the procedure described in Section 7.4. Additionally, they are required to have $p_T > 10 \text{ GeV}$ and $|\eta| < 2.5$ (except $1.37 < |\eta| < 1.52$, which falls in the transition region between the barrel and forward calorimeters). The *seed*

Figure 7.20: Hadronic decay modes of the τ -lepton.

jet axis is identified with the energy-weighted barycentre of the topoclusters forming the jet, matched to a track in the ID pointing to the PV of the event. The τ_{had} candidate vertex is defined as the vertex candidate with the highest p_T -weighted fraction of all tracks with $p_T > 0.5$ GeV within an angular distance of $R = 0.2$ around the seed jet axis [116]. τ_{had} tracks are required to have $p_T > 1$ GeV, at least seven hits in the pixel and the SCT subdetectors with at least two associated hits in the pixel, $|d_0| < 1$ mm and $|z_0 \sin \theta| < 1.5$ mm. These tracks are assigned to *core* or *isolation* regions around the τ_{had} candidate, based on a set of BDTs trained on the track p_T , number of hits in the detectors and their transverse and longitudinal impact parameters with respect to the tau vertex. Tracks in the *core* region fall in $\Delta R < 0.2$ around the jet axis and are used for τ_{had} reconstruction. The number of core tracks defines the number of prongs. For τ_{had} candidates with more than one track in the core, a secondary vertex is reconstructed from all core tracks. *Isolation* tracks, on the other hand, fall in $0.2 < \Delta R < 0.4$ of the jet axis, and are used solely for identification of τ_{had} . The reconstruction efficiency of the p_T of τ_{had} remains almost constant in the high- p_T region for 1-prong τ_{had} candidates and it deteriorates for 3-prong τ_{had} candidates, as shown in Figure 7.21.

7.5.2 Identification of τ_{had}

The τ_{had} identification algorithm is designed to reject backgrounds from quark- and gluon-initiated jets. In ATLAS, an RNN-based approach is used for this, trained on variables related to tracking, energy clusters and higher level variables calculated from track and calorimeter quantities [118]. Separate RNN algorithms are used for 1-prong and 3-prong

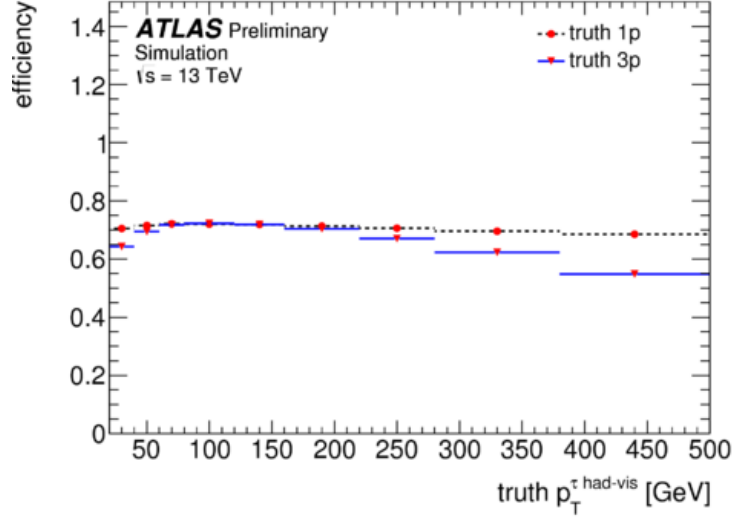


Figure 7.21: Reconstruction efficiency of τ_{had} as a function of the τ_{had} p_T for 1-prong (black) and 3-prong (blue) candidates. Figure taken from Ref. [117].

τ_{had} due to their distinct signatures in the detector. The RNN training is based on $Z/\gamma^* \rightarrow \tau\tau$ simulated events, required to decay hadronically. Reconstructed τ_{had} candidates not originating from τ_{had} decays, termed background τ_{had} , are taken from simulated dijet samples and are required to be reconstructed as 1- or 3-prong τ_{had} candidates. The background τ_{had} p_T distribution is softer compared to that of the signal τ_{had} p_T distribution from $Z/\gamma^* \rightarrow \tau\tau$ events. Thus, to ensure that no p_T -dependent bias is introduced in the trained classifiers, the p_T of the background τ_{had} is reweighted, separately for 1- and 3-track candidates, in bins of τ_{had} p_T to match the p_T distributions of true τ_{had} in $Z/\gamma^* \rightarrow \tau\tau$ signal events.

Figure 7.22 shows the rejection power for misidentified τ_{had} (from quark- or gluon-initiated jets) depending on the true τ_{had} selection efficiency, for the RNN classifier and an older BDT-based identification algorithm [117]. Four OPs with increasing background rejection (*Very loose*, *Loose*, *Medium* and *Tight*) are defined to be used by physics analyses, with selection efficiencies and the corresponding background rejection factors for the RNN classifiers shown in Table 7.23. In the 4321 analysis described in Chapter 11, the Loose RNN WP is used, which corresponds to an efficiency of 85% (75%) for 1-(3)-prong τ_{had} .

The efficiency for τ_{had} identification and combined reconstruction and identification efficiency as a function of the p_T of the τ_{had} , for 1-prong and 3-prong τ_{had} candidates is shown in Figure 7.26.

Apart from the RNN classification, an additional BDT discriminant trained on $Z \rightarrow ee$

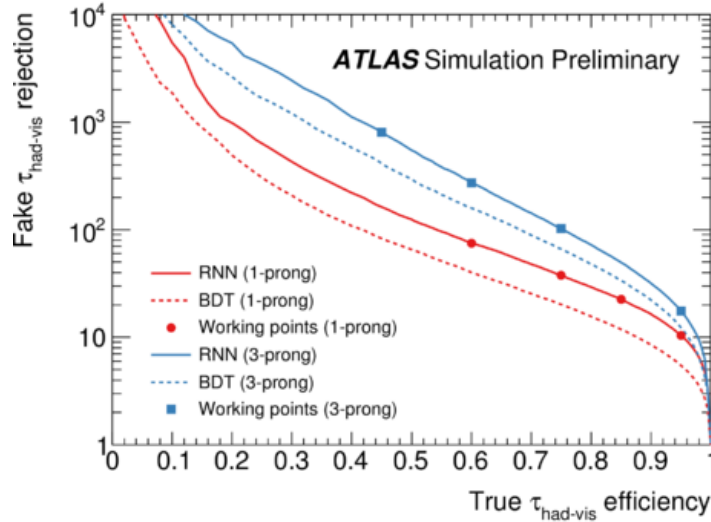


Figure 7.22: Reconstruction efficiency of τ_{had} as a function of the τ_{had} p_T for 1-prong (black) and 3-prong (blue) candidates. Figure taken from Ref. [117].

Working point	Signal efficiency	
	1-prong	3-prong
Tight	60%	45%
Medium	75%	60%
Loose	85%	75%
Very loose	95%	95%

Figure 7.23: List of defined WPs for the RNN classifier. Table modified from Ref. [117].

events is used specifically for the rejection against electron candidates as part of the τ_{had} ID. An OP of (75) 60% real τ_{had} efficiency is used, with a rejection factor of (40) 300 for (1-) 3-prong candidates, dependent on τ_{had} p_T and $|\eta|$.

7.5.3 Energy calibration of τ_{had}

Two dedicated calibration techniques have been developed in ATLAS to correct the energy of reconstructed τ_{had} candidates measured in the detector to the average value of the energy carried by the measured decay products at the generator level: the *baseline* calibration and the *boosted regression tree* (BRT) based calibration [117]. Under the *baseline calibration*,

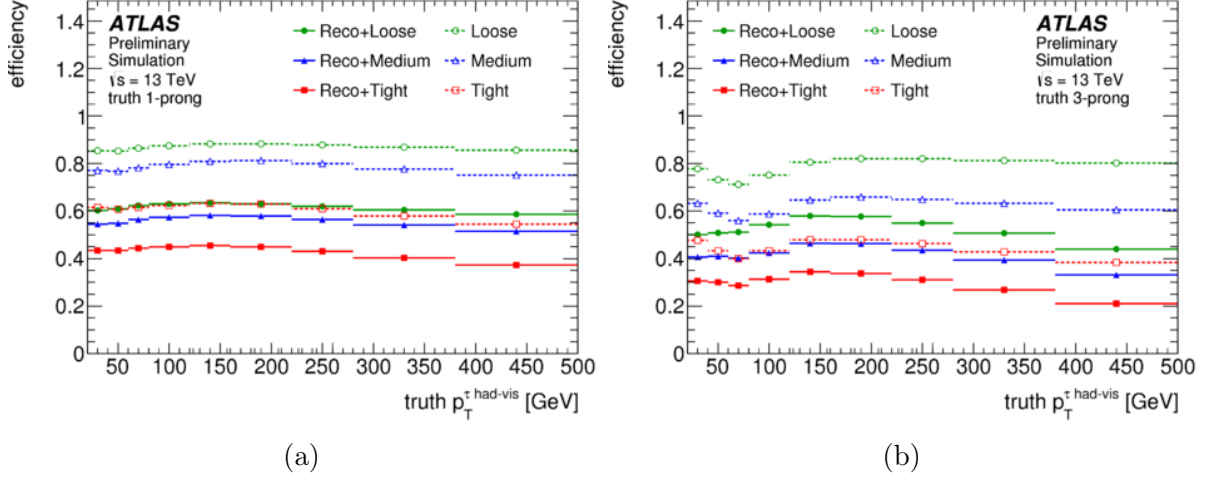


Figure 7.24: Identification efficiency for τ_{had} candidates (open symbols) together with combined reconstruction and identification efficiency (filled symbols) as a function of the p_T of the τ_{had} , for 1-prong and 3-prong τ_{had} candidates Figure taken from Ref. [117].

the correction to the τ_{had} energy (E_{calib}) is calculated as:

$$E_{\text{calib}} = \frac{E_{\text{LC}} - E_{\text{pileup}}}{\mathcal{R}(E_{\text{LC}} - E_{\text{pileup}}, |\eta|, n_p)}, \quad (7.9)$$

where E_{LC} is the correction to the LC-calibrated sum of the energy of all topoclusters within $\Delta R < 0.2$ of the τ_{had} candidate, E_{pileup} accounts for corrections from pileup and $\mathcal{R}$ is the detector response calibration. E_{pileup} increases linearly with the number of primary vertices N_{PV} and is derived as:

$$E_{\text{pileup}}(N_{\text{PV}}, |\eta|, n_p) = \mathcal{A}(|\eta|, n_p) \times (N_{\text{PV}} - \langle N_{\text{PV}} \rangle). \quad (7.10)$$

Here, n_p counts the prongness of the τ_{had} (1-prong or 3-prong) and $\mathcal{A}$ is a linear coefficient extracted from a fit of E_{LC} to simulated data, as a function of $N_{\text{PV}} - \langle N_{\text{PV}} \rangle$ in bins of $|\eta|$, shown in Figure 7.25.

Finally, $\mathcal{R}$ is extracted as the Gaussian mean of $\frac{E_{\text{LC}} - E_{\text{pileup}}}{E_{\text{vis}}}$, where E_{vis} is the true energy of the generated τ_{had} decay products excluding the contribution from neutrinos. The value of this response factor is shown in Figure 7.26 for 1-prong and 3-prong τ_{had} .

The baseline calibration is sufficient for τ_{had} candidates with high p_T , but begins to degrade for those with low p_T . The BRT calibration takes in to account information from *Tau Particle Flow* (TPF), which improves the τ_{had} energy resolution at low p_T due to the

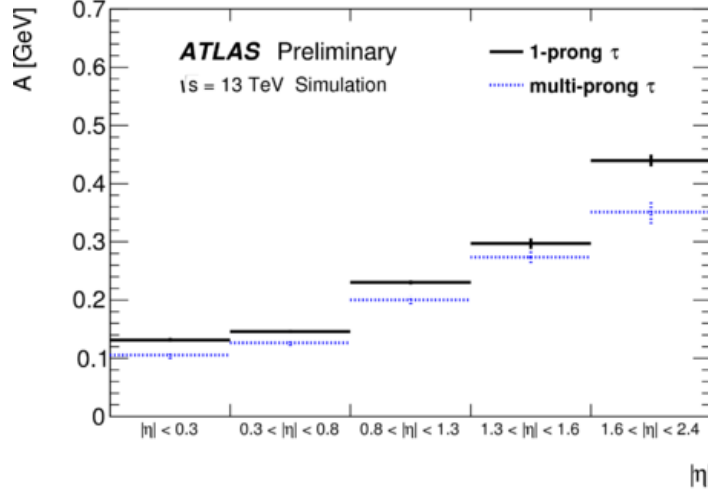


Figure 7.25: Pileup correction factor $\mathcal{A}(|\eta|, n_p)$ for 1-prong (black) and 3-prong (blue) τ_{had} candidates. Figure taken from Ref. [117].

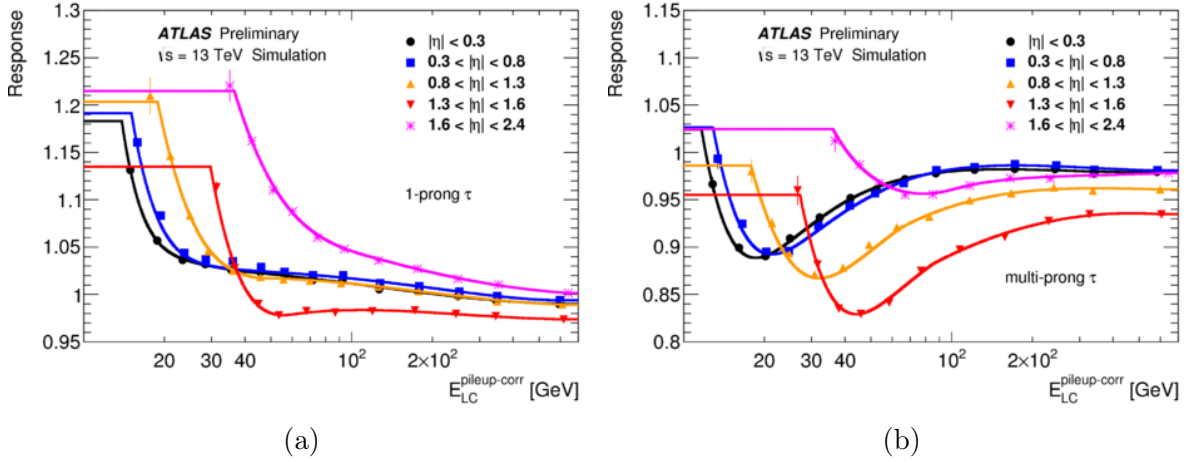


Figure 7.26: Detector response $\mathcal{R}$ for (a) 1-prong and (b) 3-prong τ_{had} decays. Figure taken from Ref. [117].

superior measurement of the charged pion momentum from the tracking system. Additional information from the tracker and calorimeters is used as an input to this BRT method. Figure 7.27 shows the resolution of the baseline and the BRT-based τ_{had} energy calibration, as a function of the τ_{had} p_T .

An additional correction to the Tau Energy Scale (TES), is derived to account for differences between data and simulation [116]. This measurement is done in the distribution of the reconstructed visible mass (m_{vis}) in $Z \rightarrow \tau_\mu \tau_{\text{had}}$ events. The τ_{had} energy scale is parameterised with an additional shift factor α , which is determined from the distribution of

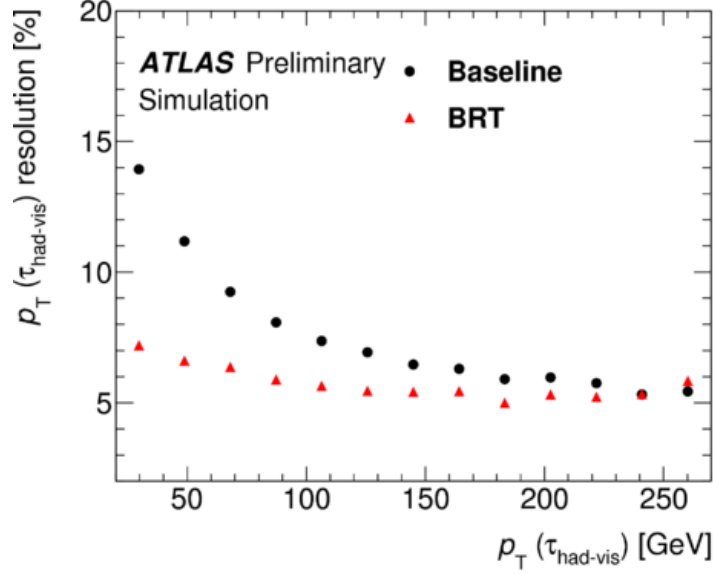


Figure 7.27: Resolution of the baseline and the BRT-based τ_{had} energy calibration, as a function of the τ_{had} p_T . Figure taken from Ref. [116].

m_{vis} in data and simulation. The muon p_T is measured independently. The total uncertainty in this correction is estimated to be about 1.2% (3%) for 1- (3-) prong τ_{had} candidates.

The probability of misidentifying an electron as a τ_{had} candidate is measured in events dominated by $Z \rightarrow ee$ processes using a tag-and-probe method. This probability ranges between 0.5% and 2.5% across the η spectrum of the τ_{had} candidate in both data and simulation [116]. Finally, the τ trigger efficiency is measured as a function of the reconstructed p_T of the τ candidate and the uncertainty in this measurement ranges from 3-8% for $p_T(\tau_{\text{had}}) < 100$ GeV to 8-14% for $100 < p_T(\tau_{\text{had}}) < 300$ GeV.

7.6 Missing transverse energy

Particles without electromagnetic or strong couplings escape undetected in the ATLAS detector. They are inferred indirectly through the energy imbalance in the event, where due to momentum conservation, the vector sum of the transverse momentum of all particles in the event should be equal to zero. Thus, the missing transverse energy in the event ($\vec{E}_T^{\text{miss}}$) is defined as the negative of the vector sum of momenta of all reconstructed and calibrated physics objects (electrons, muons, photons, hadronically decaying taus and jets):

$$\vec{E}_T^{\text{miss}} = -\sum \vec{p}_T^e - \sum \vec{p}_T^\gamma - \sum \vec{p}_T^\mu - \sum \vec{p}_T^{\text{jets}} - \sum \vec{p}_T^{\text{soft terms}} \quad (7.11)$$

An additional term called the *soft term*, $\sum \vec{p}_T^{\text{soft terms}}$, is included in Equation 7.11 to account for measured energy not included in any of the reconstructed objects. This term estimates the soft hadronic activity measured by reconstructed charged particle tracks not associated with the hard objects [119].

Common methods in multilepton searches

This chapter provides an in-depth discussion on the collision dataset, Monte Carlo simulation samples, object and event reconstruction techniques and other strategies common to the analyses presented in this dissertation.

8.1 Collision dataset

The physics analyses in this dissertation use the full Run 2 dataset collected by the ATLAS experiment from 2015 to 2018, during which pp collisions occurred at a center-of-mass energy of $\sqrt{s} = 13$ TeV with a bunch crossing interval of 25 ns. Only data collected during periods with stable beam conditions and full detector system functionality were used for analyses. These events are termed *Good For Physics* and are specified in the *Good Run List* (GRL), separately for each period of data-taking. The following GRL files are used in the analyses in this dissertation:

- 2015: data15_13TeV.periodAllYear_DetStatus-v89-pro21-02_Unknown
_PHYS_StandardGRL_All_Good_25ns.xml
- 2016: data16_13TeV.periodAllYear_DetStatus-v89-pro21-01_DQDefects-00-02-04
_PHYS_StandardGRL_All_Good_25ns.xml
- 2017: data17_13TeV.periodAllYear_DetStatus-v99-pro22-01_Unknown
_PHYS_StandardGRL_All_Good_25ns_TriggerNo17e33prim.xml
- 2018: data18_13TeV.periodAllYear_DetStatus-v102-pro22-04_Unknown
_PHYS_StandardGRL_All_Good_25ns_TriggerNo17e33prim.xml

The calculation of the total integrated luminosity of the GRL datasets and the associated uncertainty is subject to several factors and can improve depending on the algorithms and error estimation methods used. The g2HDM analysis presented in Chapter 9 uses 139 fb^{-1} of data with an uncertainty of 1.7%, following the recommendations set in Ref. [120]. A re-optimisation of the luminosity measurement following Ref. [121] recommended the full GRL dataset to be $140.1 \pm 1.2 \text{ fb}^{-1}$ with an uncertainty of 0.83%. This second estimate is used in the VLL analyses presented in Chapters 10 and 11.

After the GRL selection, additional cleaning requirements are applied to remove events with ambiguities [122]. This amounts to removing events with significant noise in the calorimeters or data corruption which satisfy the following flags:

- LAr noise burst and data corruption (`xAOD::EventInfo::LAr`),
- Tile corrupted events (`xAOD::EventInfo::Tile`),
- Events with tagged with *bad* muon(s).

8.2 Monte Carlo samples

This section describes the MC generators used for simulating different SM processes used in the analyses in this dissertation, following the discussion in Section 6.3. Table 8.1 shows the configurations used for simulating SM processes, with the samples in parentheses indicating those used to estimate the systematic uncertainties. All simulated samples, except those produced with the SHERPA event generator, utilised EVTGEN 1.2.0 to model the decays of heavy-flavour hadrons. All samples showered with PYTHIA use the A14 set of tuned parameters, whereas those showered with HERWIG use the H7-UE tune. All samples include leading-logarithm photon emission, either modelled by the parton shower generator or by PHOTOS [123]. Pile-up was modelled using events from MinBias interactions generated with PYTHIA 8.186 with the A3 tune, and overlaid onto the simulated hard-scatter events according to the luminosity profile of the recorded data. The generated events were processed through either a full simulation (FS) of the ATLAS detector geometry and response using GEANT4, or a faster simulation where the full GEANT4 simulation of the calorimeter response is replaced by a detailed parametrization of the shower shapes (*Fast Simulation* or AF2). Both types of simulated events were processed through the same reconstruction software used for the *pp* collision data and corrected to match identification, reconstruction and jet energy scale and resolution from data, with dedicated uncertainties estimated for

each of these corrections and considered in the analyses. The MC samples are normalised to their cross sections, and generated to the highest order available in perturbation theory.

Process	Generator	ME order	Parton shower	PDF	Tune
$t\bar{t}W$	SHERPA 2.2.10 (MADGRAPH5_AMC@NLO)	NLO (NLO)	SHERPA (PYTHIA 8.2)	NNPDF3.0 NNLO (NNPDF3.0 NLO)	SHERPA default (A14)
$t\bar{t}t\bar{t}$	MADGRAPH5_AMC@NLO (SHERPA 2.2.10)	NLO (NLO)	PYTHIA 8.2 (SHERPA)	NNPDF3.1 NLO (NNPDF3.0 NNLO)	A14 (SHERPA default)
$t\bar{t}H$	POWHEG-BOX (Powheg-BOX) (MADGRAPH5_AMC@NLO)	NLO (NLO) (NLO)	PYTHIA 8.2 (HERWIG7.0.4) (PYTHIA 8.2)	NNPDF3.0 NLO (NNPDF3.0 NLO) (NNPDF3.0 NLO)	A14 (H7-UE-MMHT) (A14)
$t\bar{t}(Z/\gamma^* \rightarrow l^+l^-)$	SHERPA 2.2.11 (MADGRAPH5_AMC@NLO)	NLO (NLO)	SHERPA (PYTHIA 8.2)	NNPDF3.0 NNLO (NNPDF3.0 NLO)	SHERPA default (A14)
$t\bar{t} \rightarrow W^+bW^-\bar{b}l^+l^-$	MADGRAPH5_AMC@NLO	LO	PYTHIA 8.2	NNPDF3.0 LO	A14
$t(Z/\gamma^*)$	MADGRAPH5_AMC@NLO	NLO	PYTHIA 8.2	NNPDF2.3 LO	A14
$tW(Z/\gamma^*)$	MADGRAPH5_AMC@NLO	NLO	PYTHIA 8.2	NNPDF2.3 LO	A14
$t\bar{t}W^+W^-$	MADGRAPH5_AMC@NLO	LO	PYTHIA 8.2	NNPDF2.3 LO	A14
$t\bar{t}$	POWHEG-BOX (Powheg-BOX) (MADGRAPH5_AMC@NLO)	NLO (NLO) (NLO)	PYTHIA 8.2 (HERWIG7.0.4.1.3) (PYTHIA 8.2)	NNPDF3.0 NLO (NNPDF3.0 NLO) (NNPDF3.0 NLO)	A14 (H7-UE-MMHT) (A14)
$t\bar{t}t$	MADGRAPH5_AMC@NLO	LO	PYTHIA 8.2	NNPDF2.3 LO	A14
s -, t -channel, Wt single top	POWHEG-BOX	NLO	PYTHIA 8.2	NNPDF3.0 NLO	A14
$VV, qqVV,$ $lowm_{\ell\ell}, VVV$	SHERPA 2.2.2	NLO	SHERPA	NNPDF3.0 NNLO	SHERPA default
$Z \rightarrow l^+l^-$	SHERPA 2.2.11	NLO	SHERPA	NNPDF3.0 NLO	SHERPA default
$Z \rightarrow l^+l^-$ (matCO)	POWHEG-BOX	NLO	PYTHIA 8.2	CTEQ6L1 NLO	A14
$Z \rightarrow l^+l^-+(\gamma^*)$	POWHEG-BOX	NLO	PYTHIA 8.2	CTEQ6L1 NLO	A14
W +jets	SHERPA 2.2.1	NLO	SHERPA	NNPDF3.0 NLO	SHERPA default
VH	POWHEG-BOX	NLO	PYTHIA 8.2	NNPDF3.0 NLO	A14
$t\bar{t}ZZ$	MADGRAPH	LO	PYTHIA 8.2	NNPDF2.3 LO	A14
$t\bar{t}HH$	MADGRAPH	LO	PYTHIA 8.2	NNPDF2.3 LO	A14
$t\bar{t}WH$	MADGRAPH	LO	PYTHIA 8.2	NNPDF2.3 LO	A14

Table 8.1: Configurations used for MC generation of SM processes. The samples used to estimate the systematic uncertainties are indicated in between parentheses. The mass of the top quark and SM Higgs boson were set to 172.5 GeV and 125 GeV.

For the g2HDM analysis in Chapter 9, $t\bar{t}Z$ was modelled using SHERPA 2.2.11 due to the more detailed modeling of high jet multiplicity, relevant to the analysis. On the other hand, VLL analyses in Chapters 10 and 11 use $t\bar{t}Z$ MC generated using MADGRAPH5_AMC@NLO as the nominal due to a more complete systematic recommendation for modelling the variation of the A14 tune in *Pythia 8*. Further, alternative $t\bar{t}$ samples were used in the systematic model in VLL analyses in Sections 10 and 11 exploring the $2\ell OS$ channel where this is the dominant background. Details on the simulation of signal samples specific to each model are described in the respective chapters.

8.3 Object selection and reconstruction

8.3.1 Analysis framework

Object reconstruction, calibration and event selection is performed using a two-step framework. The first framework, based on AnalysisTop, is called *Group Framework 1* (GFW1) [124] and used to produce ROOT files using HIGG8D1 physics derivations [125]. For the g2HDM analysis in Chapter 9, ANALYSISBASE 21.2.196 is used, while the VLL analyses in Chapters 10 and 11 use ANALYSISBASE 21.2.250. Output ROOT files from GFW1 are processed by *Group Framework 2* (GFW2) [126] where an event-level selection and custom analysis variables are defined. Finally, histogram creation from the GFW2 output and statistical analysis is performed using the TREXFITTER framework [127, 128], discussed further in Section 8.6.

8.3.2 Triggers

Events are required to be selected by single light lepton triggers (SLT) or dilepton triggers (DLT) respectively. The lowest p_T -threshold, un-prescaled SLT and DLT chains used in the trigger decision for the 2015, 2016, 2017 and 2018 datasets are summarised in Table 8.2. If matched, the reconstructed lepton transverse momentum is required to be 1 GeV higher than the threshold set to the online trigger object.

Single lepton triggers (2015)	
μ	HLT_mu20_iloose_L1MU15, HLT_mu50
e	HLT_e24_lhmedium_L1EM20VH, HLT_e60_lhmedium, HLT_e120_lhloose
Dilepton triggers (2015)	
$\mu\mu$ (asymm.)	HLT_mu18_mu8noL1
ee (symm.)	HLT_2e12_lhloose_L12EM10VH
$e\mu, \mu e$ ($\sim$ symm.)	HLT_e17_lhloose_mu14
Single lepton triggers (2016)	
μ	HLT_mu26_ivarmedium, HLT_mu50
e	HLT_e26_lhtight_nod0_ivarloose, HLT_e60_lhmedium_nod0, HLT_e140_lhloose_nod0
Dilepton triggers (2016)	
$\mu\mu$ (asymm.)	HLT_mu22_mu8noL1
ee (symm.)	HLT_2e17_lhvloose_nod0
$e\mu, \mu e$ ($\sim$ symm.)	HLT_e17_lhloose_nod0_mu14
Single lepton triggers (2017 / 2018)	
μ	HLT_mu26_ivarmedium, HLT_mu50
e	HLT_e26_lhtight_nod0_ivarloose, HLT_e60_lhmedium_nod0, HLT_e140_lhloose_nod0
Dilepton triggers (2017 / 2018)	
$\mu\mu$ (asymm.)	HLT_mu22_mu8noL1
ee (symm.)	HLT_2e24_lhvloose_nod0
$e\mu, \mu e$ ($\sim$ symm.)	HLT_e17_lhloose_nod0_mu14

Table 8.2: List of lowest p_T -threshold, un-prescaled single lepton and dilepton triggers used for 2015-2018 data-taking.

In addition to the above triggers, selection efficiency in the VLL4321 analysis Section 11 is improved by using the missing transverse energy (E_T^{miss}) triggers, summarised in Table 8.3. Above $E_T^{\text{miss}} > 200$ GeV, these triggers provide 100% efficiency in selection.

Trigger	Period
HLT_xe70_mht	15
HLT_xe90_mht_L1XE50	16 A - 16 D3
HLT_xe100_mht_L1XE50	16 D4 - 16 F1
HLT_xe110_mht_L1XE50	16 F2 - 16 end
HLT_xe110_pufit_L1XE55	17 B1 - 17 D5
HLT_xe110_pufit_L1XE50	17 D6 - 17 end
HLT_xe110_pufit_xe70_L1XE50	18 B - 18
HLT_xe110_pufit_xe65_L1XE50	18 C5 - 18 end

Table 8.3: List of E_T^{miss} triggers used for 2015-2018 data-taking.

8.3.3 Object preselection

The two-level GFW selects physics objects with a minimal set of cuts called *preselection* cuts, which are then tightened according to the analysis requirement. This section presents details of preselection cuts used for the reconstruction of light leptons, jets, hadronically decaying τ and missing transverse energy used in the analyses, building up on the discussion in Section 7. Tighter, analysis specific cuts are detailed in the respective chapters.

Light leptons

Electron candidates are reconstructed from energy clusters in the ECAL matched to a track in the ID and required to satisfy $p_T > 10$ GeV and $|\eta_{\text{cluster}}| < 2.47$, excluding the transition region between the endcap and barrel calorimeters ($1.37 < |\eta_{\text{cluster}}| < 1.52$). The *LooseAndBLayerLH* ID operating point (OP) and *FCLoose* isolation OP are used for identifying electrons. Muon candidates are reconstructed by performing a combined fit of the track information from the ID and MS and required to satisfy $p_T > 10$ GeV and $|\eta| < 2.5$. The *Loose* ID OP and *FCLoose* isolation OP are used for muon identification. Electron (muon) candidates are matched to the primary vertex by requiring the significance of their transverse impact parameter $|d_0/\sigma(d_0)| < 5$ (3) and their longitudinal impact parameter $|z_0 \sin \theta| < 0.5$ mm. Table 8.4 and Table 8.5 summarise the electron and muon

selection criteria used in the analyses together with additional quality and calibration flags. The lepton cuts are optimised depending on the lepton multiplicity channel, the main background processes and the expected number of events in each channel: the 2ℓ SS (2ℓ OS) channel is defined with two same-sign (opposite-sign) loose leptons, while the 3ℓ and 4ℓ channels are defined with three and four leptons respectively.

Feature	Criterion
Identification	Tight likelihood
Isolation	FCLoose/ PromptLeptonImprovedVeto Tight or VeryTight
Pseudorapidity range	$(\eta < 1.37) \quad \quad (1.52 < \eta < 2.47)$
Energy calibration	es2018_R21_v0 (ESModel)
Transverse momentum	$p_T > 10 \text{ GeV} / p_T > 20 \text{ GeV}$ (2ℓ OS/ 2ℓ SS), $p_T > 10 \text{ GeV}$ (4ℓ), $p_T > 10 \text{ GeV}$ (3ℓ)
Object quality	Not from a bad calorimeter cluster (BADCLUSELECTRON) Remove clusters from regions with EMEC bad HV (2016 data only)
Track to vertex association	$ d_0^{\text{BL}}(\sigma) < 5$ $ \Delta z_0^{\text{BL}} \sin \theta < 0.5 \text{ mm}$

Table 8.4: Summary of the electron selection criteria used in the analyses in this dissertation.

Feature	Criterion
Identification	Loose / Medium
Isolation	FCLoose/ PromptLeptonImprovedVeto Tight or VeryTight
Veto	BADMUONVETO
Momentum calibration	Sagitta correction used
Transverse momentum	$p_T > 10 \text{ GeV} / p_T > 20 \text{ GeV}$ (2ℓ OS), $p_T > 10 \text{ GeV}$ (4ℓ), $p_T > 10 \text{ GeV}$ (3ℓ)
$ \eta $ cut	< 2.5
multirow2*Track to vertex association	$ d_0^{\text{BL}}(\sigma) < 3$ $ \Delta z_0^{\text{BL}} \sin \theta < 0.5 \text{ mm}$

Table 8.5: Summary of the muon selection criteria used in the analyses in this dissertation.

Heavy-flavour non-prompt leptons are further rejected using a boosted decision tree (BDT) discriminant, referred to as the *Prompt Lepton Improved Veto* (PLIV) [129], based on isolation and lifetime information about a track-jet that matches the selected lepton. This BDT is introduced in Chapter 7.

Electrons with incorrect charge assignment, called QMisID, are suppressed using a dedicated Electron Charge Identification Selector (ECIDS) tool, based on calorimeter and tracking quantities [130]. The ECIDS tool has an efficiency of approximately 96(81)% in the barrel (endcaps) region. An ECIDS selection of $\text{BDT} > 0.7$ is used as part of the TightLH electron ID definition in all analyses.

While most electrons arising from photon conversions in the detector material (termed *material conversions*) are rejected by the standard electron identification selection, additional

requirements are imposed to remove any residual candidates. These candidates are identified as have a reconstructed, displaced vertex with radius $r > 20$ mm (including the track associated with the electron) and an invariant mass of the associated track and the closest (in $\Delta\eta$) opposite-charge track reconstructed in the silicon detector, (calculated at the conversion vertex) as < 100 MeV. *Internal conversion* candidates, which correspond to the internal photon conversions ($\gamma^* \rightarrow e^+e^-$), are identified as those failing the requirements for material conversions and with a di-track invariant mass calculated here at the primary vertex to be less than 100 MeV.

The various prompt-lepton working points used in the analyses in this dissertation are summarised in Table 8.6. After the initial categorisation based on loose leptons, the best lepton working point to further optimise the event selection is chosen, depending on the main background processes and available data in each category.

	Electron					Muon				
Lepton definition	L	L^*	M	M_{ex}	T	L	L^*	M	M_{ex}	T
Identification	Loose	Tight				Loose	Medium			
Transverse impact parameter significance $ d_0 /\sigma_{d_0}$	< 5					< 3				
Longitudinal impact parameter z_0	$ z_0 \sin \theta < 0.5 \text{ mm}$									
Isolation	Yes					Yes				
Non-prompt lepton OP	–	<i>Tight</i>	<i>Tight-not-VeryTight</i>	<i>VeryTight</i>		–	<i>Tight</i>	<i>Tight-not-VeryTight</i>	<i>VeryTight</i>	
Electron charge-misassignment veto	–	Yes				–				
Electron conversion candidate veto	–	Yes (except e^*)				–				

Table 8.6: Description of the loose inclusive (L), loose with tighter identification (L^*), medium inclusive (M), medium exclusive (M_{ex}), and tight (T) lepton definitions. The electron e^* is required to fulfil, in addition to the corresponding lepton definition requirements, those corresponding to an internal or material conversion candidate.

Jets

Jet candidates are reconstructed from particle flow objects [104] using the anti- k_T algorithm [105] with a radius parameter of $R = 0.4$. Only jet candidates with $p_T > 25$ GeV and within $|\eta| < 2.5$ are selected. Further, each jet with $p_T < 60$ GeV and $|\eta| < 2.4$ is required to satisfy the *Tight* working point of the JVT criteria [106, 107] to identify jets originating from the primary vertex. Jets are calibrated using simulation with in-situ techniques described in Section 7.4.1. A set of quality criteria is also applied to reject events containing at least one jet arising from non-collision sources or detector noise [131]. Table 8.7 summarises the jet selection criteria used in the analysis.

Feature	Criterion
Algorithm	Anti- k_T
R -parameter	0.4
Input constituent	PFlow
Analysis release number	21.2.196 or 21.2.250
CalibArea tag	
Calibration configuration	JES_MC16Recommendation_Consolidated_EMTopo_Apr2019_Rel21.config
Calibration sequence (Data)	JetArea_Residual_EtaJES_GSC_Insitu
Calibration sequence (MC)	JetArea_Residual_EtaJES_GSC_Smear
Selection requirements	
Observable	Requirement
Jet cleaning	LooseBad
BadBatMan cleaning [132]	No
p_T	$> 25\text{GeV}$
$ \eta $	< 2.5
JVT	> 0.5 for $p_T < 60\text{GeV}$, $ \eta < 2.4$

Table 8.7: Summary of the jet reconstruction criteria used in the analyses in this dissertation.

Jets containing b -hadrons are identified (b -tagged) via the DL1r algorithm mentioned in Section 7.4.3. A jet is considered b -tagged if the b -tagging score is above a certain threshold, corresponding to average expected efficiencies of 85%, 77%, 70%, or 60%, determined for jets with $p_T > 20$ GeV and $|\eta| < 2.5$ in simulated $t\bar{t}$ events. Correction factors derived from dedicated calibration samples enriched in b -jets, c -jets, or light jets, are applied to the simulated event samples [133–135]. Table 8.8 summarises the b -tagging jet selection criteria used in the analysis. An additional variable called the *pseudo-continuous b -tagging score* (PCBT) is obtained by ordering the resulting five exclusive bins from the four b -tagging WPs from higher to lower b -jet efficiency and used as input to the neural network classifiers in the respective analyses. An additional PCBT extrapolation uncertainty is derived for jets with $p_T > 400$ GeV for b -jets, 250 GeV for c -jets, and 300 GeV for light jets and used

in the 2HDM analysis, described in Chapter 9. The VLL analyses, on the other hand, use centralised PCBT uncertainty recommendations.

Feature	Criterion
	PFlow Jets
Jet collection	AntiKt4EMPFlowJets
Jet selection	$pT > 25\text{GeV}$ $ \eta < 2.5$ same JVT cuts as for jets
Algorithm	DL1r
Operating point	Pseudo-continuous Eff = 60/77%
CDI (2HDM)	2020-21-13TeV-MC16-CDI-2021-04-16_v1
CDI (VLL)	2023-21-13TeV-MC16-CDI-2023-07-18_v1

Table 8.8: Summary of the b -tagging selection criteria used in the analyses in this dissertation.

Hadronically-decaying τ leptons

Hadronically decaying τ -lepton candidates, denoted by τ_{had} , are reconstructed from energy clusters in the calorimeters and associated inner detector tracks. They are required to have either one or three associated tracks originating from the primary vertex (referred to as *one-prong* and *three-prong* τ_{had} candidates, respectively), with a total charge of ± 1 and further satisfying $p_T > 20 \text{ GeV}$ and $|\eta| < 2.5$, excluding the EM calorimeter's transition region. A recurrent neural network discriminant using calorimeter and tracking-based variables is used to identify real τ_{had} candidates and reject jet backgrounds (referred to as *fake* τ_{had} candidates) [118]. The *Loose*, *Medium* and *Tight* ID working points (WP) are created based on the RNN output. The loose WP has a target efficiency of 85% (75%) for one-prong (three-prong) τ_{had} candidates. The efficiencies for the medium working point are 75% (60%) for one-prong (three-prong) τ_{had} candidates, respectively. The tight working point has average efficiency of 60% (45%) for one-prong (three-prong) τ_{had} candidates. Electrons reconstructed as one-prong τ_{had} candidates are removed using a BDT with an efficiency of 95% for real τ_{had} candidates depending on the p_T . Additionally, τ_{had} candidates are required to be separated by $\Delta R > 0.2$ from any selected electron or muon candidates. τ_{had} reconstruction and identification efficiencies and energy scale in the simulation are

calibrated to those measured in a data control sample of $Z \rightarrow \tau^+ \tau^-$ events [116] and the associated uncertainties are considered in the analysis. Table 8.9 summarises the criteria used for selecting τ_{had} candidates in the VLL4321 analysis.

Feature	Criterion
Pseudo-rapidity range	$(\eta < 1.37) \vee (1.52 < \eta < 2.5)$
Track selection	1 or 3 tracks
Charge	$ Q = 1$
Tau energy scale	MVA TES
Transverse momentum	$p_T > 20\text{GeV}$
Jet rejection	RNN-based (Loose)
Electron rejection	BDT-based

Table 8.9: Summary of the criteria used for selecting hadronically decaying τ -lepton candidates in the VLL4321 analysis.

Missing transverse energy

The E_T^{miss} reconstruction criteria are summarised in Table 8.10.

Parameter	Value
Algorithm	Calo-based
Soft term	Track-based (TST)
MET operating point	Tight
Selection requirements	
Observable	Requirement
E_T^{miss}	No cut
$\sum E_T / E_T^{\text{miss}}$	No cut
Object-based E_T^{miss} significance	No cut

Table 8.10: Summary of the E_T^{miss} reconstruction criteria used in the analyses in this dissertation.

Overlap removal

Light leptons passing the Loose ID criteria, τ_{had} tagged with the loose RNN WP and jets passing the JVT requirement are considered for *overlap removal* to uniquely identify

these objects. If two electrons are separated by $\Delta R < 0.1$, only the one with the higher p_T is kept. If an electron and a muon overlap within $\Delta R < 0.1$, the muon is removed if it is reconstructed only from an ID track and calorimeter energy deposits consistent with a minimum-ionising particle, otherwise the electron is removed. If an electron and a selected jet are found within $\Delta R < 0.2$, the jet is removed. For each electron in the event a p_T -dependent variable-size cone of maximum size $\Delta R = 0.4$ is defined. If a selected jet, surviving all previous overlap criteria, is found in this cone, the lepton is rejected. The same procedure is also applied between jets and muons, with the exception that, if a muon and a jet overlap with $\Delta R < 0.2$, the jet is removed, unless the number of tracks in the jet is more than 2. Specific to the VLL4321 analysis which also reconstructs τ_{had} candidates, a jet is rejected if it overlaps with a τ_{had} within $\Delta R = 0.2$. Further, τ_{had} is rejected if it overlaps with an electron (muon) within $\Delta R = 0.2(0.25)$.

8.4 Analysis strategy

8.4.1 Event categorisation

In all analyses, *signal regions* (SR) are defined as the phase space where maximum signal acceptance is expected, constructed by studying the signal topology through Feynman diagrams and kinematic studies on the MC samples. Following this, major SM backgrounds living in the same phase space can be derived. A well-understood estimation of these backgrounds is important to claim discovery of a possible new signal process. The modelling of these backgrounds is checked in dedicated regions called *control regions* (CR) defined orthogonal to the SR, but as close as possible in phase space. Corrections to modelling of SM backgrounds can also be derived in such regions. In the searches for BSM particles, typically a profile likelihood fit (discussed in Section 8.6) is performed to estimate the normalisation of major SM backgrounds together with the signal strength using bins from the SRs and CRs. *Validation* regions (VRs) may be defined close to SRs by inverting a cut or two, to further test the modelling of backgrounds after the fit. An illustration of event categorisation is shown in Figure 8.1.

8.4.2 Signal-to-background discrimination

The analyses in this dissertation use deep neural networks (DNNs) in the SRs to distinguish between signal topologies and reject SM backgrounds. Discrimination between signal

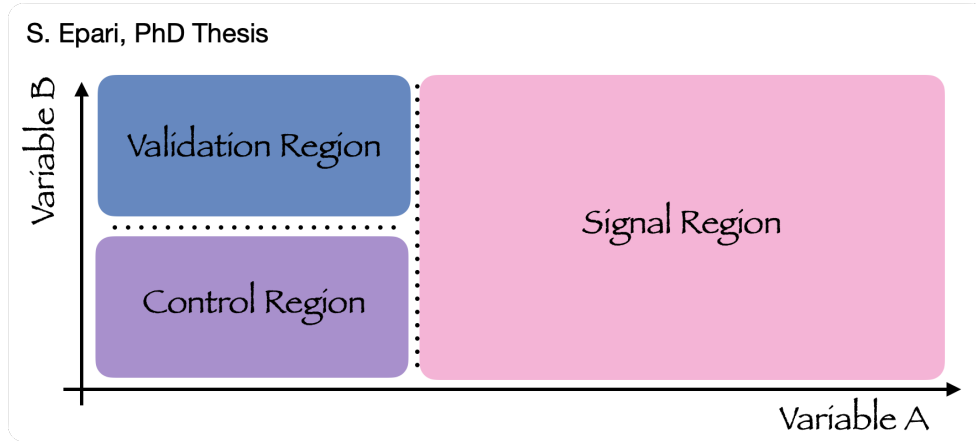


Figure 8.1: Illustration of signal, control and validation regions for a two-dimensional phase space defined using hypothetical variables. These regions are defined to be orthogonal to each other.

topologies, in particular, is an approach that is fast gaining importance because it has the potential to improve the re-usability and reach of the search, to re-interpret models with similar final states. DNNs combine the power of multiple variables into a single non-linear function, allowing for complex decision boundaries and feature extraction. Consider a simple neural network with one hidden layer, illustrated in Figure 8.2. Let x_1 and x_2 be the input variables, w_{ij} the weights, b_j the biases, and σ the activation function. The output of the hidden layer neurons can be expressed as:

$$h_j = \sigma(w_{1j}x_1 + w_{2j}x_2 + b_j)$$

where j indexes the neurons in the hidden layer. If we have two hidden neurons, the outputs are:

$$h_1 = \sigma(w_{11}x_1 + w_{21}x_2 + b_1)$$

$$h_2 = \sigma(w_{12}x_1 + w_{22}x_2 + b_2)$$

The final output y of the network, combining these hidden neurons, is given by:

$$y = \sigma(v_1h_1 + v_2h_2 + b)$$

where v_i are the weights connecting the hidden layer to the output neuron, and b is the bias term for the output neuron. *Training* the DNN on a labelled dataset with features x_1 and

x_2 amounts to estimating the best fit function y by determining the weights w_{ij} and biases b_j . *Categorical crossentropy* is a loss function used in classification tasks where the model outputs a probability distribution over multiple classes. It measures the difference between the true label distribution and the predicted probability distribution. Mathematically, for a single instance, it is defined as

$$-\sum_i y_i \log(\hat{y}_i),$$

where y_i is the true label and $\hat{y}_i$ is the predicted probability for class i . This loss function is highly effective for multiclass classification problems as it penalizes incorrect classifications more severely when the predicted probability is high. It encourages the model to output probabilities that are as close as possible to the true labels, leading to better predictive performance.

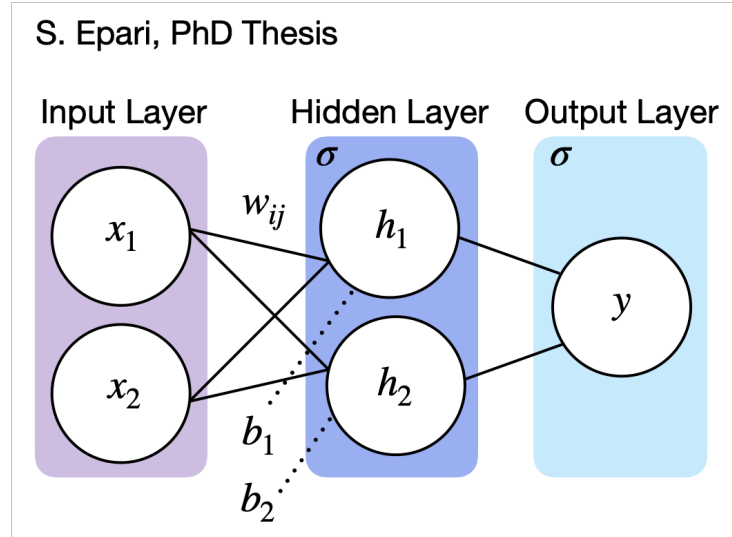


Figure 8.2: Illustration of a neural network with a single hidden layer.

A popular choice for the activation function is *Rectified Linear Unit* (ReLU), defined as $f(x) = \max(0, x)$, meaning it outputs the input directly if it is positive; otherwise, it outputs zero. Due to a constant gradient for positive values, it ensures that neurons activate and learn at a higher rate during training. *Batch training*, also known as mini-batch gradient descent, involves splitting the training dataset into smaller batches and updating the model weights iteratively for each batch. Using mini-batches helps in efficiently utilizing computational resources and reduces memory constraints, as only a subset of data needs to be loaded at any time. It also smoothens the gradient descent process by averaging out the noise introduced by individual samples, leading to more stable convergence.

The *Adaptive Moment Estimation* (Adam) optimizer [136] is an advanced optimization algorithm used in training deep learning models. Adam maintains two moment estimates: the first moment (mean) and the second moment (uncentered variance) of the gradients. These moments are used to adapt the learning rate for each parameter individually, allowing for efficient and effective training. Adam is particularly advantageous for handling sparse gradients and noisy problems. It uses adaptive learning rates that adjust based on the mean and variance of the gradients, providing robust convergence properties and typically requiring less fine-tuning of the learning rate hyperparameter compared to other optimizers.

The *learning rate* is a parameter that controls how the weights of the DNN are adjusted with respect to the loss gradient during training. A high learning rate can cause the model to converge too quickly to a sub-optimal solution or even diverge, as the updates might overshoot the optimal point. Conversely, a low learning rate can lead to a slow convergence process, requiring more time and computational resources, and can sometimes get the model stuck in local minima. Finding the right learning rate is often done through experimentation or using techniques like learning rate schedules and adaptive learning rates to dynamically adjust it during training.

The *softmax function* is used in the output layer of a neural network for multiclass classification problems. It converts uncalibrated predictions into a probability distribution over the classes. Mathematically, the softmax function for an output vector $\mathbf{z}$ is defined as

$$\text{softmax}(z_i) = \frac{e^{z_i}}{\sum_j e^{z_j}},$$

where z_i is the logit for class i . This ensures that the output probabilities sum up to 100%, making it suitable for interpreting the network's output as probabilities of different classes. Softmax is particularly useful because it highlights the predicted class while considering the relative scale of the logits, thus providing a clear and probabilistic interpretation of the model's predictions. It is typically paired with the categorical crossentropy loss during training to optimize the model's ability to predict the correct class labels.

Training of the DNNs is done using the KERAS library [137] with TENSORFLOW as a backend [138] with training variables specific to the signal model used to distinguish between signal topologies and SM background. The details of these DNNs are specified in the respective chapters.

8.5 Systematic uncertainties

This section presents a summary of experimental and theoretical systematic uncertainties included in the fit model in the analyses in this dissertation. Additional systematic uncertainties specific to the analysis are specified in the respective chapters. A smoothing algorithm based on the *MaxVariation* is used by default for all systematic uncertainties to mitigate the impact from limited MC statistics. This algorithm re-bins the distribution till the relative MC uncertainty drops below a defined threshold. Instrumental uncertainties are two-sided and symmetrized. Systematic uncertainties with an effect below 1% are *pruned* from the fit.

8.5.1 Experimental uncertainties

Experimental uncertainties included in the analyses are related to trigger efficiency, lepton reconstruction and identification, jet calibration, b-tagging and the global event activity. These recommendations are evaluated by ATLAS performance groups and are used in the analysis either as an overall event reweighting or as a re-scaling of the object energy and momentum. The list of systematic uncertainties included in the analysis is summarised in Tables [8.11](#), [8.12](#), [8.13](#) and [8.14](#).

Experimental systematics on leptons			
Type	Description		Systematics name
Trigger			
Scale Factors	e/μ Trigger Eff.		TightElMediumMuID_FCLooseIso_SLTorDLT
Scale Factors	MET Trigger Eff.		MET
Muons			
Efficiencies	Reco. and ID		MU_SF_ID_[STAT,SYST]
	Reco. and ID (low p_T)		MU_SF_ID_[STAT,SYST]_LOWPT
	Isolation		MU_SF_Isol_[STAT,SYST]
	Track-to-Vertex Association		MU_SF_TTVA_[STAT,SYST]
p_T Scale	p_T Scale		MUONS_SCALE
Resolution	ID p_T Resol.		MUONS_ID_[STAT,SYST]
	MS p_T Resol.		MUONS_MS
	MS p_T Resol. (charge dependent)		MUONS_SAGITTA_[RHO,RESBIAS]
Isolation	PLIV calib.		PLIV_Mu_*
Electrons			
Efficiencies	Reco.		EL_SF_Reco
	ID		EL_SF_ID
	Isolation		EL_SF_Isol
	PLIV calib.		PLIV_El_*
Scale Factor	Energy Scale		EG_SCALE_ALL
Resolution	Energy Resolution		EG_RESOLUTION_ALL

Table 8.11: Summary of experimental systematic uncertainties related to muons and electrons used in the analyses in this dissertation.

Experimental systematics on τ_{had}		
Type	Description	Systematics name
Hadronic Taus		
Efficiencies	Reco.	SF_RECO_TOTAL
	RNN ID	SF_RNNID_1P[2530,GE40] SF_RNNID_3P[2530,GE40]
	RNN ID (High p_T)	SF_RNNID_SYST
	Reco. (High p_T)	SF_RNNID_HIGHPT
	Electron veto BDT	SF_ELEOLR_TOTAL
p_T Scale	Electron veto BDT (truth-matched e)	SF_TRUEELECTRON_ELEOLR_TOTAL
	p_T Scale	TRUEHADTAU_SME_TES_MODEL_CLOSURE TRUEHADTAU_SME_TES_DETECTOR TRUEHADTAU_SME_TES_INSITUEXP TRUEHADTAU_SME_TES_INSITUFIT TRUEHADTAU_SME_TES_PHYSICSLIST
Fake Taus		
Scale Factors	Tau mis-ID	FakeTau_SF_[STAT,SYST]_1P[2030,ge150]
	(p_T -dependent)	FakeTau_SF_[STAT,SYST]_3P[2040,ge90]

Table 8.12: Summary of experimental systematic uncertainties on hadronically decaying tau candidates in the VLL4321 analysis.

Experimental systematic uncertainties on jets and E_T^{miss}			
Type	Origin	Systematics name	Application
Pile-up reweighting			
Pile-up reweighting			
Jets			
Jet Vertex Tagger		JVT	
Energy Scale	Calibration Method	JET_EffectiveNP_Detector1 JET_EffectiveNP_Mixed[1,3] JET_EffectiveNP_Modelling[1,4] JET_EffectiveNP_Statistical[1,6]	
	η inter-calibration	JET_EtaIntercalibration_Modelling JET_EtaIntercalibration_NonClosure JET_EtaIntercalibration_TotalStat	
	High p_T jets	JET_SingleParticle_HighPt	
	Pile-Up	JET_Pileup_OffsetNPV JET_Pileup_OffsetMu JET_Pileup_PtTerm JET_Pileup_RhoTopology	
	Non Closure	JET_PunchThrough_MC16	
	Flavour	JET_Flavor_Response JET_BJES_Response JET_Flavor_Composition	
	Resolution	JET_JER	
E_T^{miss}			
Soft Tracks Terms	Resolution	MET_SoftTrk_ResoPerp	
	Resolution	MET_SoftTrk_ResoPara	
	Scale	MET_SoftTrk_Scale	

Table 8.13: Summary of experimental systematic uncertainties in the analysis related to jets and missing transverse energy. Jet systematic uncertainties take into account effects of jets calibration method (*e.g.* in situ), η inter-calibration, high p_T jets, pile-up, non closure, flavour response and are diagonalised into effective parameters.

Experimental systematics on b -jets		
Type	Origin	Systematics name
b-tagging		
Scale Factors	DL1r b-tagger eff. on b-originated jets	weight_bTagSF_DL1r_Continuous_ FT_EFF_Eigen_B[0-19]
	DL1r b-tagger eff. on c-originated jets	weight_bTagSF_DL1r_Continuous_ FT_EFF_Eigen_C[0-19]
	DL1r b-tagger eff. on light-flavoured jets	weight_bTagSF_DL1r_Continuous_ FT_EFF_Eigen_Light[0-19]
High- p_T extrapolation uncertainties	Extrapolation of b- and c-jets	PCBT extrapolation unc bc
	Extrapolation of light-jets	PCBT extrapolation unc l

Table 8.14: Summary of experimental systematic uncertainties in the analysis related to b -tagged jets, using the DL1r tagging algorithm. In the g2HDM analysis, PCBT extrapolation uncertainties are estimated using an in-house recipe due to the absence of official ATLAS recommendations at the time.

The implementation of JES uncertainties uses the *Category Reduction* scheme while the *Full JER* scheme is used for JER uncertainties. The uncertainty in the luminosity measurement is 1.7% in the g2HDM analyses and the re-processed value of 0.83% was used in the VLL analyses. This uncertainty is used as an independent nuisance parameter in the fit. Uncertainties related to τ_{had} are included only in the fits performed in the VLL4321 analyses and are listed in Table 8.12.

8.5.2 Theoretical uncertainties

Theoretical uncertainties common to all analyses are shown in Table 8.15. Systematic uncertainties in the signal modelling, background corrections and fake estimation specific to an analysis are described in the dedicated chapters. For the dominant background processes where there is an alternative MC sample available, the 2-point systematic built from the comparison between the nominal and the alternative MC samples is taken as a nuisance parameter. This is the case for $t\bar{t}W$, $t\bar{t}Z$, $t\bar{t}H$, $t\bar{t}$, and $t\bar{t}t\bar{t}$. For $t\bar{t}H$, $t\bar{t}W$, $t\bar{t}Z$, and VV , variations of the re-normalisation and factorisation scale by a factor of 0.5 and 2, available via internal weights are taken as additional modelling uncertainties. Uncertainties due to PDF effects are estimated by taking the differences with respect to alternative PDF sets where available. Normalisation uncertainties are included for all processes whose normalisation is not obtained from the likelihood fit: 20% [139], 11% [140] and 5% [141] respectively on the $t\bar{t}t\bar{t}$, $t\bar{t}H$ and tZ simulations. Finally, as a conservative estimate, a 50% cross section uncertainty is assigned to small backgrounds like VH , tWZ , tWH , $tHbj$, $t\bar{t}WH$, $t\bar{t}HH$, $t\bar{t}ZZ$, $t\bar{t}WW$ and triboson backgrounds. In the VLL analyses where prompt $t\bar{t}$ is a leading background, additional uncertainties are applied due to iterative reweighting of events at the next-to-next-to leading order theory predictions in terms of top quark p_T , $p_{T,t\bar{t}}$, and $m_{t\bar{t}}$ [142]. In the same analysis, Z+jets is also a dominant background in some channels, and dedicated uncertainties in the re-summation and CKKW merging scale are derived and used. A detailed description of these uncertainties is described in Section 10.4.

Theory systematic uncertainties		
Systematics name	Analysis	
	2HDM	VLLs
$t\bar{t}$ systematic uncertainties		
Parton shower and hadronisation	X	Y
Matrix element and parton shower matching	X	Y
FSR μ_R	X	Y
Pythia8 A14 Var3c	X	Y
Matrix element μ_R	X	Y
Matrix element μ_F	X	Y
$t\bar{t}$ NNLO iterative reweighting	X	Y
(scaling of top p_T , $m_{t\bar{t}}$, and $p_T^{t\bar{t}}$; μ_R and μ_F variations of top p_T ; μ_R and μ_F variations of $m_{t\bar{t}}$)		
Single top systematic uncertainties		
tW diagrams removal vs subtraction	X	Y
Z+jets systematic uncertainties		
Z+jets CKKW	X	Y
Z+jets QSF	X	Y
Z+jets alternative LO-EW matching weight	X	Y
$t\bar{t}Z$ systematic uncertainties		
$t\bar{t}Z$ generator and shower	Y	Y
$t\bar{t}Z$ μ_R variation	Y	Y
$t\bar{t}Z$ μ_F variation	Y	Y
$t\bar{t}W$ systematic uncertainties		
$t\bar{t}W$ generator and shower	Y	Y
$t\bar{t}W$ μ_R variation	Y	Y
$t\bar{t}W$ μ_F variation	Y	Y
$t\bar{t}H$ systematic uncertainties		
$t\bar{t}H$ cross-section normalisation (11%)	Y	Y
$t\bar{t}H$ generator acceptance	Y	Y
$t\bar{t}H$ parton shower	Y	Y
$t\bar{t}H$ μ_R variation	Y	Y
$t\bar{t}H$ μ_F variation	Y	Y
Diboson systematic uncertainties		
VV cross-section normalisation (3% in the 2HDM analysis)	Y	Y
VV μ_R , variation	Y	Y
VV μ_F , variations	Y	Y
Four top systematic uncertainties		
$tt\bar{t}\bar{t}$ cross-section normalisation (20% in 2HDM and 29% in VLL analyses)	Y	Y
$tt\bar{t}\bar{t}$ generator	Y	Y
Other rare processes systematic uncertainties		
tZ cross-section normalisation (5%)	Y	Y
VH cross-section normalisation (50%)	Y	Y
tWZ cross-section normalisation (50%)	Y	Y
tWH cross-section normalisation (50%)	Y	Y
$tHbj$ cross-section normalisation (50%)	Y	Y
VVV cross-section normalisation (50%)	Y	Y
$ttWW$ cross-section normalisation (50%)	Y	Y
ttt cross-section normalisation (50%)	Y	Y
$ttZZ$, $t\bar{t}HH$, $t\bar{t}WH$ cross-section normalisation (50%)	Y	Y

Table 8.15: Summary of common theoretical systematic uncertainties in the analysis from the background modelling. Y (X) indicates that the corresponding systematic is (not) included in the fit model of the analysis.

8.6 Statistical analysis

The final state of a particle collision can be compatible with a multitude of theoretical frameworks, each known to limited precision due to computational and practical reasons. Further, the number of collision events recorded and the reconstruction of the final state of these events is affected by our understanding of detector response. Due to these limitations, experimental results in particle physics need to be interpreted within a statistical framework which takes into account these theoretical and experimental uncertainties in order to reach a robust conclusion. This section discusses briefly some of the theoretical and practical tools used for statistical analyses of datasets collected by the ATLAS experiment. A *frequentist's* approach to probability is going to form the basis of the discussion that is about to follow: given n independent experiments that make n independent observations of a property of the event, the probability of the event is understood as the fraction of favorable outcomes in the total number of repetitions of an experiment.

8.6.1 Constructing the likelihood function

The recorded properties of a collision event may include information about the number and properties of jets, leptons, missing transverse energy and other complex variables. Mathematically, this information can be encoded in a vector of length n associated with each event: $\vec{x} = (x_1, x_2, \dots, x_n)$. The *probability distribution function (pdf)*, denoted by $f(\vec{x}|\vec{\theta})$, describes the likelihood of observing the data $\vec{x}$ given a physics model with a set of parameters $\vec{\theta} = (\theta_1, \theta_2, \dots, \theta_n)$.

The goal of a physics analysis is to estimate the most probable values of $\vec{\theta}$ given the measured variables $\vec{x}$. The *likelihood function*, denoted by $L(\vec{\theta}|\vec{x})$, evaluates how likely it is for the observed data $\vec{x}$ have originated from a model with parameters $\vec{\theta}$. Maximizing the likelihood function provides the set of parameters that make the observed data $\vec{x}$ most probable. In Run 2, the ATLAS experiment recorded an estimated 100 million $t\bar{t}$ events. $t\bar{t}$ is one of the major backgrounds in the VLL analyses and reduces by about a factor of ten after preselection. Such a large number of events makes computation of the likelihood function and its maximization an expensive problem. The solution is to store the variables in histograms and use the number of events to construct an approximate likelihood. The expected number of events in each bin, n_i , is assumed to be Poisson distributed, so the likelihood function for the observed data to be produced by the model becomes:

$$L(\vec{\theta}|\vec{x}) = \prod_{i=1}^M \frac{\mu_i(\vec{\theta})^{n_i} e^{-\mu_i(\vec{\theta})}}{n_i!}, \quad (8.1)$$

where x_i is the observed number of events in bin i and $n_i \vec{\theta}$ is the expected number of events in that bin according to the model parameters $\vec{\theta}$.

The expected number of events in each bin comes with an associated uncertainty, arising from both statistical and systematic sources. Statistical uncertainties arise due to the finite number of events in each bin, while systematic uncertainties arise from our modeling of the detector response, the background processes, etc. The effect of systematic uncertainties can be included in the likelihood function through the use of *nuisance parameters (NPs)*. These NPs can be modeled through pdfs called *priors*, denoted as $\rho(\theta)$, that penalize the likelihood function and are estimated by auxiliary measurements. Depending on the NP, the pdf can assume different forms, shown in Figure 8.3:

- *Gaussian prior*, used for most systematic uncertainties that change the shape of the final discriminant, such as the jet energy scale.
- *Log-normal prior*, for normalization uncertainties.
- *Gamma prior*, used for statistical uncertainties associated with the number of selected MC events per bin.

The full likelihood can then be written as:

$$L(\vec{\theta}|\vec{x}) = \prod_{i=1}^M \frac{\mu_i(\vec{\theta})^{n_i} e^{-\mu_i(\vec{\theta})}}{n_i!} \times \prod_{k=1}^{N_{\text{NP}}} \rho(\theta_k^{\text{NP}}), \quad (8.2)$$

where $\mu_i(\vec{\theta})$ is the expected number of events in bin i , n_i is the observed number of events in bin i and θ_k^{NP} represents the nuisance parameters, each with its own prior $\rho(\theta_k^{\text{NP}})$.

8.6.2 Hypothesis testing

The discovery of a new particle involves testing the new BSM theory against the existing hypothesis, the SM. This comparison allows to assess the level of compatibility of the data with each hypothesis. Based on this comparison, statements about the existence or exclusion of a certain BSM theory can be made.

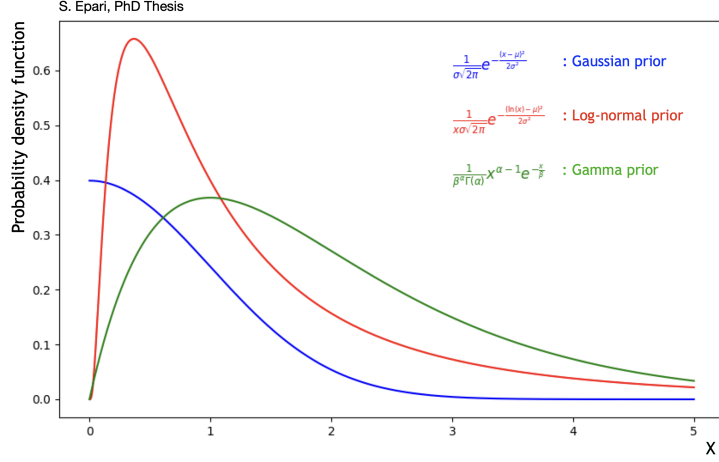


Figure 8.3: Comparison of Gaussian (blue), Log Normal (red), and Gamma (green) probability density functions. Each distribution is defined with parameters: Gaussian (mean = 0, std = 1), Log Normal (mean = 0, std = 1), and Gamma (shape = 2, rate = 1).

Traditionally, two hypotheses are defined as follows:

- H_0 or the *null hypothesis*, which corresponds to the SM hypothesis. This is also called the background-only (B-only) hypothesis.
- H_1 or the *alternative hypothesis*, which corresponds to the new signal model together with the SM hypothesis. This is also called the signal plus background (S+B) hypothesis.

The two hypotheses can be accommodated in the likelihood function (Equation 8.2) by introducing a signal strength parameter μ that modifies the number of expected events in a bin i as:

$$\mu_i(\vec{\theta}) = \mu s_i + b_i. \quad (8.3)$$

In terms of the NPs, the expected number of events b_i (or s_i) get modified as:

$$b_i = b_i^0 \left(1 + \sum_k \Delta b_i \theta_k^{\text{NP}} \right), \quad (8.4)$$

where b_i^0 is the expected number of background events in bin i without considering any systematic uncertainties and Δb_i represents the relative change in the expected number of events in bin i due to the k^{th} nuisance parameter θ_k^{NP} .

The B-only hypothesis is recovered for $\mu=0$ while $\mu \geq 1$ is the S+B hypothesis. The full likelihood can then be written as:

$$L(\vec{x}|\mu, \vec{\theta}) = \prod_{i=1}^M \frac{(\mu s_i + b_i)^{n_i} e^{-(\mu s_i + b_i)}}{n_i!} \times \prod_{k=1}^{N_{\text{NP}}} \rho(\theta_k^{\text{NP}}). \quad (8.5)$$

To simplify comparison with prefit values, NPs are redefined to be centered at 0 with unit width. This redefinition makes it easier to interpret the results of the fit in terms of *pulls* and *constraints*:

- **Pulls:** A fitted NP centered at a value different from 0 indicates a *pull*, meaning that the nominal background prediction has been modified by the fit, often using additional information from CRs or other constraints in the data. This suggests that the data provide evidence for a shift in the expected background relative to the prefit prediction.
- **Constraints:** A fitted NP with an uncertainty significantly smaller than 1 indicates a *constraint*. This means that the prefit uncertainty assigned to this NP has been reduced by the fit, implying that the observed data provided enough statistical power to constrain the NP more tightly than initially assumed.

This, if a fitted NP is centered at 0 with an error close to 1, it indicates that the fit did not have enough statistical power to significantly *pull* this NP or reduce its prefit uncertainty. In contrast, a post-fit *constraint* on an NP indicates that the prefit uncertainty was likely too large and has been refined using the observed data.

The compatibility of the observed data with a given hypothesis is tested using a *test statistic*. The most commonly used test statistic is called q_μ , computed from the likelihood function as:

$$q_\mu = -2 \ln \lambda(\mu) = -2 \ln \frac{L(\mu, \hat{\hat{\theta}}(\mu))}{L(\hat{\mu}, \hat{\theta})}, \quad (8.6)$$

where $L(\hat{\mu}, \hat{\theta})$ denotes the unconditional maximum likelihood and $L(\mu, \hat{\hat{\theta}}(\mu))$ is the conditional maximum likelihood computed for a fixed value of μ .

From the test statistic, a *p-value* can be computed as:

$$p_\mu = \int_{\text{data}}^{\infty} f(q_\mu|\mu) dq_\mu, \quad (8.7)$$

where $f(q_\mu|\mu)$ is the pdf of q_μ under the hypothesis μ and the integral is taken from the observed value of the test statistic to positive infinity. This integral represents the probability of obtaining a test statistic at least as extreme as the one observed, assuming the hypothesis μ is true.

If the p-value computed for the test hypothesis is lower than a predefined threshold, the hypothesis is excluded at a certain confidence level (CL). In particle physics, this threshold is typically set to 0.05, which corresponds to a 95% CL exclusion. This means that if the p-value is below 0.05, the hypothesis μ is rejected with 95% confidence. The test statistic used for discovery in particle physics often focuses on estimating the probability to reject the background-only hypothesis (denoted as H_0) if it is true. This specific p-value, referred to as p_0 , measures the significance of the observed excess over the expected background. Very low values of p_0 suggest that the background-only hypothesis is unlikely, which could indicate the presence of new physics. When p_0 is sufficiently low, it signals potential discovery, as the data significantly deviate from what is expected under the background-only scenario.

The p-value can be converted to the corresponding Gaussian *significance* denoted by Z , defined as:

$$Z = \Phi^{-1}(1 - p_0) \quad (8.8)$$

Here, Φ^{-1} is the inverse of the cumulative distribution function of the Gaussian distribution. The quantity, Z , measures the number of standard deviations that correspond to an upper-tail probability of p_μ for a Gaussian distributed variable. The following thresholds are commonly used in particle physics:

- *Exclusion* of a physics process occurs for values of Z below 1.68 ($p = 0.05$). This is referred to as the 95% Confidence Limit (CL).
- *Evidence* of a physics process is claimed at $Z = 3$ ($p = 0.0027$).
- *Discovery* of a physics process is claimed at $Z = 5$ ($p = 2.7 \times 10^{-7}$).

The pdf $f(q_\mu|\mu)$ is typically computed using pseudo-experiments and can be computationally expensive. For large statistics, assuming data to be distributed according to a strength parameter μ' , Wald's approximation [143] can be used to write:

$$q_\mu = -2 \ln \lambda(\mu) = \frac{(\mu - \hat{\mu})^2}{\sigma^2} + \mathcal{O}(1/\sqrt{N}). \quad (8.9)$$

Here, $\hat{\mu}$ is the fitted signal strength that follows a Gaussian distribution with mean μ' and standard deviation σ and N is the total number of events in the sample. The value of σ is

estimated from an artificial dataset called the *Asimov* dataset, defined as the one where the pseudo-data is equal to the sum of background predictions.

The pdf $f(q_\mu|\mu)$ simplifies to:

$$f(q_\mu, \Lambda) = \frac{1}{2\sqrt{q_\mu}} \frac{1}{\sqrt{2\pi}} \left[\exp\left(-\frac{1}{2}(\sqrt{q_\mu} + \sqrt{\Lambda})^2\right) + \exp\left(-\frac{1}{2}(\sqrt{q_\mu} - \sqrt{\Lambda})^2\right) \right], \quad (8.10)$$

on ignoring the $\mathcal{O}(1/\sqrt{N})$ term and the parameter Λ is defined as:

$$\Lambda = \frac{(\mu - \hat{\mu})^2}{\sigma^2} \quad (8.11)$$

This is known as the *asymptotic approximation* [143] and is used in this dissertation to compute the relevant p -values.

8.6.3 The CL_s method

In the event of a downward fluctuation in the observed number of events due to a lack of statistics, the p -value discussed in the previous section may lead to accidental exclusions of hypotheses. Essentially, the statistical fluctuation might suggest a false signal or deviation from the background-only hypothesis, which can lead to misleading conclusions if the fluctuation is interpreted as significant when it is actually a random fluctuation rather than a genuine effect. To resolve this issue, the CL_s method [144] is used, with a figure of merit defined as:

$$\text{CL}_s = \frac{\text{CL}_{s+b}}{\text{CL}_b} = \frac{p_{s+b}}{1 - p_b}, \quad (8.12)$$

with

$$p_{s+b} = P(q_\mu \geq q_{\mu,\text{obs}}|H_1) = \int_{q_{\mu,\text{obs}}}^{\infty} f(q_\mu|H_1) dq_\mu,$$

$$p_b = P(q_\mu \leq q_{\mu,\text{obs}}|H_0) = \int_0^{q_{\mu,\text{obs}}} f(q_\mu|H_0) dq_\mu.$$

A value of μ is excluded at $\geq 95\%$ confidence level (CL) if the CL_s value is ≤ 0.05 . The highest value of μ that can be excluded according to this criterion is known as the upper limit on μ and is denoted by μ_{up} . The upper limit computed from simulated data is referred to as the *expected* upper limit, while the upper limit computed from observed data

is called the *observed* upper limit. For simulated data, the confidence intervals associated with μ_{up} are determined by considering all potential values of μ_{up} that could be obtained if the experiment were repeated. These intervals reflect the range of μ_{up} values for which the null hypothesis H_0 cannot be rejected. The boundaries of the CIs, $\mu_{\text{up}}^{\pm 1\sigma}$ and $\mu_{\text{up}}^{\pm 2\sigma}$ are found at the $\pm 1\sigma$ and $\pm 2\sigma$ significance points of the $f(\mu_{\text{up}}|H_0)$ distribution and reported for all signal mass points in a search.

8.6.4 TRexFitter framework

Statistical analysis is performed using the TRexFitter framework [127, 128], which builds statistical models in the HistFactory format [145]. In all analyses, profile-likelihood fits are conducted using all bins of the signal and control regions, incorporating systematic uncertainties to extract the signal strength and normalisation factors for major background processes. The test statistic is evaluated with the RooFit package [146, 147]. Upper limits are derived using the CL_s method on the test statistic q_μ , implemented in the RooFit package. The Asimov dataset is used to estimate the expected sensitivity. The significance is obtained from the test statistic using the asymptotic formula [143].

Search for heavy Higgs bosons from a g2HDM in multilepton plus b -jets final states

The chapter presents the first-ever search for a general two Higgs doublet model (g2HDM) with flavor changing neutral currents (FCNC) in the extended Higgs sector. Section 9.1 provides an introduction to the g2HDM and discusses the specific g2HDM model that forms the content of this analysis. The following sections discuss the analysis strategy, estimation of SM backgrounds, systematic uncertainties and concludes with presenting the results of the analysis in Section 9.5. The search is also used to set limits on R-parity violating supersymmetric models, motivated by flavor anomalies. These results are discussed in Section 9.6.

9.1 Simplified model

A g2HDM is an extension of the SM consisting of two complex Higgs doublets, Φ_1 and Φ_2 :

$$\Phi_1 = \begin{pmatrix} \phi_1^+ \\ \frac{v_1 + \phi_1^0 + i\eta_1}{\sqrt{2}} \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} \phi_2^+ \\ \frac{v_2 + \phi_2^0 + i\eta_2}{\sqrt{2}} \end{pmatrix}. \quad (9.1)$$

where ϕ_1^0 (ϕ_2^0) and η_1 (η_2) denote the real parts and imaginary components and v_1 (v_2) denote the VEV of the Higgs field(s). This extension results in eight degrees of freedom in the model, reduced to five after electroweak symmetry breaking as three of the modes are absorbed by the W^+ , W^- and Z bosons. The remaining five degrees of freedom

corresponding to five physical Higgs states: two CP-even neutral scalars (h, H), one CP-odd neutral scalar (A), and two charged scalars ($H^\pm$). The CP-even Higgs mass eigenstates, h and H , are related to the gauge eigenstates, ϕ_1^0 and ϕ_2^0 , by a mixing angle α :

$$\begin{pmatrix} h \\ H \end{pmatrix} = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \phi_1^0 \\ \phi_2^0 \end{pmatrix}. \quad (9.2)$$

The angle β is defined with the ratio of the VEVs of the two Higgs doublets as:

$$\tan \beta = \frac{v_2}{v_1}. \quad (9.3)$$

Generally, a discrete Z_2 symmetry is imposed on the Lagrangian to prevent tree-level flavor-changing neutral currents (FCNCs), defined as:

$$\Phi_1 \rightarrow \Phi_1 \quad \text{and} \quad \Phi_2 \rightarrow -\Phi_2.$$

The *alignment limit* is a special case in the g2HDM where the Z_2 symmetry is dropped and one of the CP-even Higgs bosons, typically the lighter one h , has SM-like couplings to the gauge bosons and fermions [148]. This occurs when the mixing angle α in the CP-even Higgs sector aligns in such a way that:

$$\cos(\beta - \alpha) \rightarrow 0. \quad (9.4)$$

In this limit, the couplings of h to the gauge bosons ($W^\pm$ and Z) and fermions match those of the SM Higgs boson, making it phenomenologically indistinguishable from the Higgs boson observed at the LHC, thus, consistent with current experimental data. The other CP-even scalar H and the other Higgs bosons (A and $H^\pm$) can still have different properties, potentially leading to new physics signals. This the kind of g2HDM model, explored in this chapter, with extra top Yukawa couplings is phenomenologically interesting since they can explain the generation of the baryon asymmetry in the universe [149].

The production and decay modes of the BSM Higgs are shown in Figure 9.1. Only couplings involving top-quarks, namely ρ_{tt} , ρ_{tc} and ρ_{tu} (collectively termed ρ_{tq}) are considered and no distinction is made between ρ_{tq} and ρ_{qt} . This search targets two same-sign tops (Figures 9.1a and 9.1b), three-tops (Figures 9.1c and 9.1d) and four-tops (Figure 9.1e), producing multiple light leptons and b -jets in the final state. Many of the production modes are expected to be charge-asymmetric: processes initiated by uu or ug (Figure 9.1a-9.1c)

have a much larger cross-section due to a much larger PDF for the valence quarks compared to sea anti-quark PDFs (discussed in Figure 6.2).

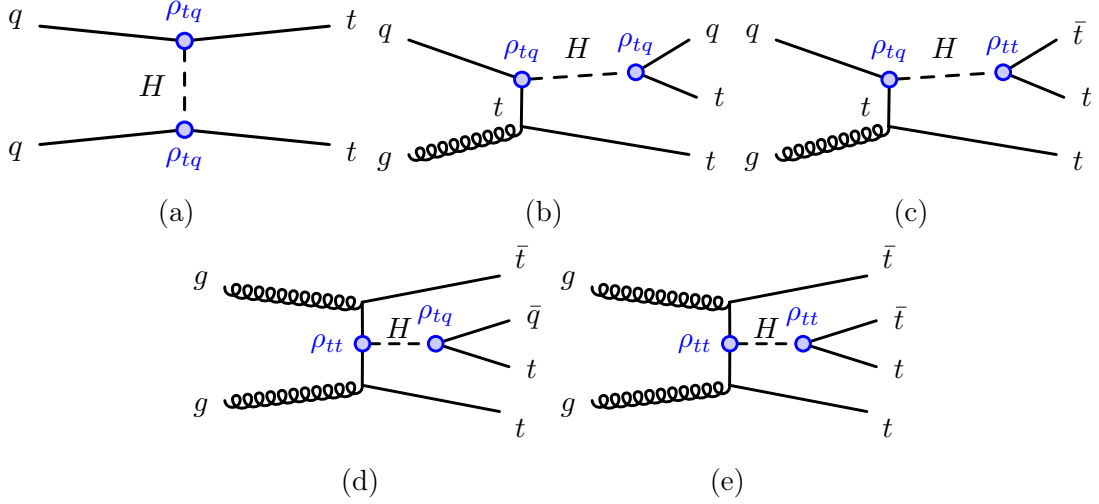


Figure 9.1: Illustrative Feynman diagrams for the dominant production and decay modes of the BSM Higgs scalar, H , considered in the analysis.

This analysis is the first to target the g2HDM model, and BSM production leading to three-top final states which has been highlighted as a sensitive probe of new physics [150–153]. The production of four-tops in the SM or via heavy scalars has been targeted previously by ATLAS [154–157] and CMS [158–162].

A benchmark of $\rho_{tt} = 0.4$ and $\rho_{tq} = 0.20$ with $m_H = 400$ GeV is chosen for analysis design and optimisation. The values are chosen so that the signal would be responsible for the higher $t\bar{t}W$ and $t\bar{t}t\bar{t}$ yields observed in ATLAS analyses: the $t\bar{t}H/t\bar{t}W$ analyses in ATLAS fit a normalization of the $t\bar{t}W$ background about 60% above the next-to-leading order (NLO) prediction [163–165] while several four-top measurements fit a normalization of the $t\bar{t}t\bar{t}$ process a factor two above the NLO prediction [154, 166, 167]. Further limits on the couplings can be derived from LHC Higgs measurements and B physics [168], leading to $\rho_{tt} < 2$ and $\rho_{tc} < 1.06$. Additional constraints can be obtained from K - $\bar{K}$ mixing and D - $\bar{D}$ mixing: $|\rho_{tc}\rho_{tu}^*| < 0.01$ assuming a negligible ρ_{ut} [169]. These constraints are derived assuming $m(H) \approx m(H^+) = 500$ GeV, and become weaker for higher masses.

9.2 Datasets, trigger and object definition

The full Run 2 dataset, corresponding to an integrated luminosity of 139 fb^{-1} with an uncertainty of 1.7%, at the centre-of-mass energy $\sqrt{s} = 13 \text{ TeV}$ is used for this search. Events with two or more light leptons are pre-selected using a logical OR of single and di-lepton triggers (SLT OR DLT). Details about these triggers are summarised in Table 8.2. Physics objects are reconstructed using the definitions established in Chapter 8 and τ_{had} candidates are vetoed from the search. Events are separated into channels with two same-sign ($2\ell\text{SS}$), three (3ℓ) and four (4ℓ) light leptons using the loose light lepton definitions established in Chapter 8. For electrons (muons), the TightLH (Medium) ID and FCLoose isolation WP is used to pre-select events. PLIV cuts are used to suppress non-prompt leptons from heavy flavor decays. A hybrid b -jet tagging criteria, using the 60% and 77% WP is developed in the analysis, discussed more in detail in Section 9.3.2.

Signal samples were generated at leading order (LO) with MADGRAPH v2.9.3 with NNPDF23LO. PYTHIA 8.245 with the A14 tune was used as the showering algorithm. Signal events were generated for masses in the range of 200 GeV to 1 TeV with a 100 GeV step, with the set of couplings $\rho_{tt} = \rho_{tq} = 0.1$ and re-weighted to obtain the corresponding cross-sections and branching ratios per production and decay mode for different values of the couplings. Approximately 500k MC signal events were generated for each campaign (mc16a, mc16d, mc16e) and each mass point. The NLO generator cross-section was used for the normalisation of the signals. Detector level effects were incorporated using ATLAS *Fast Simulation* as described in Chapter 6.

9.3 Analysis strategy

The presence of two same-sign top quarks (Figures 9.1a and 9.1b) or three or more top quarks (Figures 9.1c-9.1e) in the signal processes lead to final states with two same-sign ($2\ell\text{SS}$), three (3ℓ) or four (4ℓ) leptons. Thus, the search is structured in the $2\ell\text{SS}$, 3ℓ , and 4ℓ channels, defined in terms of the loose light lepton multiplicity after overlap removal discussed in Chapter 8. Additionally, events are required to have at least one b -jet tagged at the 60% WP or at least two b -jets tagged at the 77% WP to suppress diboson backgrounds that rarely contain b -tagged jets. If events contain pairs of opposite-sign charge and same-flavour leptons (OSSF), as in the 3ℓ and 4ℓ channels, all pairs are required to satisfy a mass requirement on the dilepton system mass of $m_{\ell^+\ell^-}^{\text{OS-SF}} > 12 \text{ GeV}$ and $|m_{\ell^+\ell^-}^{\text{OS-SF}} - m_Z| > 10$

GeV, to further suppress SM backgrounds from WZ and ZZ processes in the respective channels.

Events are categorised into orthogonal signal regions (SRs) targeting the different decay modes in Figure 9.1 using the number of leptons, total lepton charge (Q) and a multi-output deep neural network classifier to distinguish between various signal processes. A second deep neural network is trained in each of the SRs to discriminate the signal from the backgrounds. Orthogonal control regions (CRs) are defined in order to fit the normalisation of the main backgrounds and a maximum-likelihood fit is performed across categories in order to test for a possible signal and constrain the leading backgrounds simultaneously.

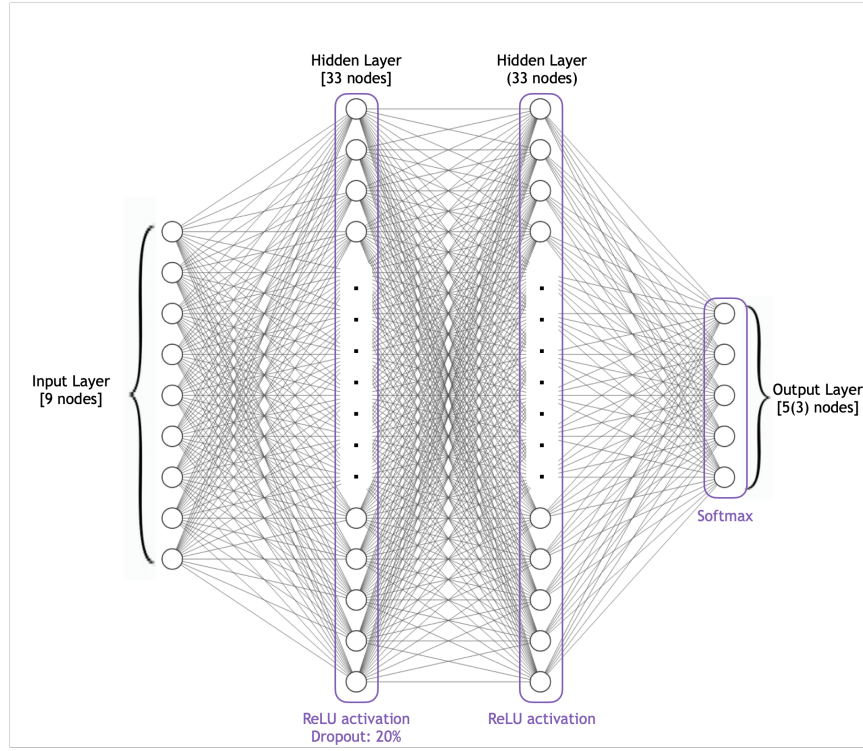
9.3.1 Signal region definition

SRs targeting the different decay modes in Figure 9.1, i.e sstt, ttq, ttt, ttq, tttt, are defined using a signal-vs-signal categorisation deep neural network (DNN^{cat}). This network is trained separately for the $2\ell\text{SS}$ and 3ℓ channels because different signal processes contribute to each of these channels. In contrast, the 4ℓ channel does not require a DNN since only a single signal diagram contributes to it.

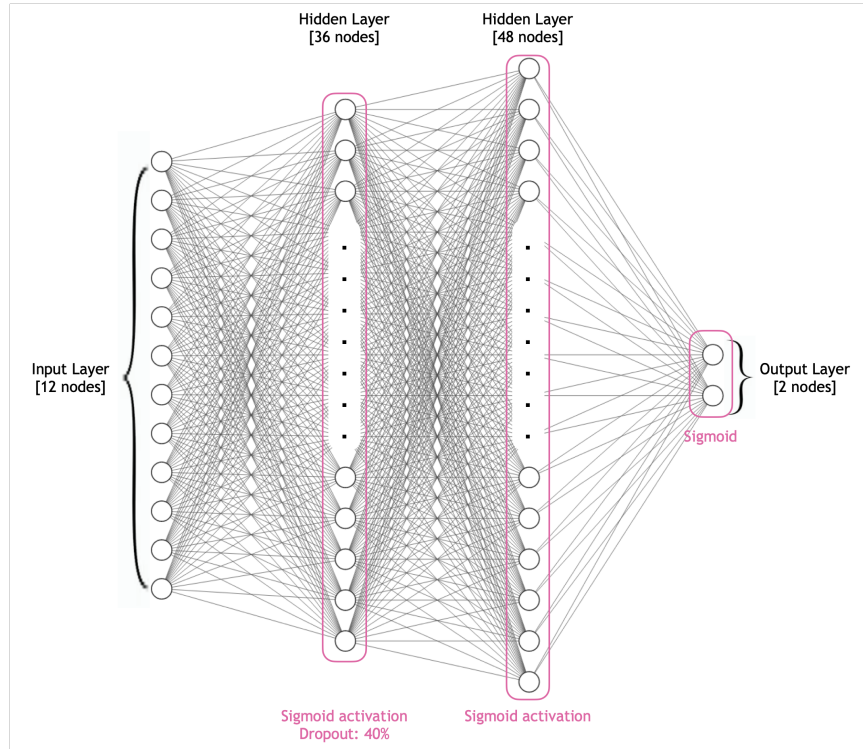
The training is done using the KERAS library [137] with TENSORFLOW as a backend [138] and Adam optimiser [136]. Hyperparameters are optimised with the TALOS library [170]. The architecture of this DNN is shown in Figure 9.2a. The network is trained with batch size of 2000 and up to 100 epochs, using all the available signal mass points using cross-training. The input variables used in training are summarised in Table 9.1. The output categories correspond to the 5 (3) top quark topologies expected to populate the $2\ell\text{SS}$ (3ℓ) channel.

Variable	DNN^{cat}	DNN^{SB}
Number of jets (N_{jets})	Y	Y
Sum of pseudo-continuous b-tagging scores of jets (sumPCB)	Y	Y
Pseudo-continuous b-tagging score of 1 st , 2 nd , 3 rd leading jet in p_T	Y	Y
Sum of p_T of the jets and leptons ($H_{T,\text{jets}}, H_{T,\text{lep}}$)	Y	Y
Angular distance of leptons, $dR(l, l)$	Y	Y
Missing transverse energy (E_T^{miss})	Y	Y
Leading p_T of jet	-	Y
Invariant mass of leading lepton and missing transverse energy (MT(lept, E_T^{miss}))	-	Y
Di/tri/quad-lepton type variable (associated to the number of electrons/muons in event)	-	Y

Table 9.1: Input variables for training of the DNN^{cat} and DNN^{SB} classifiers. Y indicates that the variable was used in the training.



(a)



(b)

Figure 9.2: (a) Architecture of the DNN^{cat} classifiers trained separately for $2\ell\text{SS}$ and 3ℓ channels. The output categories correspond to the 5 (3) decay modes in the $2\ell\text{SS}$ (3ℓ) channel. (b) Architecture of the DNN^{SB} classifiers trained in each SR.

The distributions of the signal and background shapes in the training variables used in the NNs is shown in Appendix A, for signal processes from the benchmark set of couplings, i.e, $\rho_{tt} = 0.4$ and $\rho_{tq} = 0.20$ with $m_H = 400$ GeV. The performance of the DNN^{cat} classifiers in $2\ell\text{SS}$ and 3ℓ is evaluated using a confusion matrix: each row of the matrix represents the instances in an actual class while each column represents the instances in a predicted class. The diagonal entries can be interpreted as the probability of correctly classifying a labelled event. Figure 9.3 shows the performance of the network in validation data for $2\ell\text{SS}$ and 3ℓ channels, respectively.

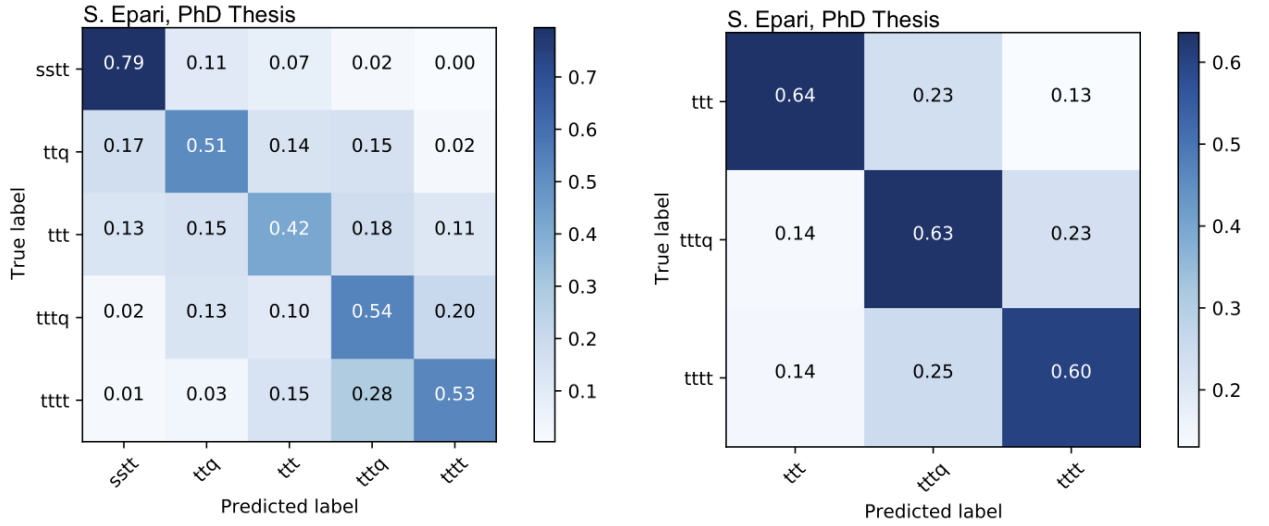


Figure 9.3: Normalised confusion matrices for DNN^{cat} classifiers trained in the (a) $2\ell\text{SS}$ and (b) 3ℓ channel.

To exploit the charge-asymmetric nature of the probed signal processes, all the $2\ell\text{SS}$ and 3ℓ SRs are further split into two categories using total lepton charge: ‘++’ or ‘--’. However, training of the DNN classifiers is done inclusively over charge, so that the DNN shape is not biased when categorizing events by total charge. The selections used to define SRs is summarised in Table 9.2. A total of 17 SRs (10 in $2\ell\text{OS}$, 6 in 3ℓ and 1 in 4ℓ) are defined in the analysis.

Figures 9.4a and 9.4b show the normalized distributions of the target signals from a scalar mass of 400 GeV or 1000 GeV, compared to the expected background distribution

Lepton category	2ℓSS	3ℓ	4ℓ
Lepton definition	(T, T) with ≥ 1 $b^{77\%}$ (T, M) with ≥ 2 $b^{85\%}$	(L, T, M) with ≥ 1 $b^{77\%}$ (L, M, M) with ≥ 2 $b^{85\%}$	(L, L, L, L)
Lepton p_T [GeV]	(20, 20)	(10, 20, 20)	(10, 10, 10, 10)
$m_{\ell^+\ell^-}^{\text{OS-SF}}$ [GeV]	–	>12	
$ m_{\ell^+\ell^-}^{\text{OS-SF}} - m_Z $ [GeV]	–	>10	
N_{jets}		≥ 2	
$N_{b\text{-jets}}$		≥ 1 $b^{77\%}$ ≥ 2 $b^{85\%}$	
Region split	$(\text{sstt}, \text{ttq}, \text{ttt}, \text{tttq}, \text{tttt}) \times (Q^{++}, Q^{--})$	$(\text{ttt}, \text{tttq}, \text{tttt}) \times (Q^+, Q^-)$	–
Region naming	2ℓSS ++ CAT sstt 2ℓSS ++ CAT ttq 2ℓSS ++ CAT ttt 2ℓSS ++ CAT tttq 2ℓSS ++ CAT tttt 2ℓSS -- CAT sstt 2ℓSS -- CAT ttq 2ℓSS -- CAT ttt 2ℓSS -- CAT tttq 2ℓSS -- CAT tttt	3ℓ ++ CAT ttt 3ℓ ++ CAT tttq 3ℓ ++ CAT tttt 3ℓ -- CAT ttt 3ℓ -- CAT tttq 3ℓ -- CAT tttt	4ℓ

Table 9.2: Event selection summary in the SRs. Light leptons definitions from Table 8.6 are used. Leptons are ordered by p_T in the 2ℓSS and 4ℓ regions. In the 3ℓ regions the lepton with opposite-sign charge is taken first, followed by the two same-sign leptons in p_T order.

across the various categories described in Table 9.2. At high signal mass, a strong migration is observed from the $t\bar{t}t$ to the $t\bar{t}t\bar{q}$ category due to the high probability of additional radiation.

A DNN^{SB} classifier is trained in each SR to separate the targeted signal from the sum of backgrounds. The architecture of this DNN is shown in Figure 9.2b and Table 9.1 summarises the input variables used for training. Good sensitivity over the large range of signal masses is ensured by de-correlating the output of the classifier from the signal mass by introducing an additional term to the loss function via distance correlation [172, 173]. The same DNN^{SB} is used in both positive- and negative-charge regions. The performance of the DNN^{SB} classifiers is evaluated using *Receiver Operating Characteristic* (ROC) curves, shown in Figure 9.5.

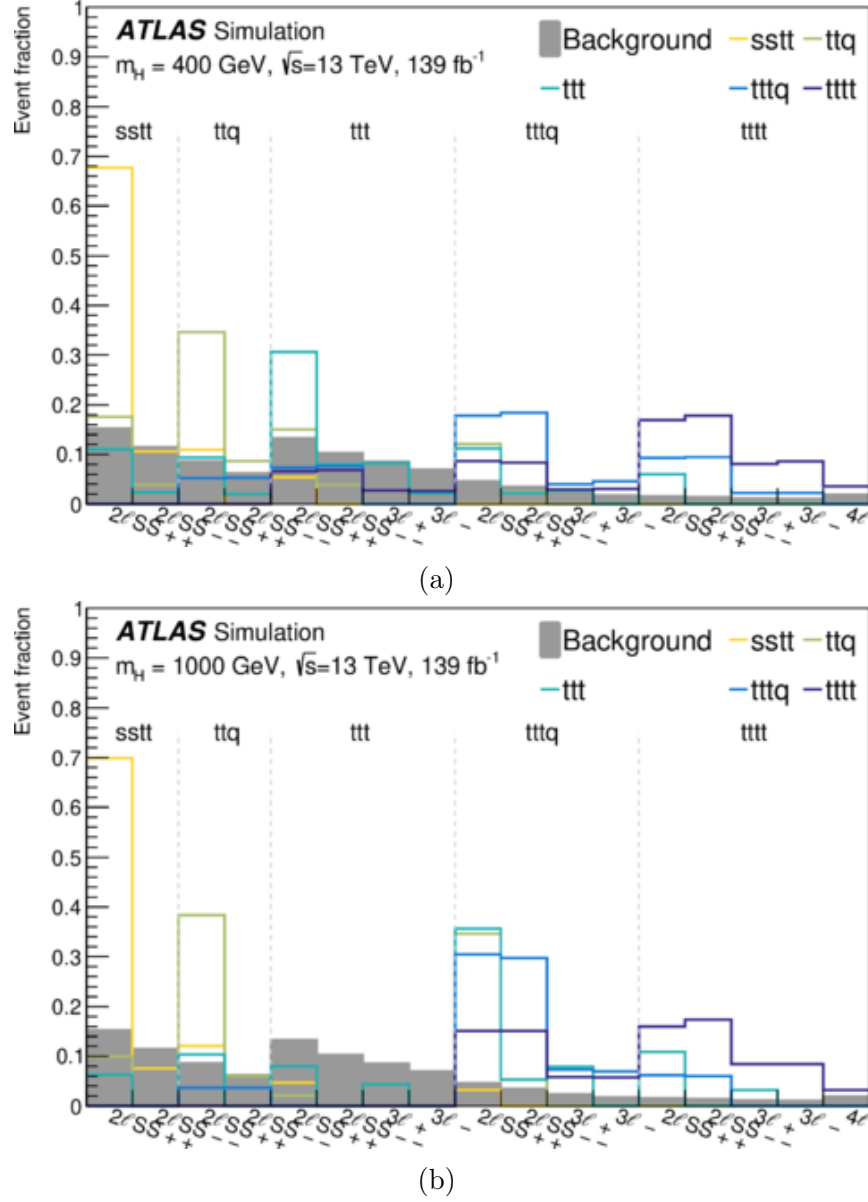


Figure 9.4: Distributions for each signal process category compared to the total expected background, for (a) $m_H = 400$ GeV and (b) $m_H = 1000$ GeV. All distributions are normalised to unity. Figures taken from Ref. [171].

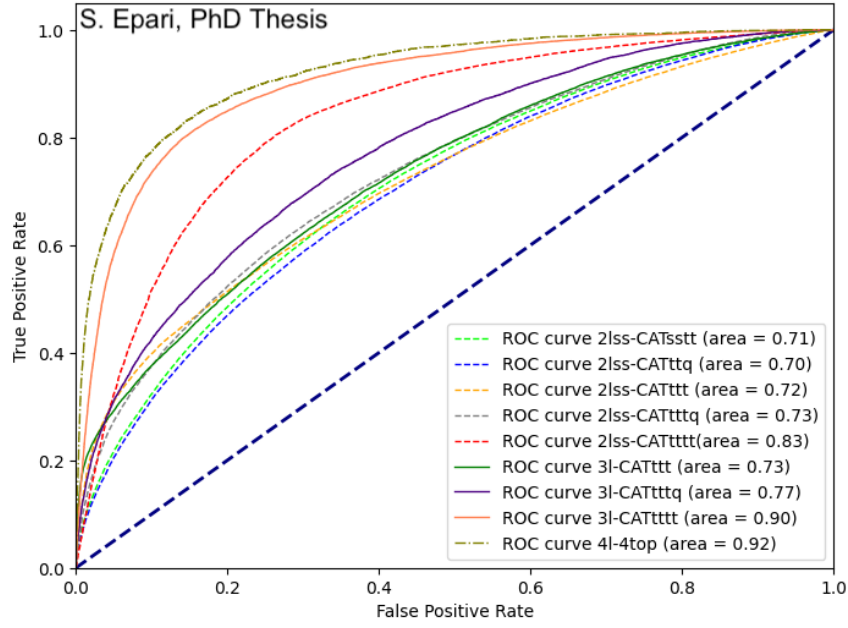


Figure 9.5: ROC curves with *area under curve* values per categories for each DNN^{SB} classifier.

Figure 9.6 shows the DNN^{SB} distribution of the targeted signal, total signal and sum of SM background in each signal-enriched category.

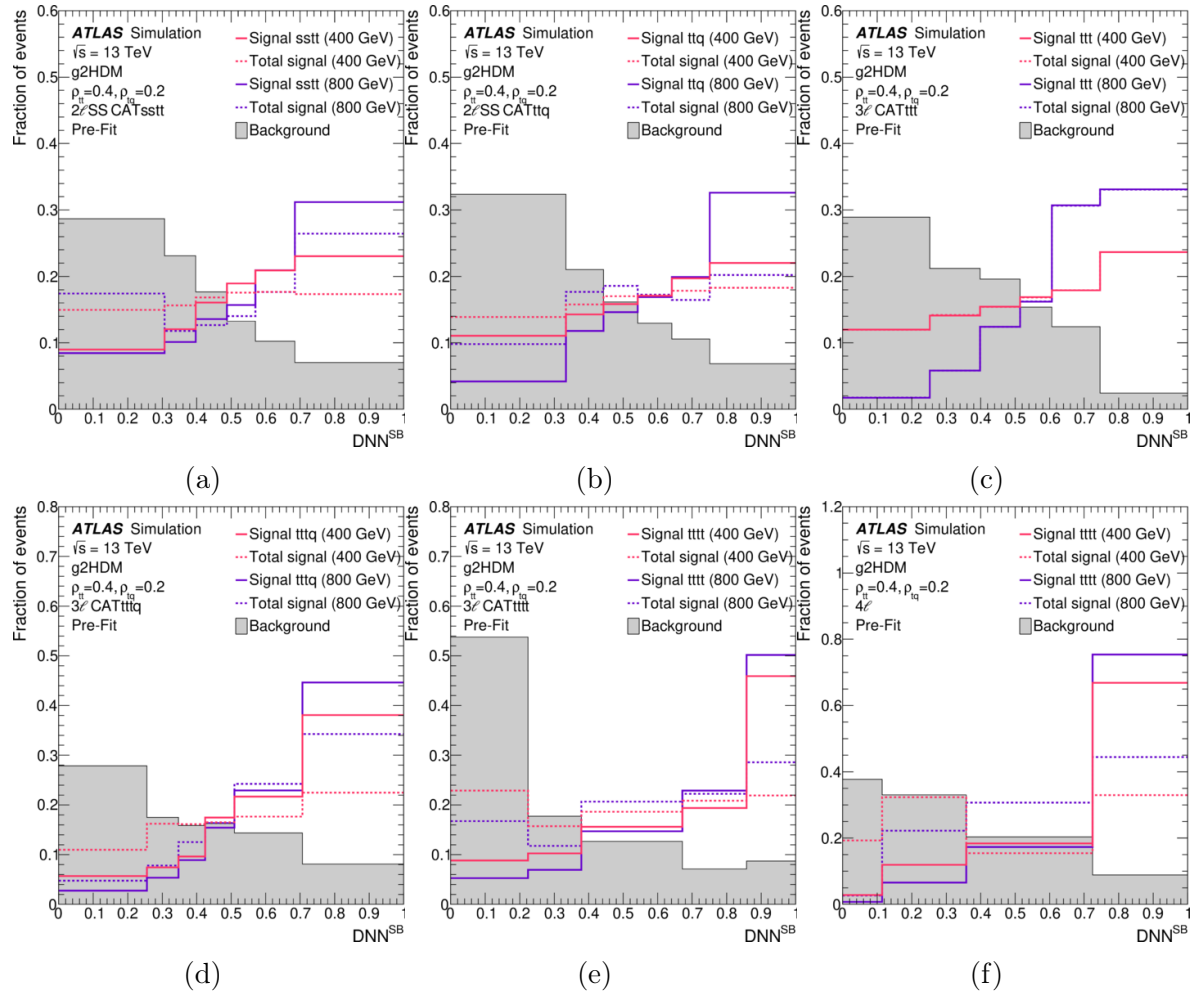


Figure 9.6: Comparison of the DNN^{SB} distribution of the targeted signal (solid line), the total signal (dashed line) and the background (filled grey area) in the (a) 2 ℓ SS CAT sstt, (b) 2 ℓ SS CAT ttq, (c) 3 ℓ CAT ttt, (d) 3 ℓ CAT tttq, (e) 3 ℓ CAT tttt, and (f) 4 ℓ categories, for an assumed $m_H = 400$ GeV (pink) and $m_H = 800$ GeV (violet), with couplings $\rho_{tt} = 0.4$ and $\rho_{tq} = 0.2$. All distributions are normalised to unity. Figures taken from Ref. [171].

9.3.2 Control regions

Figure 9.7 highlights the main SM backgrounds expected in the SRs. The main *prompt*-lepton backgrounds originate from $t\bar{t}W$, $t\bar{t}t\bar{t}$ and $t\bar{t}\gamma^*$ production, followed by VV (in particular $W\gamma^*$) and $t\bar{t}H$ production, and have final states and kinematic properties similar to the g2HDM signal. Smaller contributions originate from the following rare processes: tZ , tW , tWZ , $ttWW$ and VVV production. Fake-lepton backgrounds come from a mixture of semi-leptonic b -decays (HFe or $HF\mu$), material conversions and charge mis-identification (QMisID). Dedicated CRs are defined to estimate major backgrounds common to the SRs, summarised in Table 9.3.

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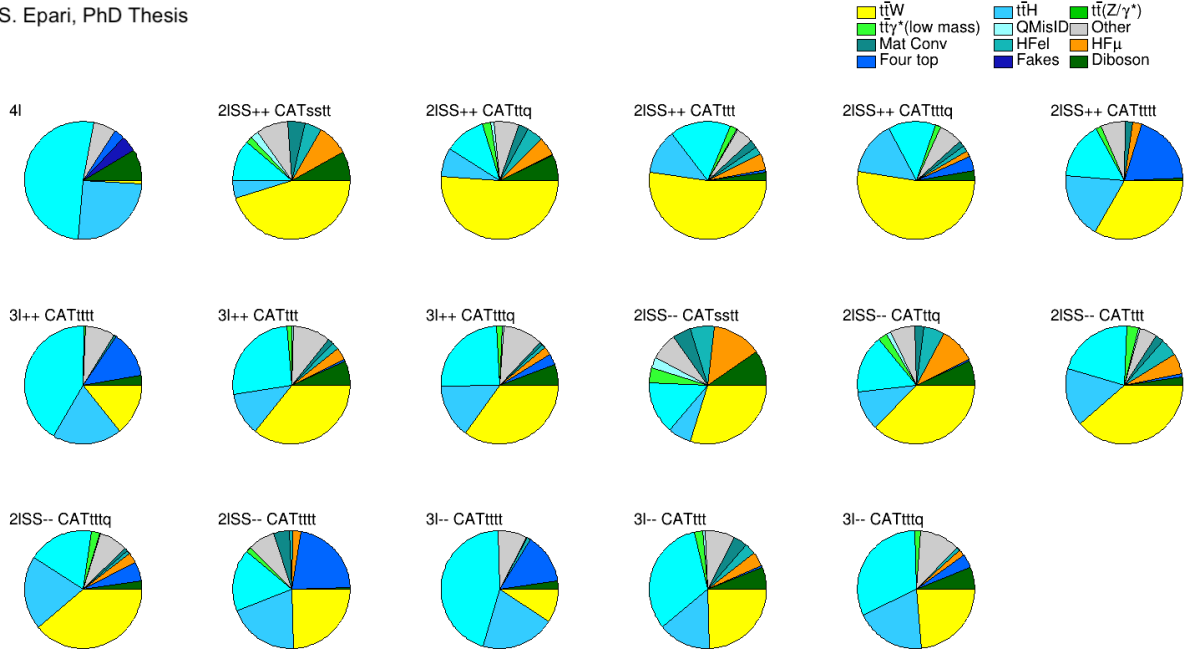


Figure 9.7: Background composition in the g2HDM SRs.

Except for the QMisID background, all other backgrounds are estimated using the simulated samples described in Section 8.5.2. Event kinematics of the simulated $t\bar{t}$ and VV backgrounds require dedicated corrections to better describe the data, described in this section. Yields of $t\bar{t}W$, $t\bar{t}Z$, VV and non-prompt-lepton backgrounds, are adjusted via normalisation factors that are determined by performing a likelihood fit to data across all event categories, shown in Section 9.5.

Control regions	WZ	$t\bar{t}Z$	Conversions	HF non-prompt
N_{jets}	2 or 3	≥ 4	≥ 0	≥ 2
$N_{b\text{-jets}}$	≥ 1	$b^{77\%} \parallel \geq 2$	$b^{85\%}$	1
Lepton requirement		3ℓ	$\mu\mu e^*$	$2\ell\text{SS}$
Lepton definition		(L, M, M)		$(T, M_{\text{ex}}) \parallel (M_{\text{ex}}, T) \parallel (M_{\text{ex}}, M_{\text{ex}})$
Lepton p_T [GeV]		$(10, 20, 20)$		$(20, 20)$
$m_{\ell^+\ell^-}^{\text{OS-SF}}$ [GeV]		>12	>12	–
$ m_{\ell^+\ell^-}^{\text{OS-SF}} - m_Z $ [GeV]		<10	>10	–
$ m_{\ell\ell} - m_Z $ [GeV]		–	<10	–
$m_T(\ell_0, E_T^{\text{miss}})$ [GeV]		–		< 250
Region split	–	–	internal / material	subleading $e/\mu \times [(T, M_{\text{ex}}), (M_{\text{ex}}, T), (M_{\text{ex}}, M_{\text{ex}})]$
Region naming	$3\ell\text{VV}$	$3\ell\text{tt}Z$	$3\ell\text{IntC}$	$2\ell\text{tt}(e)_{(T, M_{\text{ex}})}, 2\ell\text{tt}(e)_{(M_{\text{ex}}, T)}, 2\ell\text{tt}(e)_{(M_{\text{ex}}, M_{\text{ex}})}$
			$3\ell\text{MatC}$	$2\ell\text{tt}(\mu)_{(T, M_{\text{ex}})}, 2\ell\text{tt}(\mu)_{(M_{\text{ex}}, T)}, 2\ell\text{tt}(\mu)_{(M_{\text{ex}}, M_{\text{ex}})}$

Table 9.3: Event selection summary in the CRs. Light leptons definitions from Table 8.6 are used. The notation e^* is used to denote material conversion or internal conversion candidates. In the HF non-prompt lepton region naming, “ $2\ell\text{SS}(\text{e})$ ” (“ $2\ell\text{SS}(\mu)$ ”) refer to the CRs enriched in non-prompt electrons (muons) from semi-leptonic b -decays originating mostly from $t\bar{t}$ and with the lepton flavours for the leading and subleading leptons corresponding to “ $ee, \mu e$ ” (“ $\mu\mu, e\mu$ ”). The additional (T, M_{ex}) , (M_{ex}, T) , and $(M_{\text{ex}}, M_{\text{ex}})$ subscripts refer to the lepton definitions required for the leading and subleading leptons in each region.

Diboson background

The main SM background in the 3ℓ region is $W\gamma^*$ (instead of WZ because of the Z veto). To check the modelling of this background, a VR enriched in WZ events is defined by inverting the Z veto in the 3ℓ channel. The selection for this VR, called $3\ell VV0b$, is defined in Table 9.3, with the additional requirement of zero b -jets (at the 85% WP) to suppress the $t\bar{t}Z$ background in the region. Figure 9.8a shows the jet multiplicity distribution in the $3\ell VV0b$ VR, with a disagreement of up to 30% at high jet multiplicity. A data-driven correction is derived from this VR to correct this mis-modelling, as the ratio of the diboson contribution to the data (subtracted by the non-diboson backgrounds), fitted with a polynomial of the form:

$$f(x) = a + \frac{b}{x^c} \quad (9.5)$$

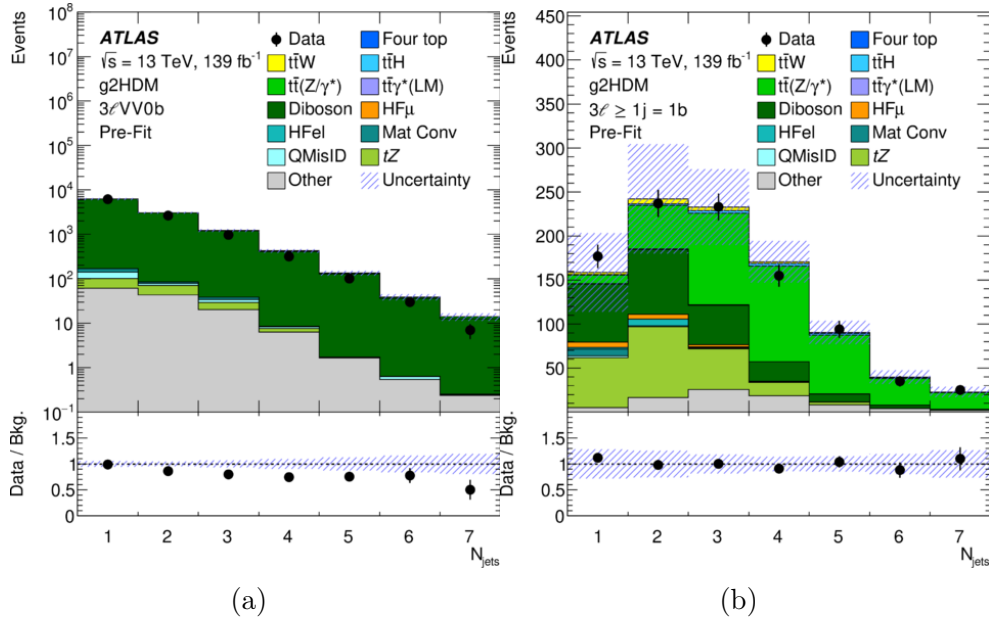


Figure 9.8: Comparison between data and the background prediction for the distribution of the number of jets in the (a) $3\ell VV0b$ region before the VV jet multiplicity correction and (b) 3ℓ region with at least one jet and exactly one b -jet defined with the 60% WP after the VV jet multiplicity correction. Figures taken from Ref. [171].

The following parameters are determined from the fit:

$$a = -0.693 \pm 0.012, b = -0.563 \pm 0.014, c = 0.246 \pm 0.018.$$

After the correction is applied to VV , the good modelling is observed in the jet multiplicity distribution in an inclusive 3ℓ VR enriched in both WZ and $t\bar{t}Z$, as shown in Figure 9.8b. The modelling of VV and $t\bar{t}Z$ is checked for different variables in dedicated CRs (defined in Table 9.3), shown in Figures 9.9 and 9.10. A systematic uncertainty derived for the VV correction is included in the search as a nuisance parameter, described in Section 9.4.

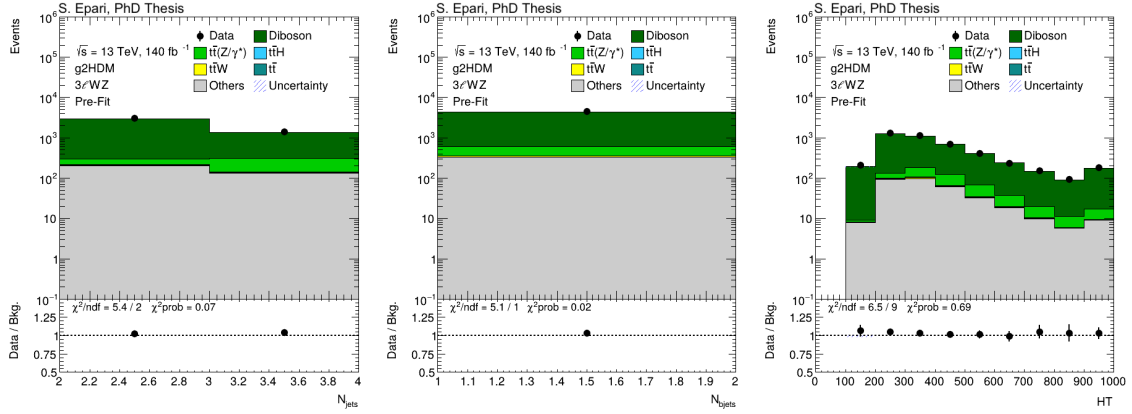


Figure 9.9: Comparison between data and the background prediction for the distribution of the number of jets, b -tagged jets and HT (defined as the sum of p_T of jets and leptons) in the WZ control region after the VV jet multiplicity correction.

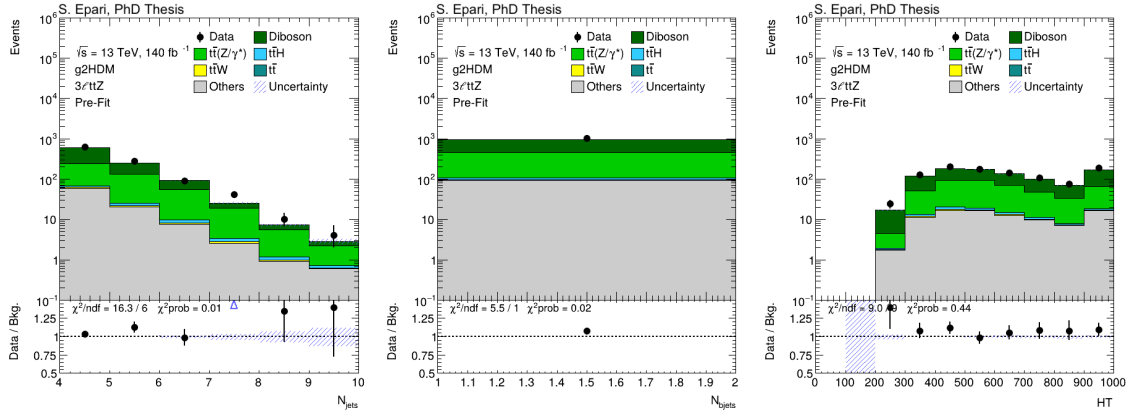


Figure 9.10: Comparison between data and the background prediction for the distribution of the number of jets, b -tagged jets, HT (defined as the sum of p_T of jets and leptons) in the $t\bar{t}Z$ control region after the VV jet multiplicity correction.

Estimation of events with charge-misassigned leptons

QMisID electrons arise predominantly from $t\bar{t}$ production, with one electron having undergone a hard bremsstrahlung as well as an asymmetric conversion ($e^\pm \rightarrow e^\pm \gamma^* \rightarrow e^\pm e^+ e^-$) or a mis-measured track curvature. These events usually populate channels with ee or $e\mu$. Events with QMisID electrons surviving the ECIDS criteria mentioned in Chapter 8 are estimated in data using samples of $Z \rightarrow e^+ e^-$ events. These rates are derived as a function of electron p_T and $|\eta|$, for electrons in the internal and material conversion CRs and in SRs using the TightLH electron definition. The fraction of events with charge-flipped muon candidates is negligible in the p_T range of the analysis.

The QMisID rates for the leading and subleading p_T electron (ϵ_i and ϵ_j respectively) are estimated using the fraction of 2ℓ OS events reconstructed as same-sign:

$$\epsilon_i(1 - \epsilon_j) + \epsilon_j(1 - \epsilon_i) = \epsilon_i + \epsilon_j - 2\epsilon_i\epsilon_j, \quad (9.6)$$

These rates are used to compute the expected number of events with misidentified same-sign leptons (N_{SS}) from the total number of observed opposite-sign events (N_{OS}):

$$N_{SS} = \frac{\epsilon_i + \epsilon_j - 2\epsilon_i\epsilon_j}{1 - (\epsilon_i + \epsilon_j - 2\epsilon_i\epsilon_j)} N_{OS} \quad \text{and} \quad N_{SS} = \frac{\epsilon_i}{1 - \epsilon_i} N_{OS}, \quad (9.7)$$

for the ee and $e\mu$ channel respectively. The QMisID rates are estimated from the fraction of $Z \rightarrow ee$ events reconstructed as same-sign pairs ($\tilde{N}_{SS}^{ij}$) around the Z boson peak, given the total number of electron pairs N^{ij} as:

$$\tilde{N}_{SS}^{ij}(\epsilon_i, \epsilon_j) = N^{ij}(\epsilon_i + \epsilon_j - 2\epsilon_i\epsilon_j). \quad (9.8)$$

This rate can be estimated as the mean of the Poisson distribution:

$$f(N_{SS}^{ij} | \tilde{N}_{SS}(\epsilon_i, \epsilon_j)) = \frac{[\tilde{N}_{SS}^{ij}]^{N_{SS}^{ij}} e^{-\tilde{N}_{SS}^{ij}}}{N_{SS}^{ij}!}.$$

This expression is integrated into a likelihood formalism:

$$\mathcal{L}(\vec{\epsilon} | N_{SS}) = \prod_{i,j} f(N_{SS}^{ij} | \tilde{N}_{SS}(\epsilon_i, \epsilon_j)),$$

which is maximised to obtain the rates that best describe the data. The QMisID rate, for electrons in the internal and material conversion CRs and in SRs using the TightLH

electron definition, parameterized in the electron p_T and η is illustrated in Figure 9.11 and varies from about 10^{-5} for low- p_T electrons ($17 \leq p_T \leq 50$ GeV) with $|\eta| \leq 1.37$, to about 3×10^{-4} for high- p_T electrons ($p_T \geq 100$ GeV) with $1.52 \leq |\eta| \leq 2$.

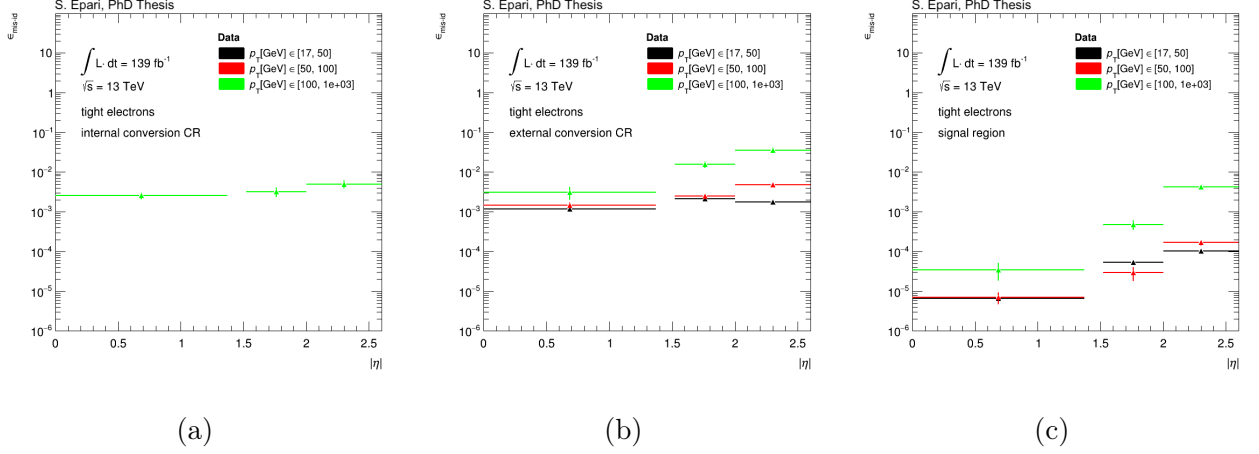


Figure 9.11: Electron QMisID rates derived from the data with the likelihood method for the *Tight* electron definition and the *VeryTight* PLIV WP. The rates are presented as a function of $|\eta|$ and p_T of the electron for (a) internal conversion (b) material conversion and (c) candidates passing the TightLH WP in the SRs.

The total systematic uncertainty in the estimation of QMisID rates is defined in a single nuisance parameter, calculated as the quadratic sum of the following contributions:

- The statistical uncertainty from the likelihood maximization, which depends on the sample size in the regions where the rates are extracted.
- The difference between the rates measured using the likelihood method and those obtained through truth-matching with simulated $Z \rightarrow ee$ events.
- The variation of the rates based on the Z mass window.
- The difference in QMisID rates between electrons and positrons.

Fake-lepton background estimation

The non-prompt light lepton background in the $2\ell\text{SS}$, 3ℓ , and 4ℓ channels comprises of a mixture of *non-prompt* leptons originating from semi-leptonic heavy flavour (HF) decays, photon conversions and charge mis-identified leptons. The main contribution to non-prompt lepton background comes from $t\bar{t}$, followed by a much smaller contribution from $V + \text{jets}$ and single top.

The *template fit* method is a semi-data-driven method that uses Monte Carlo events to model major non-prompt backgrounds and adjusts their normalisation to data together with that from other major prompt backgrounds. Based on the truth classification of events containing a non-prompt lepton [174, 175], the following main contributions are distinguished and one or more free-floating normalisation factors (NF) are assigned to each of them:

- λ_e^{ExtCO} : normalisation factor applied to events with one electron from a material (photon) conversion. These electrons have a truth origin 5 and decay radius above 20 mm.
- λ^{IntCO} : normalisation factor applied to events with internal conversions ($\gamma^* \rightarrow \ell\ell$). These electrons have a truth origin 5 and decay radius below 20mm.
- λ_e^{HF} : normalisation factor applied to events with one non-prompt electron from b - or c -hadron decays. The NF is further decorrelated for different PLIV WPs. Non-prompt leptons from b -hadron decays have truth origin = 26, 29 or 33 and those from c -hadron decay have truth origin = 25, 27, 28 or 32.
- λ_μ^{HF} : normalisation factor applied to events with one non-prompt muon from b - or c -hadron decays. The NF is further decorrelated for different PLIV WPs. Non-prompt leptons from b -hadron decays have truth origin = 26, 29 or 33 and those from c -hadron decays have truth origin = 25, 27, 28 or 32.

Dedicated regions targeting each kind of non-prompt leptons are defined and shown in Table 9.3. The $2\ell\text{SS}/\text{OS}$ heavy-flavor fake-enriched CRs are defined with one or more leptons that do not pass the *VeryTight PromptLeptonImprovedVeto* (PLIV) isolation requirement, but do pass the *Tight* one (denoted by M). These CRs are orthogonal to the SRs, where both leptons are required to pass the *VeryTight* PLIV WP (denoted by T). The lepton p_T of the fake candidate lepton is used as discriminating variable in all fake related CRs. The

fake lepton is assumed to be the subleading lepton except for the MT region, where the leading lepton is assumed to be the fake one. Additional cuts, such as requiring exactly 1 b -tagged jet (77% WP) and an upper bound to the transverse mass $M_T(\text{leading } \ell, E_T^{\text{miss}}) < 250$ GeV are used to reduce $t\bar{t}W$ contamination in these CRs.

Internal conversion and material conversion CRs are defined based on electron variables defined in Chapter 8. The background contribution with charge-misidentified electrons is estimated with a dedicated data-driven method, as explained in Section 9.3.2. Two CRs enriched in $t\bar{t}Z$ and VV , shown in Table 9.3, are built to constrain the normalisation factors of $t\bar{t}Z$ and VV respectively. Pre-fit distributions of the template fit regions are shown in Figure 9.12.

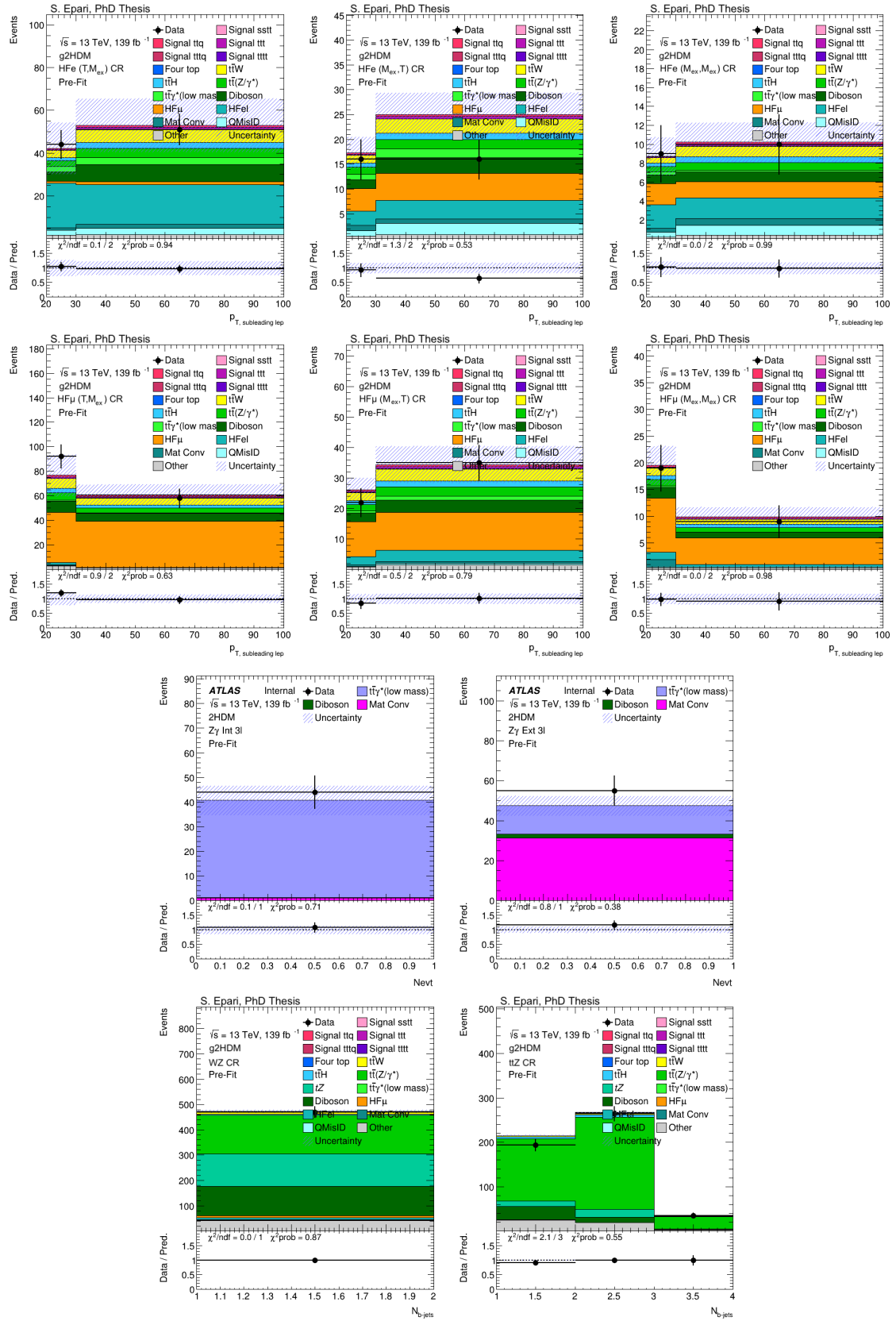


Figure 9.12: Comparison between data and the background prediction for the control region variables used in the template fit (pre-fit). The blue hashed band includes both statistical and systematic uncertainties.

Non-prompt lepton and $t\bar{t}$ corrections

Additional corrections are applied to correct the modelling of extra heavy flavor jets in the non-prompt $t\bar{t}$ background in 2ℓ SS. The $t\bar{t} + \geq 1b$ jets contribution to the fake-lepton background is scaled by a factor of 1.3 and then a bin-by-bin correction is applied to correct the modelling of the number of b-tagged jets in HF CRs by requiring the sub-leading lepton to be *Loose*. Figure 9.13 shows the per-bin correction for the electron and muon channels separately. The statistical uncertainty associated with this correction is added as a nuisance parameter in the final fit.

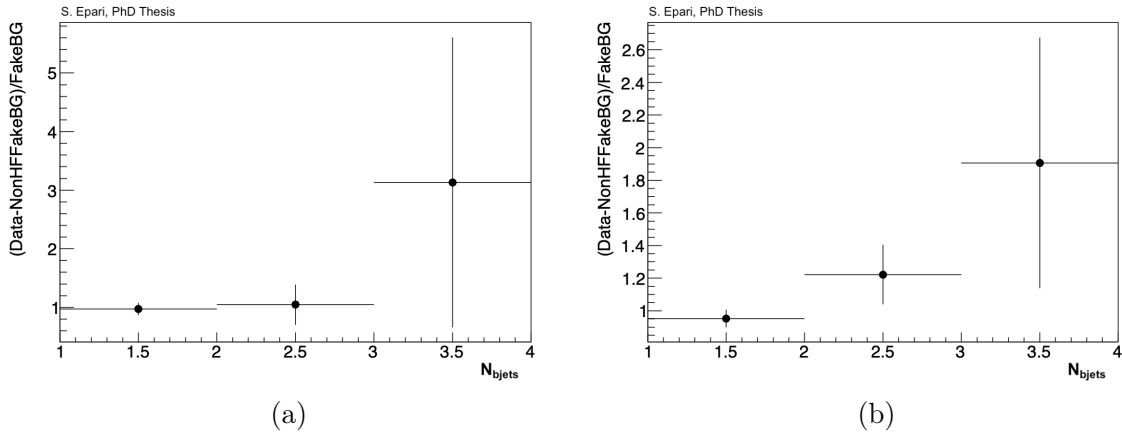


Figure 9.13: Data-driven correction for fakes as a function of $N_{b\text{-jets}}$ bin, derived in the (a) TL HFe VR and (b) TL HF μ VR. .

$t\bar{t}W$ background

The $t\bar{t}W$ background represents the leading background in several event categories and is estimated from simulation with a dedicated normalisation factor from the low score bins of the DNN^{SB} discriminant in the SRs. Signal processes initiated by uu or ug interactions are more charge-asymmetric than the $t\bar{t}W$ background. Therefore, categorizing SRs by the total charge of light leptons provides additional separation between the $t\bar{t}W$ background and the signal processes.

9.3.3 Summary of analysis regions

A summary of the analysis regions defined in the analysis, emphasizing the orthogonality selections, is illustrated in Figure 9.14. A total of 17 SRs (Table 9.2) and 10 CRs (Table 9.3) are defined in the analysis.

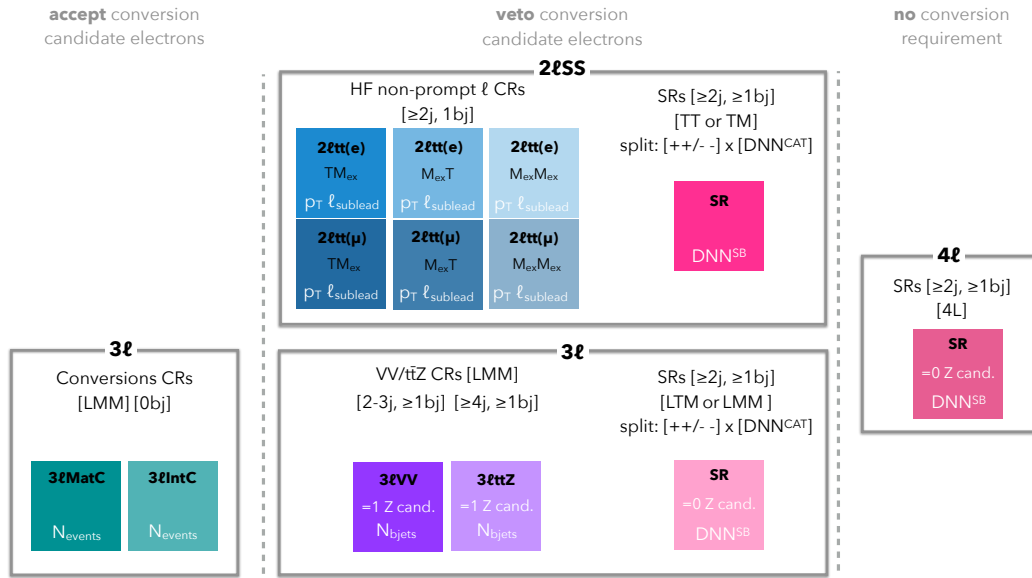


Figure 9.14: Illustrative sketch of regions defined in the g2HDM analysis.

9.4 Systematic uncertainties

This section describes the systematic uncertainties considered in the fit to data, in addition to the experimental and theoretical uncertainties defined in Section 8.

b-tagging systematics

The flavour-tagging calibration uncertainties for pseudo-continuous *b*-tagging for light jets with $p_T > 300$ GeV, *b*-jets with $p_T > 400$ GeV and *c*-jets with $p_T > 250$ GeV were not available by the ATLAS performance group and thus derived in-house. These uncertainties were derived for each flavor, p_T and WP bin are shown as a function of the *b*-tagging WP in

Figure 9.15, considering effects from various sources of tracking or calorimetry performance.

Signal modelling

The uncertainties in the modelling of the signal samples are evaluated through independent variations of the factorisation and re-normalisation scales by a factor two up and down with respect to the nominal values. Additional uncertainties due to PDF effects are estimated by taking the difference to alternative PDF sets. These uncertainties are estimated independently for each mass point at the benchmark coupling and have a negligible impact on the sensitivity of the search.

Non-prompt lepton modelling uncertainties

The following uncertainties are applied to various non-prompt lepton corrections:

- Shape-only systematic uncertainties to cover residual disagreements between data and MC of the PLIV input variables.
- Since the HF non-prompt normalisation factor is correlated between T and M leptons, a *Medium-to-Tight* extrapolation uncertainty of 20% is derived comparing the nominal $t\bar{t}$ MC (POWHEG+PYTHIA 8) vs an alternative $t\bar{t}$ MC (POWHEG+HERWIG 7.1.3) and used as a nuisance parameter in the fit.
- 50% normalisation uncertainty de-correlated between the $t\bar{t} + b$ and $t\bar{t} + c$ background processes.
- Uncertainties in electron conversions extrapolation from Z-enriched to $t\bar{t}$ -enriched regions, of 50% and 10% on internal and material conversion respectively.
- Uncertainties in QMisID estimation from a quadratic sum of uncertainties from the statistical size of the sample, difference from truth-level rates and variation of the rates with the m_Z window.

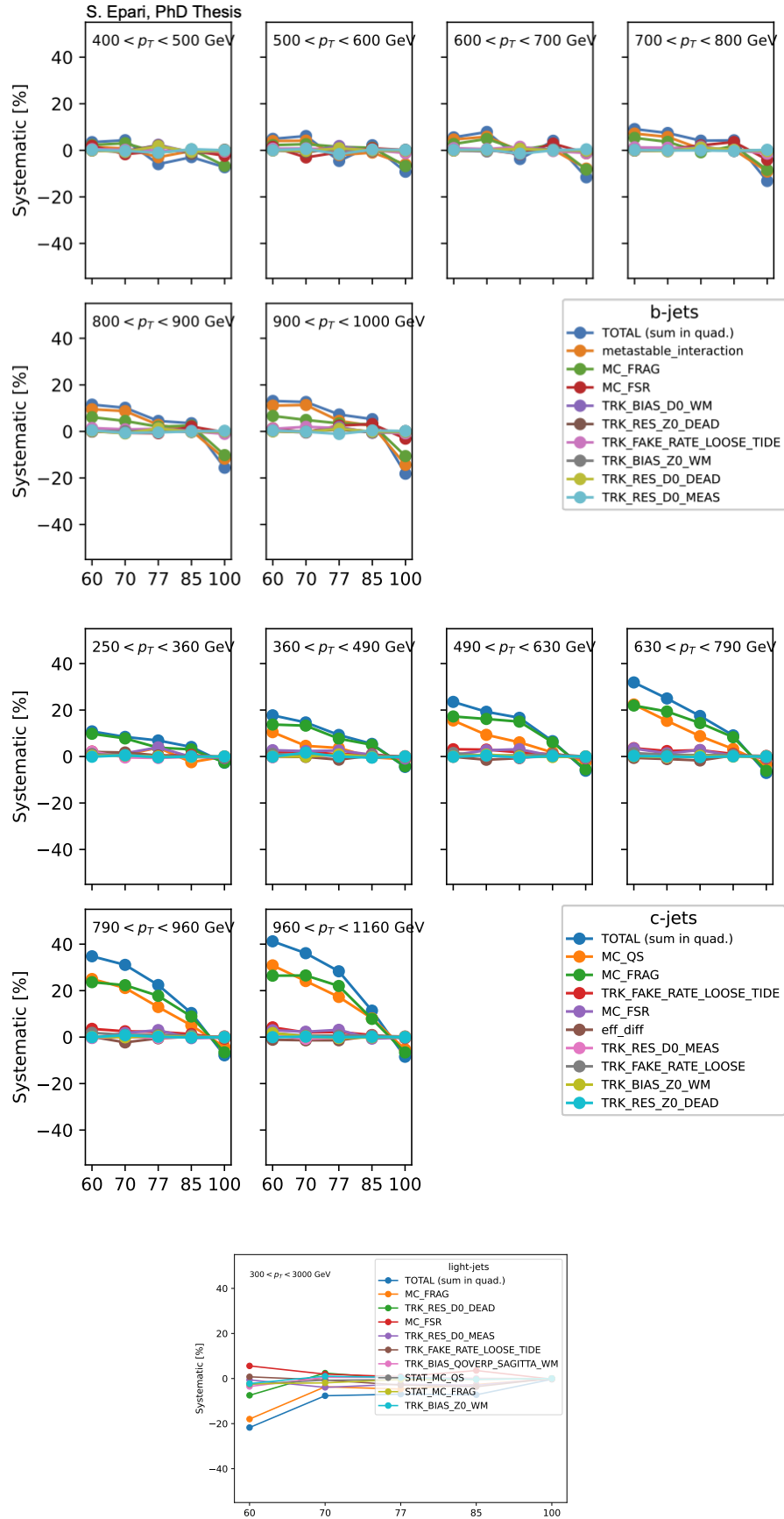


Figure 9.15: High- p_T PCBT extrapolation uncertainties for each jet flavour: b -jets (top), c -jets (middle), light-jets (bottom), shown as a function of the b -tagging WP.

Diboson re-weighting uncertainty

Systematic variations about the nominal fit function are calculated by varying the eigen function characterizations of Equation 10.1, taking into account correlations between the fit parameters. The shape-only effect of a 3σ variation of largest eigen function is used as the systematic uncertainty for the diboson re-weighting, correlated between light and heavy flavour. This envelope covers the variations at high jet multiplicity, as shown in Figure 10.18.

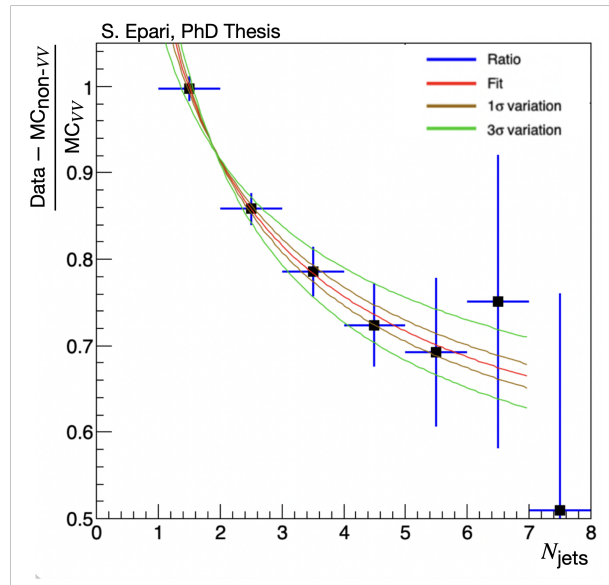


Figure 9.16: Ratio of data to VV MC in the jet multiplicity bins of the $3\ell VV0b$ VR, fitted with a polynomial (red). The 1σ variation of the largest eigen function is shown in brown, while the corresponding 3σ variation is shown in green. The 3σ variation is chosen as the systematic uncertainty because it covers the variations at high jet multiplicity.

Summary of systematic uncertainties

A summary of all systematic uncertainties included in the analysis is given in Table 9.4. A total of 207 systematics, including experimental and theoretical uncertainties are considered in the analysis.

Systematic uncertainty	Components	Systematic uncertainty	Components
Signal modelling		Luminosity	1
Cross section (N)	1	Pileup re-weighting	1
$t\bar{t}W$ modelling		Physics objects	
QCD scale	3	Electron	6
Generator	2	Muon	15
Electroweak cross section	1	Electron Non-prompt BDT	14
Additional heavy-flavour	1	Muon Non-prompt BDT	20
$t\bar{t}Z/\gamma^*$ (high mass) modelling		Jet energy scale	30
QCD scale	2	Jet energy resolution	12
Generator	2	Jet vertex fraction	1
Additional heavy-flavour	1	Jet flavour tagging	62
$t\bar{t}H$ modelling		E_T^{miss}	3
Cross section (N)	1	Total (Experimental)	165
Parton shower and hadronization model	1	Data-driven reducible background estimates	
Generator	1	Material conversions modelling	1
QCD scale	1	Internal conversions modelling	1
Additional heavy-flavour	1	Charge misassignment	1
WZ modelling		HF non-prompt	8
QCD scale	1	$t\bar{t}$ additional heavy-flavour	2
Cross section (N)	1	Total (Data-driven reducible background)	13
Extra-jets correction	1	Total (Overall)	207
$t\bar{t}t\bar{t}$ modelling			
Generator	1		
Cross section (N)	1		
Other background modelling			
Cross section (N)	6		
Total (Signal and background modelling)	29		

Table 9.4: Summary of systematic uncertainties considered in the analysis. N means that the uncertainty is taken as normalisation-only for all processes and channels affected. Some of the systematic uncertainties are split into several components, as indicated by the number in the rightmost column.

9.5 Results

Separate maximum likelihood fits are performed to data in the various 10 CRs and 17 SRs defined in the Tables 9.2 and 9.3 under the background-only hypothesis (*B-only*), and the signal plus background (*S+B*) hypothesis considering signals from models with all possible allowed couplings and masses. In these fits, the normalisation of $t\bar{t}W$, $t\bar{t}Z$, VV , conversions (internal and material) and non-prompt leptons ($\text{HF}e$, $\text{HF}\mu$) is estimated with dedicated factors. In the *S+B* fits, in addition to the above, the g2HDM signal strength is free-floated. Figure 9.17 shows the normalisation factors (NFs) measured between the *B-only* fit and *S+B* fit for the benchmark signal hypothesis ($\rho_{tt} = 0.4$, $\rho_{tq} = 0.20$ and $m_H = 400$ GeV). In both fits, the normalisation factor of $t\bar{t}W$ is measured higher than unity, while those of other backgrounds are measured to be compatible with unity. In the *S+B* fit, the g2HDM signal strength is measured compatible with zero, implying failure to reject the *B-only* hypothesis for the benchmark signal. The nuisance parameters (NPs) measured in the *B-only* fit, together with correlations above 20%, between various NFs and NPs, is shown in Figure 9.18, with small pulls and constraints, consistent with the expectation.

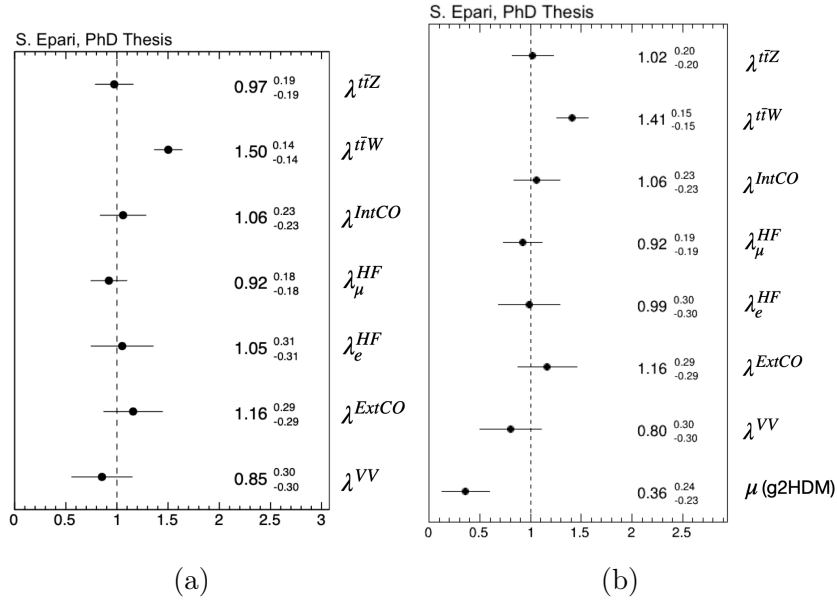


Figure 9.17: Fitted NFs from the (a) *B-only* and (b) *S+B* fit for the benchmark signal hypothesis.

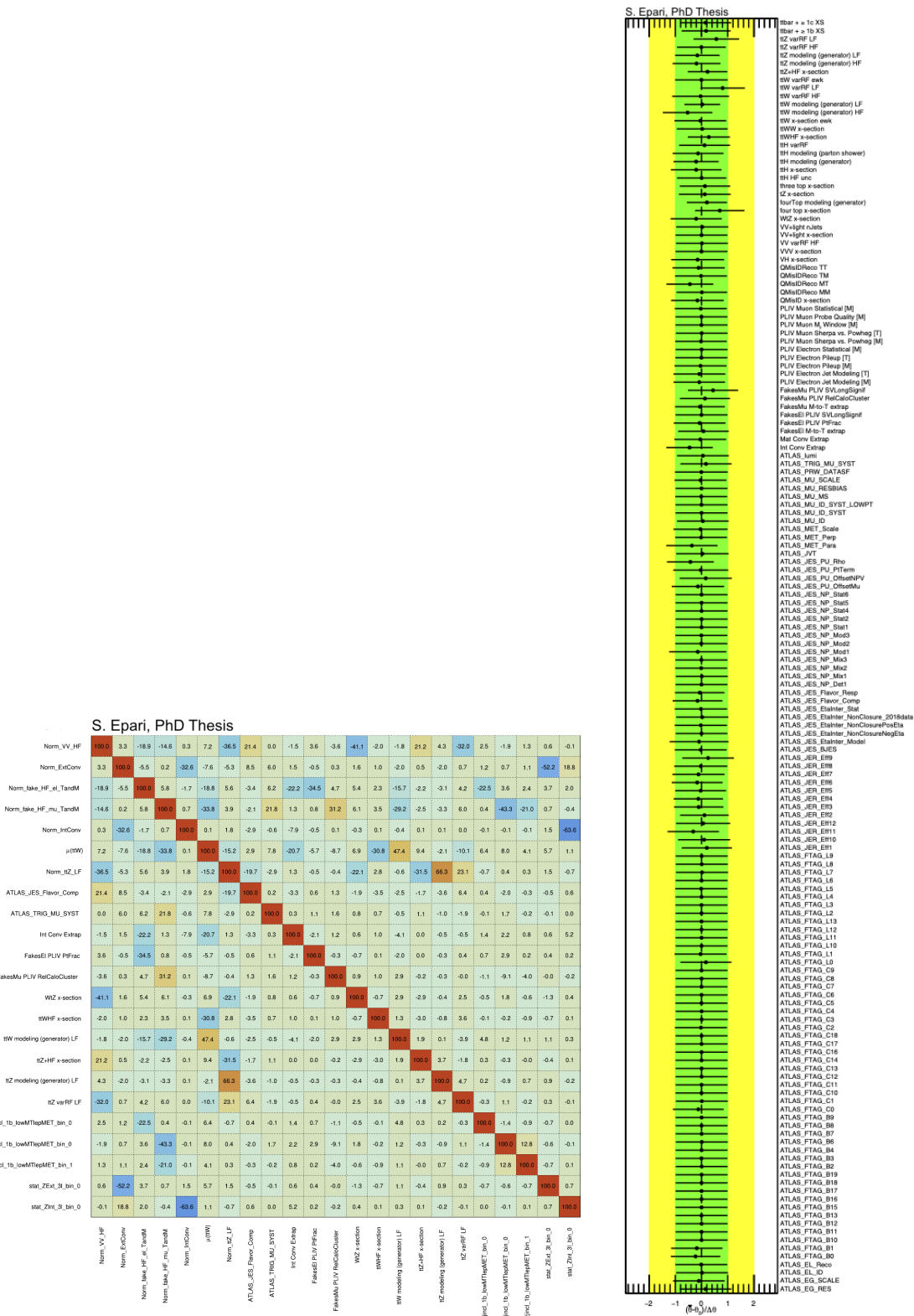


Figure 9.18: NPs measured in the *B-only* fit together with correlations between various NPs and NFs above 20%.

A 4-dimensional scan was performed over allowed choices of masses and couplings to determine the most significant excess. Figure 9.19 shows the local significance as a function of the three couplings normalised to the sum of the couplings for $m_H = 400, 700, 1000$ and 1300 GeV.

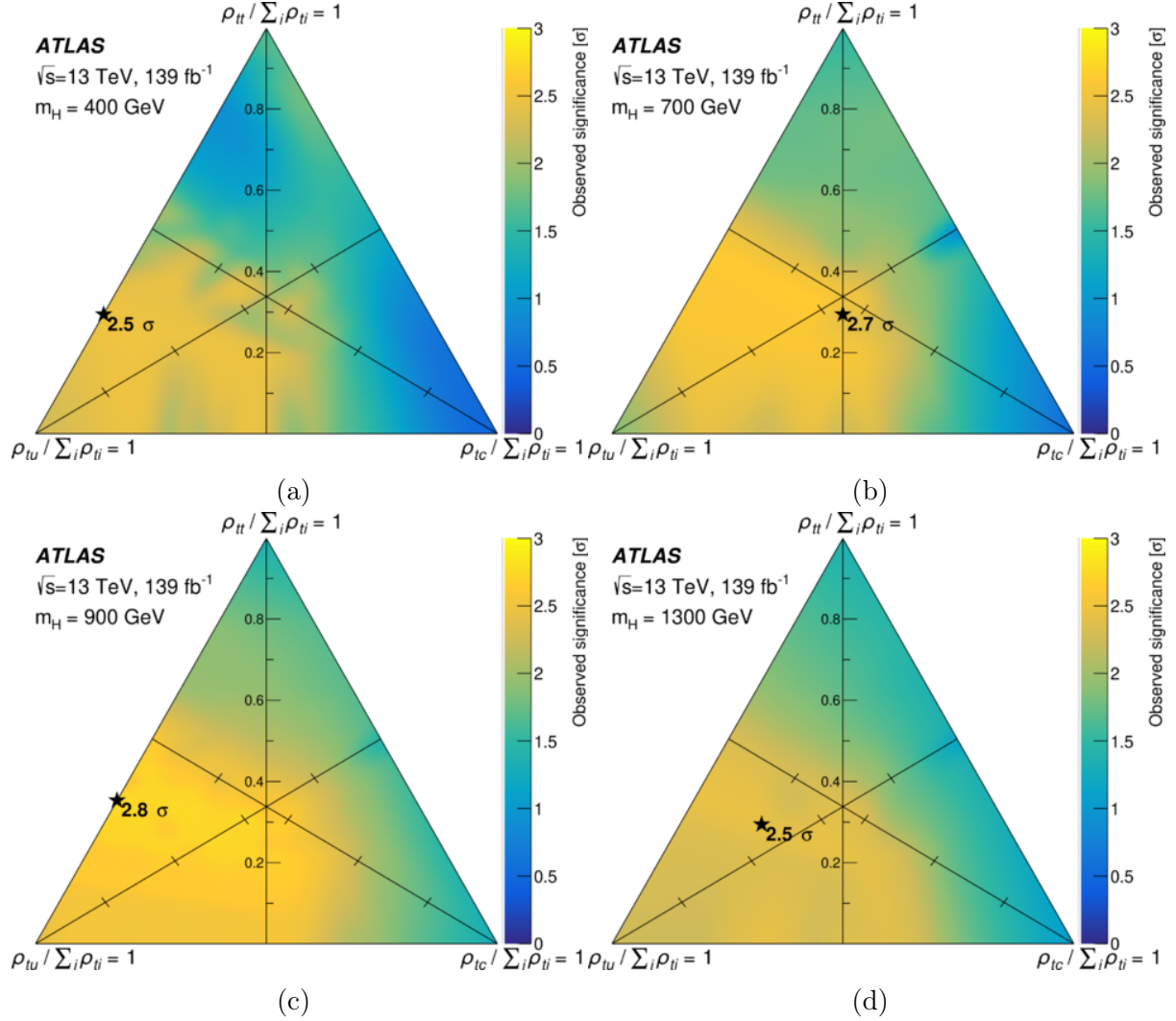
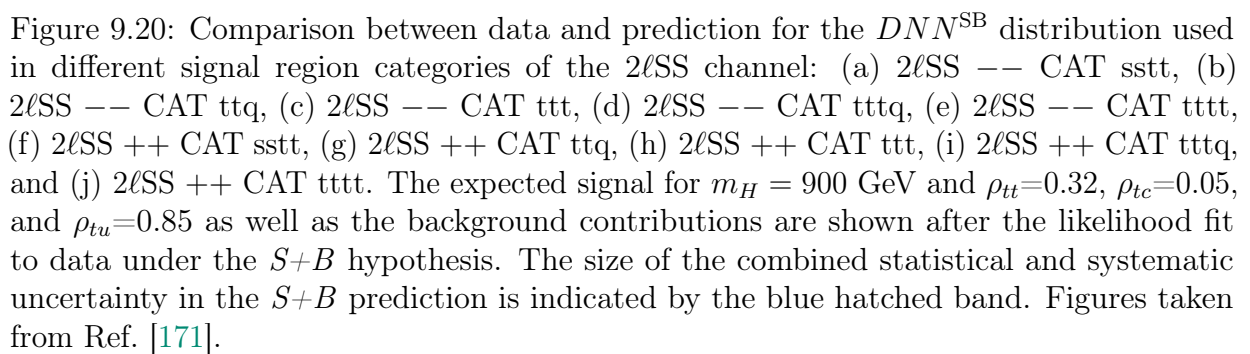


Figure 9.19: Observed significance for a heavy scalar with a mass of (a) 400 GeV (b) 700 GeV (c) 1000 GeV and (d) 1300 GeV as a function of the three couplings normalised to the sum of the couplings. The star indicates the coupling configuration leading to the highest observed significance for the given mass. Figures taken from Ref. [171].

A local significance of 2.81 standard deviations is observed when assuming a signal with $m_H = 900$ GeV and $\rho_{tt}=0.32$, $\rho_{tc}=0.05$ and $\rho_{tu}=0.85$. The signal cross section resulting from the fit to data for this g2HDM signal hypothesis is 138 fb, with fractional contributions of 71% ttq, 20% sstt, and 9% ttt. Comparisons between data and the background prediction for the DNN^{SB} distributions used in the different SRs for this set of parameters is shown in Figures 9.20 and 9.21. The corresponding post-fit yields for the SRs can be found in Tables 9.5, 9.6, and 9.7 for the 2 ℓ SS positively-charged, 2 ℓ SS negatively-charged, and 3 ℓ and 4 ℓ SRs, respectively.



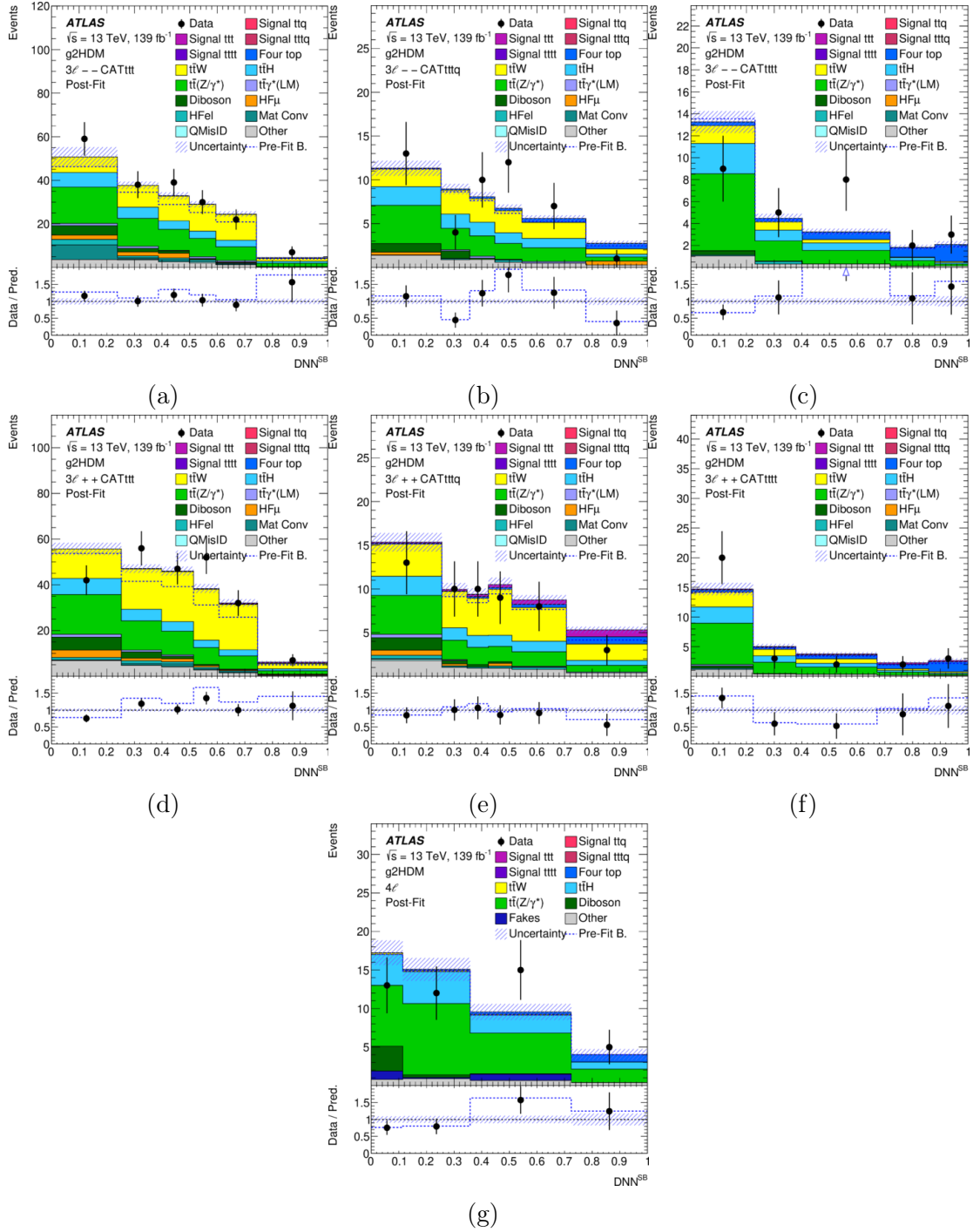


Figure 9.21: Comparison between data and prediction for the DNN^{SB} distribution used in different signal region categories of the 3ℓ and 4ℓ channels: (a) 3ℓ -- CAT tttq, (b) 3ℓ -- CAT tttt, (c) 3ℓ -- CAT tttt, (d) 3ℓ ++ CAT ttt, (e) 3ℓ ++ CAT tttq, (f) 3ℓ ++ CAT tttt, and (g) 4ℓ . The expected signal for $m_H = 900$ GeV and $\rho_{tt}=0.32$, $\rho_{tc}=0.05$, and $\rho_{tu}=0.85$ as well as the background contributions are shown after the likelihood fit to data under the $S+B$ hypothesis. The size of the combined statistical and systematic uncertainty in the $S+B$ prediction is indicated by the blue hatched band. Figures taken from Ref. [171].

	2 ℓ SS ++ CAT sstt	2 ℓ SS ++ CAT ttq	2 ℓ SS ++ CAT ttt	2 ℓ SS ++ CAT ttq	2 ℓ SS ++ CAT tttt
Signal	8 $\pm$ 4	16 $\pm$ 7	3.8 $\pm$ 1.7	23 $\pm$ 10	4.2 $\pm$ 1.9
$tt\bar{t}\bar{t}$	0.2 $\pm$ 0.1	0.4 $\pm$ 0.1	2.3 $\pm$ 0.5	4.6 $\pm$ 0.9	7.8 $\pm$ 1.4
$t\bar{t}W$	231 $\pm$ 19	139 $\pm$ 10	219 $\pm$ 16	68 $\pm$ 7	15 $\pm$ 2
$t\bar{t}H$	17 $\pm$ 3	15 $\pm$ 2	37 $\pm$ 5	14 $\pm$ 3	6.1 $\pm$ 1.4
$t\bar{t}(Z/\gamma^*)$	43 $\pm$ 5	24 $\pm$ 3	53 $\pm$ 5	14 $\pm$ 1	5.5 $\pm$ 0.8
$t\bar{t}\gamma^*$ (low mass)	5.3 $\pm$ 3.0	4.0 $\pm$ 2.4	4.9 $\pm$ 2.8	1.3 $\pm$ 0.8	0.6 $\pm$ 0.4
VV	22 $\pm$ 7	11 $\pm$ 4	5.2 $\pm$ 1.9	2.2 $\pm$ 0.9	0.2 $\pm$ 0.1
tZ	24 $\pm$ 1	9.3 $\pm$ 0.6	5.2 $\pm$ 0.4	0.7 $\pm$ 0.1	0.01 $\pm$ 0.01
Non-prompt ℓ	45 $\pm$ 17	20 $\pm$ 7	19 $\pm$ 6	4.2 $\pm$ 1.9	0.8 $\pm$ 0.7
Mat Conv	19 $\pm$ 5	5.9 $\pm$ 1.6	7.2 $\pm$ 2.1	1.7 $\pm$ 0.7	0.9 $\pm$ 0.2
QMisID	7.4 $\pm$ 2.7	1.7 $\pm$ 0.6	1.4 $\pm$ 0.5	0.2 $\pm$ 0.1	0.02 $\pm$ 0.01
Other	5.8 $\pm$ 2.0	4.0 $\pm$ 1.3	8.0 $\pm$ 2.2	6.1 $\pm$ 1.9	2.4 $\pm$ 0.6
Total	428 $\pm$ 15	250 $\pm$ 9	367 $\pm$ 12	141 $\pm$ 9	43 $\pm$ 3
Data	434	261	342	138	46

Table 9.5: Post-fit yields of the 2 ℓ SS (++) SRs. The best-fit signal for $m_H = 900$ GeV and ($\rho_{tt}=0.32$, $\rho_{tc}=0.05$, and $\rho_{tu}=0.85$) is shown for a $\mu = 1.8 \pm 0.8$. Tables taken from Ref. [171].

	2 ℓ SS -- CAT sstt	2 ℓ SS -- CAT ttq	2 ℓ SS -- CAT ttt	2 ℓ SS -- CAT ttq	2 ℓ SS -- CAT tttt
Signal	1.0 $\pm$ 0.4	2.1 $\pm$ 1.0	0.5 $\pm$ 0.2	3.0 $\pm$ 1.3	0.6 $\pm$ 0.3
$tt\bar{t}\bar{t}$	0.2 $\pm$ 0.1	0.5 $\pm$ 0.1	2.4 $\pm$ 0.6	4.7 $\pm$ 0.9	7.8 $\pm$ 1.4
$t\bar{t}W$	115 $\pm$ 9	72 $\pm$ 5	126 $\pm$ 9	37 $\pm$ 4	9.4 $\pm$ 1.4
$t\bar{t}H$	17 $\pm$ 3	15 $\pm$ 2	38 $\pm$ 6	15 $\pm$ 3	6.1 $\pm$ 1.4
$t\bar{t}Z/\gamma^*$	42 $\pm$ 5	23 $\pm$ 3	53 $\pm$ 5	14 $\pm$ 2	5.5 $\pm$ 0.8
$t\bar{t}\gamma^*$ (low mass)	9 $\pm$ 5	3.3 $\pm$ 1.9	6.2 $\pm$ 3.5	1.4 $\pm$ 0.9	0.3 $\pm$ 0.3
VV	21 $\pm$ 6	7.7 $\pm$ 2.7	3.9 $\pm$ 1.5	1.4 $\pm$ 0.5	0.1 $\pm$ 0.1
tZ	13 $\pm$ 1	5.5 $\pm$ 0.3	3.2 $\pm$ 0.3	0.27 $\pm$ 0.02	0.04 $\pm$ 0.02
Non-prompt ℓ	54 $\pm$ 16	23 $\pm$ 8	25 $\pm$ 8	2.6 $\pm$ 0.8	0.8 $\pm$ 0.5
Mat Conv	16 $\pm$ 4	3.9 $\pm$ 1.1	6.7 $\pm$ 1.8	0.8 $\pm$ 0.5	1.4 $\pm$ 0.6
QMisID	7.4 $\pm$ 2.7	1.7 $\pm$ 0.6	1.4 $\pm$ 0.5	0.2 $\pm$ 0.1	0.02 $\pm$ 0.01
Other	6.4 $\pm$ 2.1	3.8 $\pm$ 1.2	7.7 $\pm$ 2.3	5.7 $\pm$ 1.8	2.3 $\pm$ 0.6
Total	302 $\pm$ 10	161 $\pm$ 5	273 $\pm$ 8	86 $\pm$ 4	34 $\pm$ 2
Data	296	158	282	78	35

Table 9.6: Post-fit yields of the 2 ℓ SS (--) SRs. The best-fit signal for $m_H = 900$ GeV and ($\rho_{tt}=0.32$, $\rho_{tc}=0.05$, and $\rho_{tu}=0.85$) is shown for a $\mu = 1.8 \pm 0.8$. Tables taken from Ref. [171].

	$3\ell ++$ CAT tttt	$3\ell ++$ CAT tt	$3\ell ++$ CAT ttq	$3\ell --$ CAT tttt	$3\ell --$ CAT tt	$3\ell --$ CAT ttq	4ℓ
Signal	1.2 ± 0.5	1.6 ± 0.7	2.9 ± 1.3	0.2 ± 0.1	0.2 ± 0.1	0.4 ± 0.2	0.05 ± 0.02
$t\bar{t}t\bar{t}$	3.7 ± 0.7	0.8 ± 0.2	1.7 ± 0.3	3.7 ± 0.7	0.9 ± 0.2	1.7 ± 0.3	1.5 ± 0.9
$t\bar{t}W$	4.6 ± 0.6	100 ± 7	23 ± 3	2.7 ± 0.4	55 ± 4	12 ± 2	0.5 ± 0.1
$t\bar{t}H$	4.8 ± 1.0	23 ± 3	7.5 ± 1.5	4.8 ± 1.0	23 ± 3	7.6 ± 1.4	10 ± 3
$t\bar{t}Z/\gamma^*$	11 ± 1	55 ± 6	13 ± 2	11 ± 1	56 ± 6	13 ± 2	24 ± 3
$t\bar{t}\gamma^*$ (low mass)	0.2 ± 0.2	2.6 ± 1.5	0.7 ± 0.4	0 ± 0	3.2 ± 1.8	0.5 ± 0.3	0 ± 0
VV	0.5 ± 0.2	11 ± 4	2.4 ± 0.9	0.4 ± 0.2	7.9 ± 3.0	2.1 ± 0.6	3.6 ± 1.3
tZ	0.27 ± 0.02	13 ± 1	2.5 ± 0.2	0.11 ± 0.01	7.2 ± 0.4	1.2 ± 0.1	0 ± 0
Non-prompt ℓ	0 ± 0	11 ± 4	1.9 ± 0.8	0.2 ± 0.1	12 ± 6	1.1 ± 0.6	2.1 ± 0.3
Mat Conv	0.2 ± 0.1	3.2 ± 1.1	0.5 ± 0.3	0.1 ± 0.1	8 ± 5	0.04 ± 0.01	0 ± 0
Other	1.9 ± 0.5	7.4 ± 2.3	3.3 ± 1.0	1.8 ± 0.5	5.9 ± 2.0	3.3 ± 1.0	2.7 ± 0.9
Total	28 ± 2	229 ± 6	60 ± 3	25 ± 2	180 ± 7	43 ± 2	45 ± 3
Data	30	236	53	27	195	47	45

Table 9.7: Post-fit yields of the 3ℓ and 4ℓ SRs. The best-fit signal for $m_H = 900$ GeV and ($\rho_{tt}=0.32$, $\rho_{tc}=0.05$, and $\rho_{tu}=0.85$) is shown for a $\mu = 1.8 \pm 0.8$. Tables taken from Ref. [171].

Figures 9.22a and 9.22b show the summary of the regions after the profile likelihood fit, together with the pre-fit background expectation. The SRs with the largest pre-fit tension between data and the background yields at high values of the DNN^{SB} are the $t\bar{t}t\bar{t}q$, the $t\bar{t}t\bar{t}$, the $sstt$, and the ttq regions. Within this model, the $\hat{\lambda}_{t\bar{t}W}$ remains higher than 1, as observed by other analyses. However, charge-asymmetric tensions both at low and high jet and b -jet multiplicities are accommodated by the best fit g2HDM signal, where the largest signal contributions in the $t\bar{t}t\bar{t}q$ and the $t\bar{t}t\bar{t}$ regions originate mainly from ttq and $t\bar{t}t$ processes (excess at high jet multiplicities), and the largest signal contributions in the tt and the ttq regions originate mainly from the corresponding targeted signals tt and ttq processes (excess at low jet multiplicities). The systematic uncertainties with the largest impact on the signal strength originate from the modelling of $t\bar{t}W$ with and without additional heavy flavour jets, $t\bar{t}Z$, $t\bar{t}H$, and $t\bar{t}t\bar{t}$ processes. The search is dominated by statistical uncertainties.

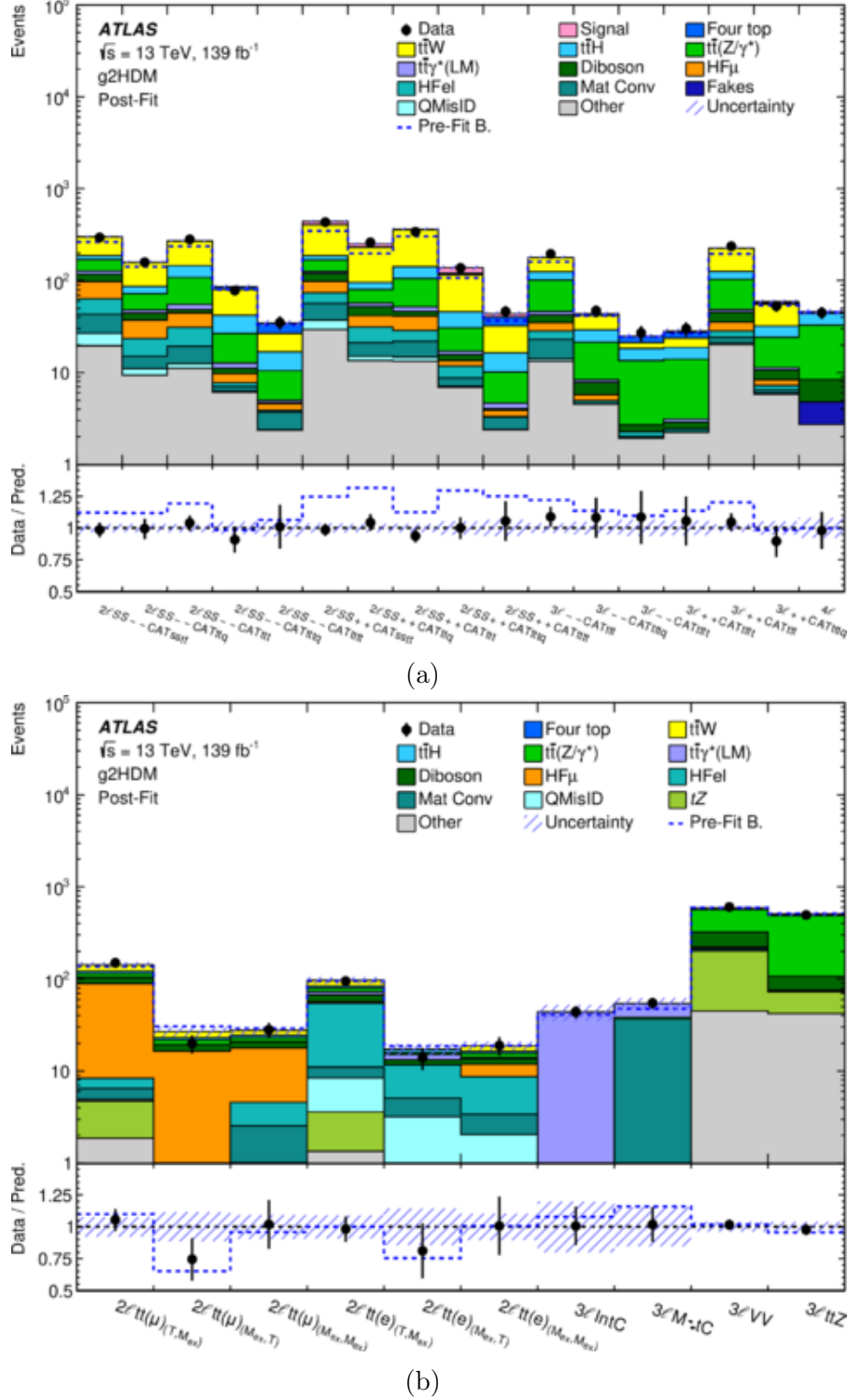


Figure 9.22: Comparison between data and the background prediction for the event yields in the (a) 17 SRs and the (b) 10 CRs. The expected signal for $m_H = 900$ GeV and ($\rho_{tt}=0.32$, $\rho_{tc}=0.05$, and $\rho - tu=0.85$) as well as the background contributions are shown after the likelihood fit to data under the $S+B$ hypothesis. The total background prediction before the likelihood fit to data is shown as a dashed blue histogram in the upper panel. The blue hatched band includes both statistical and systematic uncertainties. Figures taken from Ref. [171].

9.5.1 Expected and observed upper limits

Exclusion limits on the BSM Higgs boson mass are set for different choices of the couplings, as shown in Figure 9.23. An observed (expected) limit on the Higgs boson mass of 620 (840) GeV is set in the benchmark scenario with couplings $\rho_{tt} = 0.4$ and $\rho_{tq} = 0.2$. For a scenario without coupling to two top quarks, i.e. $\rho_{tt} = 0$, $\rho_{tc} = 0.2$, $\rho_{tu} = 0.2$, an observed (expected) limit of 350 (580) GeV on the heavy Higgs boson mass is set. No limits can be set on scenarios without off-diagonal couplings leading only to four-top final states with a coupling set $\rho_{tt} = 1$, $\rho_{tc} = 0$, $\rho_{tu} = 0$, but the search could have potentially excluded larger allowed ρ_{tt} values ($\rho_{tt} < 2$ is allowed by existing constraints [168]). Broad excesses across the Higgs boson mass spectrum are observed in all three scenarios. A real signal would also be expected to lead to such excesses are expected due to the search's poor mass resolution, which results from the lack of mass reconstruction variables in the training of the neural networks. The sensitivity of the analysis on the four-top final state is similar to previous ATLAS analyses [156]. The excluded mass is also presented as a function of two couplings under different assumptions, as shown in Figure 9.24.

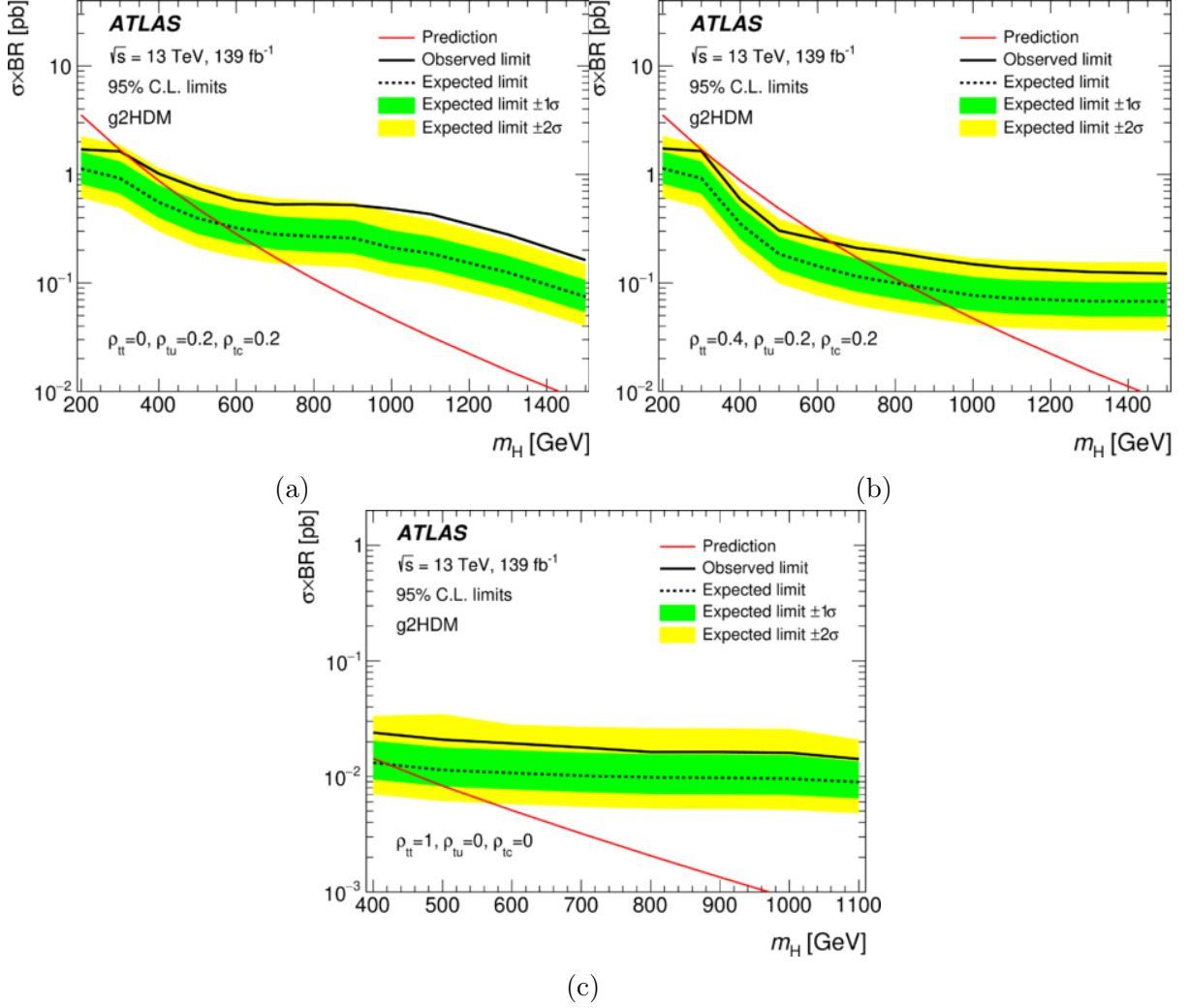


Figure 9.23: Observed and expected exclusion limits at 95% confidence level on the heavy Higgs boson mass for the g2HDM signal model for different couplings choices: (a) $\rho_{tt} = 0$, $\rho_{tc} = 0.2$, $\rho_{tu} = 0.2$, (b) $\rho_{tt} = 0.4$, $\rho_{tc} = 0.2$, $\rho_{tu} = 0.2$ and (c) $\rho_{tt} = 1$, $\rho_{tc} = 0$, $\rho_{tu} = 0$. The yellow and green contours of the band around the expected limit are the $\pm 1\sigma$ and $\pm 2\sigma$ variations including all uncertainties, respectively. The theoretical prediction for the signal production cross section is also shown as a red line. The production cross section is the sum of the five production modes considered in the search. Figures taken from Ref. [171].

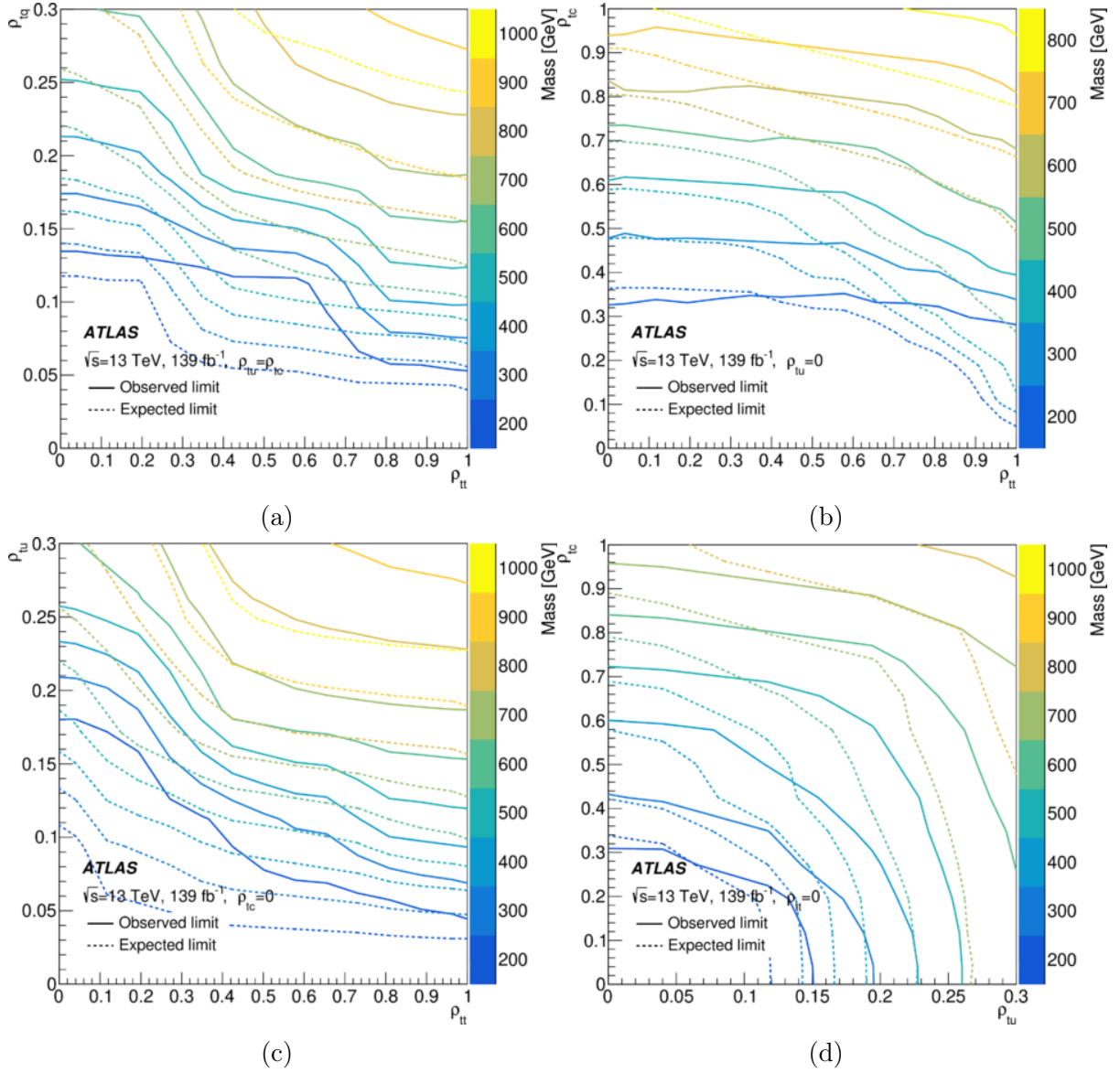


Figure 9.24: Observed (solid line) and expected (dashed line) exclusion limits on the scalar mass as a function of the coupling under different assumptions: (a) $\rho_{tc} = \rho_{tu}$, (b) $\rho_{tu} = 0$, (c) $\rho_{tc} = 0$, and (d) $\rho_{tt} = 0$. Figures taken from Ref. [171].

9.6 Re-interpretation in RPV SUSY models

This search is also used to set limits on RPV SUSY models featuring multiple light leptons and b -jets in the final state, using the existing DNNs that were trained for the g2HDM model. The models are motivated by flavour anomalies [176–183] and the $(g - 2)_\mu$ anomaly [184] and can provide a successful explanation with different choices of particles, masses, and couplings [185–194]. The first model features electroweakino production (wino or Higgsino) which decays via a lepton-number-violating RPV coupling (λ'_{i33} , with $i \in 2, 3$) to a lepton and third-generation quarks. Relevant diagrams for the production and decay are shown in Figures 9.25a and 9.25b. The second model features direct smuon production decaying to a bino-like neutralino, which in turn decays via the same RPV coupling (λ'_{i33}), as shown in Figure 9.25c.

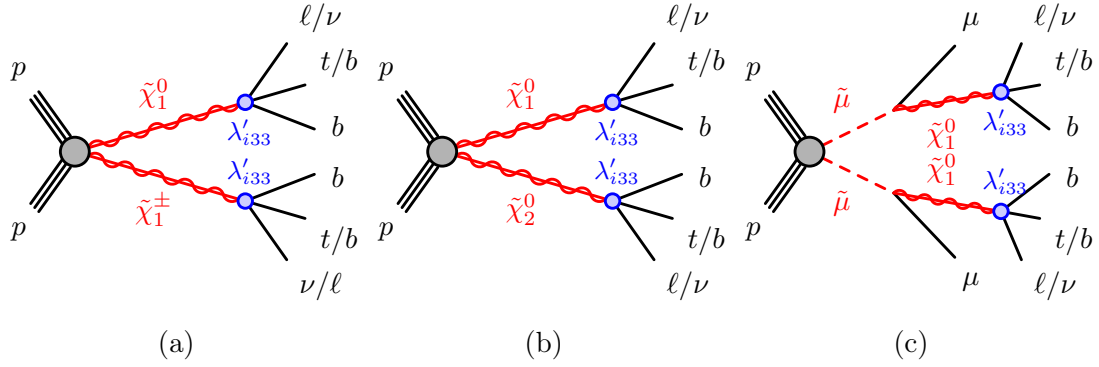


Figure 9.25: Feynman diagrams for the RPV SUSY signals used as additional interpretation in the analysis. The subsequent decay can lead to a final state with high multiplicity of leptons and b -jets which is targeted by the search

The DNNs trained for the g2HDM model were re-used for the SUSY re-interpretation, with the distributions of the SUSY signal processes compared to the total expected background shown in the various DNN^{cat} categories in Figure 9.26.

Figures 9.27a and 9.27b show the exclusion limits obtained on the higgsino and wino models respectively. Higgsinos (winos) with masses up to 585 (670) GeV are excluded. Figure 9.28 shows limits on the smuon-bino model. Smuon masses up to 460 GeV are excluded, with weaker exclusion limits for small mass splittings between the smuon and the neutralino.

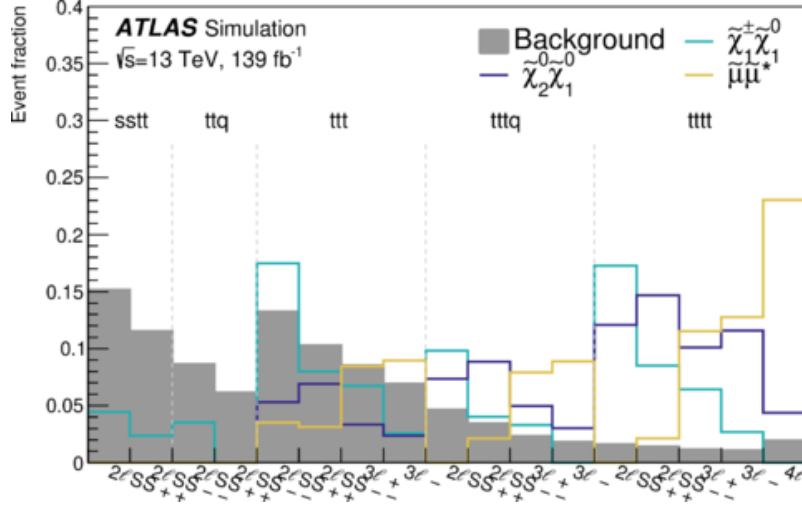


Figure 9.26: Distributions for the SUSY signal processes compared to the total expected background in the DNN^{cat} categories of the g2HDM search. All distributions are normalised to unity. Figure taken from Ref. [171].

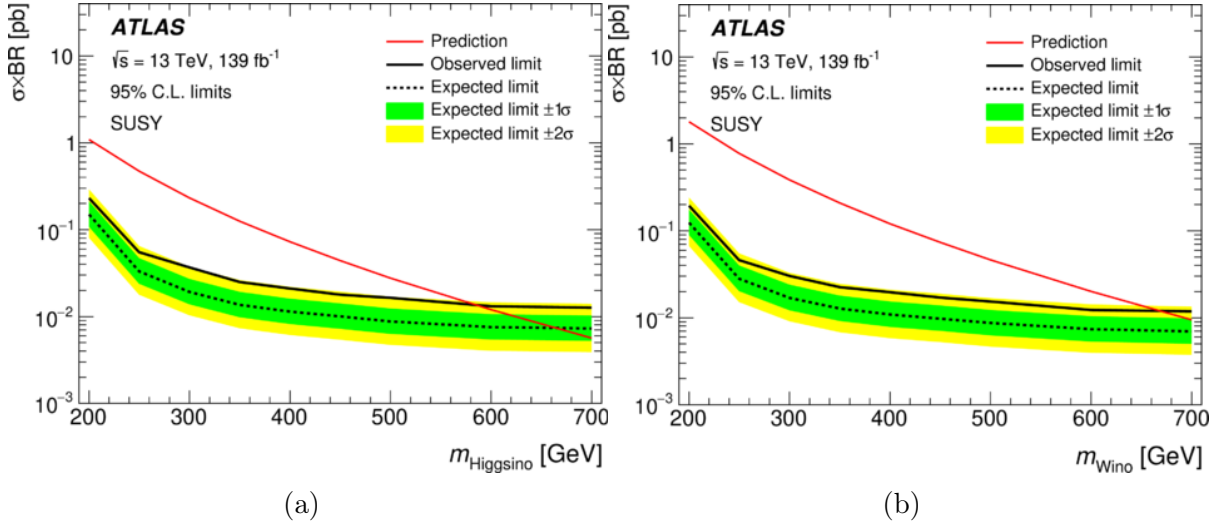


Figure 9.27: Expected and observed exclusion limits on the cross section times branching ratio of electroweakino production in RPV SUSY models as a function of the sparticle masses: (a) higgsino model, and (b) wino model. The yellow and green contours of the band around the expected limit are the $\pm 1\sigma$ and $\pm 2\sigma$ variations including all uncertainties, respectively. The theoretical prediction for the signal production cross section is also shown as a red line. Figures taken from Ref. [171].

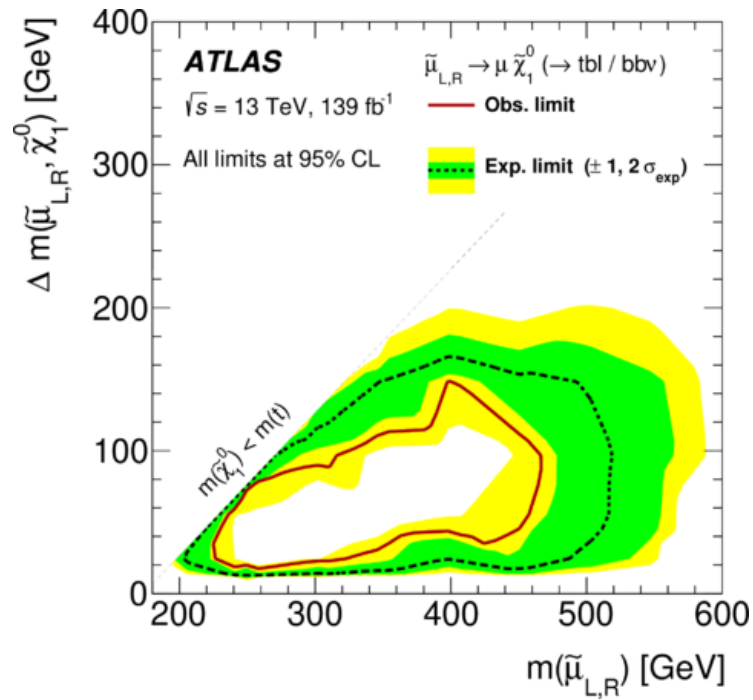


Figure 9.28: Expected and observed exclusion limits on the smuon plus bino RPV SUSY model. The yellow and green contours of the band around the expected limit are the $\pm 1\sigma$ and $\pm 2\sigma$ variations including all uncertainties, respectively. The diagonal grey lines indicates the allowed kinematic limit for the decays. The neutralino is assumed to decay to $t\bar{b}l$ or $b\bar{b}\nu$ with equal probability. Figure taken from Ref. [171].

9.7 Conclusions

This chapter presented the first LHC search for flavour violating heavy Higgs bosons decaying to multilepton plus multi b -jets final states, performed using the full Run 2 dataset of proton-proton collisions collected at $\sqrt{s} = 13$ TeV, corresponding to an integrated luminosity of 139 fb^{-1} , by the ATLAS experiment. The results are interpreted in terms of a general two Higgs doublet (g2HDM) model involving an additional scalar with couplings to the top-quark and the three up-type quarks (ρ_{tt} , ρ_{tc} , and ρ_{tu}). The targeted signals lead to final states with either a same-sign top-quark pair, three top-quarks, or four top-quarks. Events are categorised depending on the multiplicity of light charged leptons (electrons or muons), total lepton charge, and a deep-neural-network-based categorisation to enhance the purity of each of the signals. A broad excess is observed over the Standard Model expectation corresponding to a maximum local significance of 2.8 standard deviations for a signal with $m_H = 900$ GeV and $\rho_{tt}=0.32$, $\rho_{tc}=0.05$ and $\rho_{tu}=0.85$. Exclusion limits at 95% confidence are set on the mass and couplings of the heavy Higgs boson. An additional scalar boson with couplings $\rho_{tt} = 0.3$, $\rho_{tc} = 0.15$, and $\rho_{tu} = 0.15$ is observed (expected) to be excluded at 95% confidence level for masses up to $m_H = 570$ (760) GeV. Additional interpretations are provided in models of R -parity violating supersymmetry, motivated by the recent flavour and $(g - 2)_\mu$ anomalies. The results of this search is published at JHEP 12 (2023) 081 [171].

Search for vector-like light leptons in multilepton final states

This chapter presents the results of the first direct LHC search for vector-like electrons and muons, collectively termed vector-like light leptons (VLLs). Section 10.1 provides a brief introduction to the simplified models containing VLLs, motivation for these particles and highlights the challenging nature of this search. The analysis strategy is discussed in the subsequent sections and the chapter concludes presenting results of this search.

10.1 Simplified model

Vector-like fermions are hypothetical particles whose left- and right-handed chiral components have the same transformation properties under the weak-isospin $SU(2)$ gauge group [195–199]. These particles are expected to be sub-TeV in mass and arise in many BSM models, such as composite Higgs models [200, 201], models with extra spatial dimensions [202, 203], supersymmetric models [204, 205], and grand unified theories [206–208]. These fermions are expected to mix with SM fermions and provide an explanation to the flavour puzzle [209, 210], or even a dark matter candidate [211–214]. A broad search program has been developed for vector-like quarks or particles with color charge, produced via the strong interaction (see e.g. Section 6.2 of Ref. [215]). On the other hand, VLLs are only recently gaining interest. Compared to VLQs, these searches are challenging because VLLs are expected to be produced via the electroweak interaction and thus, have much lower production cross-sections. Models containing these particles might explain the observed tensions between the measured and predicted values of the anomalous moment of the

muon [216, 217] and the electron [218–220] and the *Cabibbo angle anomaly* [221–223].

The simplest extension of the SM includes VLLs occurring either as an $SU(2)$ doublet or an $SU(2)$ singlet. The production and decay modes for VLLs depend on the assumed $SU(2)$ representation and are shown in Figure 10.1 [224, 225].

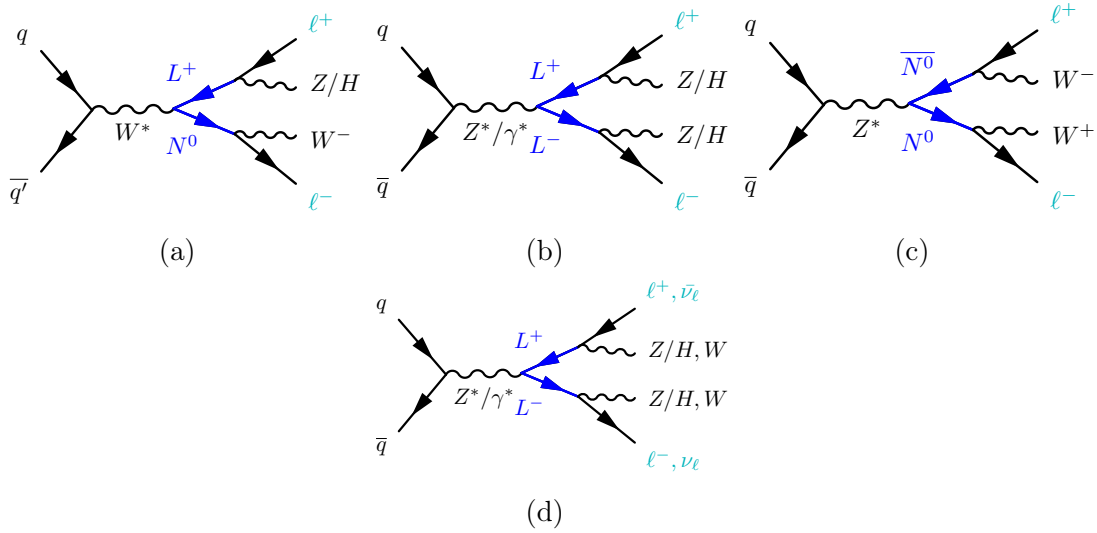


Figure 10.1: Feynman diagrams illustrating the pair production and decay of vector-like leptons from (a-c) the $SU(2)$ doublet and (d) $SU(2)$ singlet models.

The $SU(2)$ doublet model consists of one electrically charged ($L^\pm$) and one electrically neutral (N^0) VLL. They can be produced either together or in pairs via a virtual W , Z or photon exchange and decay to a charged SM lepton and a weak (W/Z) or Higgs boson, conserving lepton flavor, total charge and other quantum numbers. The $SU(2)$ singlet model, on the other hand, consist of just the charged VLLs ($L^\pm$), with additional couplings that allow decays to SM neutrinos, in addition to charged leptons. Lepton flavor and other quantum numbers are conserved in these decays. Figure 10.2 shows the total production cross sections (assuming all modes), calculated at next-to-leading order, for VLLs from both the doublet and singlet models. The charged and the neutral VLL from the doublet model have been assumed to be mass-degenerate. The production cross-sections for the doublet model are enhanced by the W -mediated production modes, which have a much larger cross-section than those mediated by Z/γ^* .

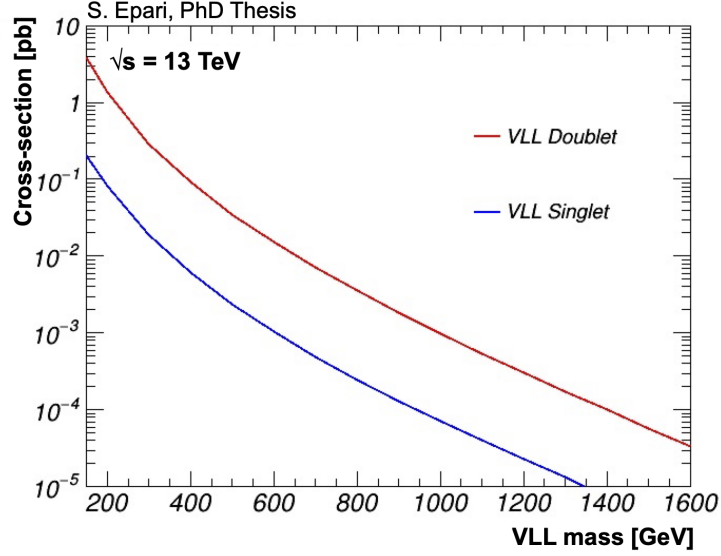


Figure 10.2: Total production cross-sections for vector-like leptons from the $SU(2)$ singlet (blue) and $SU(2)$ doublet (red) model, calculated at next-to-leading order, as a function of VLL mass (m_{VLL}).

As shown in Figure 10.3, the branching ratio of the charged VLL from the doublet model to either the Higgs or Z boson become equal and plateau at high VLL masses, following the Goldstone boson equivalence theorem [226]. Further, decays to the Z boson are kinematically favorable at low VLL mass. On the other hand, in the singlet model, the additional W decay mode is always higher in branching ratio than the decay modes to the Higgs or Z boson.

Searches at the LEP collider excluded vector-like leptons with mass less than ~ 100 GeV at the 95% confidence level (CL) [227], for both the doublet and singlet models. At the LHC, using a data sample of pp collisions at a centre-of-mass energy of $\sqrt{s} = 8$ TeV corresponding to an integrated luminosity of 20.3 fb^{-1} , the ATLAS Collaboration excluded vector-like electrons (muons) in the mass range 129–176 GeV (114–168 GeV), except for 144–163 GeV (153–160 GeV), in the doublet scenario [228]. Both the ATLAS and CMS Collaborations searched for vector-like τ -leptons using the full LHC Run 2 dataset at $\sqrt{s} = 13$ TeV, corresponding to about 140 fb^{-1} . Assuming the doublet scenario, the ATLAS search excluded vector-like τ -leptons in the mass range of 130–900 GeV [229]. The CMS search considered both the doublet and singlet scenarios, excluding vector-like τ -leptons in the mass ranges of 100–1045 GeV and 125–150 GeV, respectively [230].

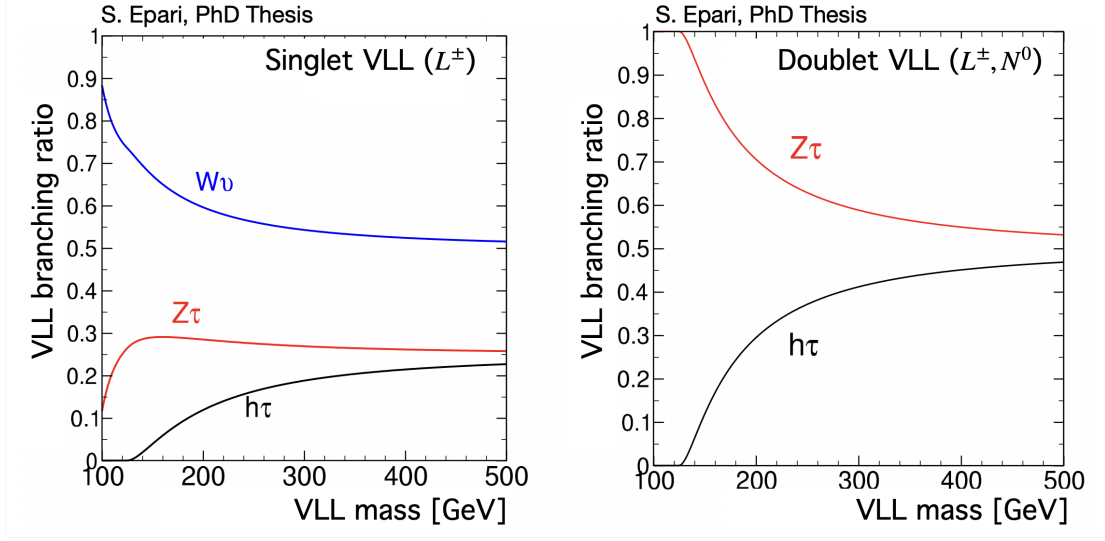


Figure 10.3: Branching ratios for a VLL from an $SU(2)$ singlet (left) and mass-degenerate VLLs from an $SU(2)$ doublet (right) as a function of the VLL mass. Figure adapted from Ref [224].

10.2 Datasets, trigger and object definition

The full Run 2 dataset, corresponding to an integrated luminosity of 140 fb^{-1} with an uncertainty of 0.83%, at a centre-of-mass energy $\sqrt{s} = 13 \text{ TeV}$ is used for this search. Events with two or more light leptons are pre-selected using a logical OR of single and di-lepton triggers (SLT OR DLT). Details about these triggers are summarised in Table 8.2. Physics objects are reconstructed using the definitions established in Chapter 8 and τ_{had} candidates are vetoed from the search. Events are separated into channels with two opposite-sign ($2\ell\text{OS}$), three (3ℓ) and four (4ℓ) light leptons using the loose light lepton definitions established in Chapter 8. For electrons (muons), the TightLH (Medium) ID and FCLoose isolation WP is used to pre-select events. B -jets are tagged at the 77% DL1r WP.

Signal samples for vector-like electrons ($VLLe$) and vector-like muons ($VLL\mu$) from $SU(2)$ singlet and doublet models were generated using MADGRAPH v2.9.5 at NLO with NNPDF30_nlo_as_0118 and PYTHIA 8.245 with the A14 tune for modelling the parton shower. The mass values of these VLLs were chosen to be in $[150, 200, 300, 400, \dots, 1300] \text{ GeV}$. For each model ($VLLe$ singlet, $VLLe$ doublet, $VLL\mu$ singlet, $VLL\mu$ doublet), approximately 300k events were generated for each campaign (mc16a, mc16d, mc16e) and mass point. The NLO generator cross-section was used for the normalisation of the signals.

Detector level effects were incorporated using ATLAS *Fast Simulation*, as described in Chapter 6

10.3 Analysis strategy

The search targets $VLLe$ and $VLL\mu$ from both the models separately in channels with at least two light leptons by placing requirements on the flavor of the leptons entering the channel. Channels with at least two opposite sign electrons are used to target $VLLe$ while those with at least two opposite sign muons are used to target $VLL\mu$. These channels, also termed *multilepton* channels, are defined with up to four light leptons, and have backgrounds that are easy to model and suppress. Thus, the $2\ell OS$, 3ℓ , and 4ℓ channels are defined in terms of loose light lepton multiplicity after overlap removal as explained in Section 8. This ensures orthogonality of events entering the various channels. The 4ℓ channel with two opposite sign electrons and muons is assigned to be a $VLLe$ channel if the sum of transverse momentum of the electrons is greater than that of the muons, and a $VLL\mu$ channel if the opposite is true.

Signal regions (SRs) targeting distinct signal topologies or SM background are defined in the $2\ell OS$ and 3ℓ depending on the number of hadronically or leptonically decaying $h/W/Z$ and leptons using dedicated *signal-vs-signal-vs-background* categorisation deep neural networks (CAT DNN). *PromptLeptonImprovedVeto* (PLIV) is used to suppress fakes from heavy flavor decays in the 3ℓ channel and electron conversions are suppressed in all channels using a derivation-level flag to veto objects that resemble those originating from a conversion. Leptonically decaying $Z \rightarrow l\bar{l}$ candidates, reconstructed within a 10 GeV window around the Z mass, are vetoed from the $2\ell OS$ and 3ℓ channels. Orthogonal control regions (CRs) are defined in order to accurately estimate the normalisation of the main backgrounds in the SRs, described in Section 10.3.2. Finally, a maximum-likelihood fit is performed across event categories, separately for each model, in order to test for a possible signal.

10.3.1 Signal region definition

Distinct signal topologies can be defined in each channel ($2\ell OS$ and 3ℓ) depending on the kinds of SM boson decays expected to populate these final states. VLLs from the $SU(2)$ doublet have two charged leptons originating from the VLL and any missing transverse energy (E_T^{miss}) can only come from boson decays. Thus, these topologies are expected

to have lower E_T^{miss} . On the other hand, VLLs from the $SU(2)$ singlet can have much larger E_T^{miss} due to at least one possible neutrino from the VLL in the final state, and the branching ratio to this state being higher than to the charged lepton states. In the $2\ell\text{OS}$ channel, three low E_T^{miss} and two high E_T^{miss} topologies can be defined, sensitive to both VLL models:

- $\ell\ell\text{HH}$: low E_T^{miss} topology targeting two hadronic Higgs boson candidates. Characterised by a high number of b -jets.
- $\ell\ell\text{HV}$: low E_T^{miss} topology targeting a hadronic Higgs boson candidate and a hadronic W/Z boson candidate. Characterised by a high number of a mix of light and heavy-flavour (b - or c -) jets.
- $\ell\ell\text{VV}$: low E_T^{miss} topology targeting two hadronic W/Z boson candidates. Characterised by a high number of light-flavour jets.
- $\ell\nu\text{HW}$: high E_T^{miss} topology targeting a hadronic Higgs boson candidate and a leptonic W boson candidate. Characterised by heavy-flavour jets.
- $\ell\nu\text{WZ}$: high E_T^{miss} topology targeting a hadronic Z boson candidate and a leptonic W boson candidate. Characterised by light-flavour jets.

Each of the above topologies have their own unique ad-mixture of heavy flavor jets. An additional *SM-like* category is defined to capture events which fall into none of the above topologies. This category is expected to be low in signal but capture a lot of the SM background.

A similar exercise is repeated in the 3ℓ channel, merging topologies that are theoretically or experimentally harder to distinguish, and the following topologies were defined in addition to the background *SM-like* category:

- $\ell\ell\text{HH} + \text{HW}$: low E_T^{miss} topology targeting a hadronic Higgs boson candidate and a leptonic W boson candidate (prompt or from the other Higgs boson decay). Characterised by a high number of b -jets.
- $\ell\ell\text{HV} + \text{VV}$: low E_T^{miss} topology targeting a Higgs boson $H \rightarrow WW$ candidate, with one of the W bosons decaying into a lepton and a neutrino, and a hadronic W/Z boson candidate. Characterised by a high number of light-flavour jets.

- $\ell\nu\text{HV}$: high $E_{\text{T}}^{\text{miss}}$ topology targeting a Higgs boson $H \rightarrow WW$ candidate, with both W bosons decaying into a lepton and a neutrino, and a hadronic W/Z boson candidate. Characterised by a high number of light-flavour jets.

The advantage of defining the above topologies is to design SRs sensitive to not only the VLL models, but also any similar non-VLL like topology that falls into one of the above categories. In the absence of an overall excess in the search, this categorisation is valuable to possibly pin-point the features of a different BSM signal by looking at the topologies which show the most disagreement with data, as input to future studies. The analysis uses a multi-class deep neural network (DNN), trained separately in the $2\ell\text{OS}$ and 3ℓ channels to classify events into one of the signal categories or background. The variables listed in Table 10.1 are used to discriminate between the categories. These variables are independent of lepton flavor and independent of the mass of the VLL, ensuring the same training can be used for both $\text{VLL}e$ and $\text{VLL}\mu$, for all mass points.

Signal categorisation neural network input variables
Number of jets (N_{jets})
Sum of pseudo-continuous b -tagging scores of jets (sumPCB)
Number of hadronic W or Z bosons ($n\text{WZ}_{\text{had}}$)
Number of hadronic h bosons ($N_{h \rightarrow bb}$)
Missing transverse energy ($E_{\text{T}}^{\text{miss}}$)

Table 10.1: Input variables for categorisation neural network for the $2\ell\text{OS}$ and 3ℓ channels.

The shapes of these variables for signal topologies defined in the $2\ell\text{OS}$ channels is shown in Figure 10.4. A powerful variable counting the weighted sum of the number of light and heavy flavor jets in an event, called the sum of pseudo-continuous b -tagging scores of jets (sumPCB), is created. Distributions of $\ell\ell\text{HH}$ and $\ell\ell\text{HV}$ in the topologies show separation in sumPCB and N_{jets} , from the rest of the topologies which have either lower jet multiplicity or light flavor jets. The $E_{\text{T}}^{\text{miss}}$ distribution is useful in separating out most events in the topologies with neutrinos in the final state. The algorithm for reconstructing the number of $h \rightarrow bb$ candidates searches for a single b -tagged jet with mass in the window 90–140 GeV (for reconstructing boosted $h \rightarrow bb$ candidates), and in the absence of such a jet, looks for two b -tagged jets with an invariant mass in the said mass window (to target reconstructing resolved $h \rightarrow bb$ candidates). Similarly, $W \rightarrow qq$ or $Z \rightarrow qq$ candidates are reconstructed by first searching for a non- b -tagged jet in the mass window 60–110 GeV (for reconstructing boosted $W/Z \rightarrow qq$ candidates), and in the absence of such a jet,

looks for two non- b -tagged jets with an invariant mass in the said mass window (to target reconstructing resolved $W/Z \rightarrow qq$ candidates). No distinction is made between a $W \rightarrow qq$ and $Z \rightarrow qq$ candidate due to similar masses of the two resonances. These algorithms have efficiencies up to about 80% for events with two leptons. Similarly, the shapes of the DNN training variables for signal topologies defined in the 3ℓ channel is shown in Figure 10.5. The $\ell\ell HH + HW$ topology, with a high number of b -tagged jets is separated well from the remaining topologies and the SM background by the sumPCB variable.

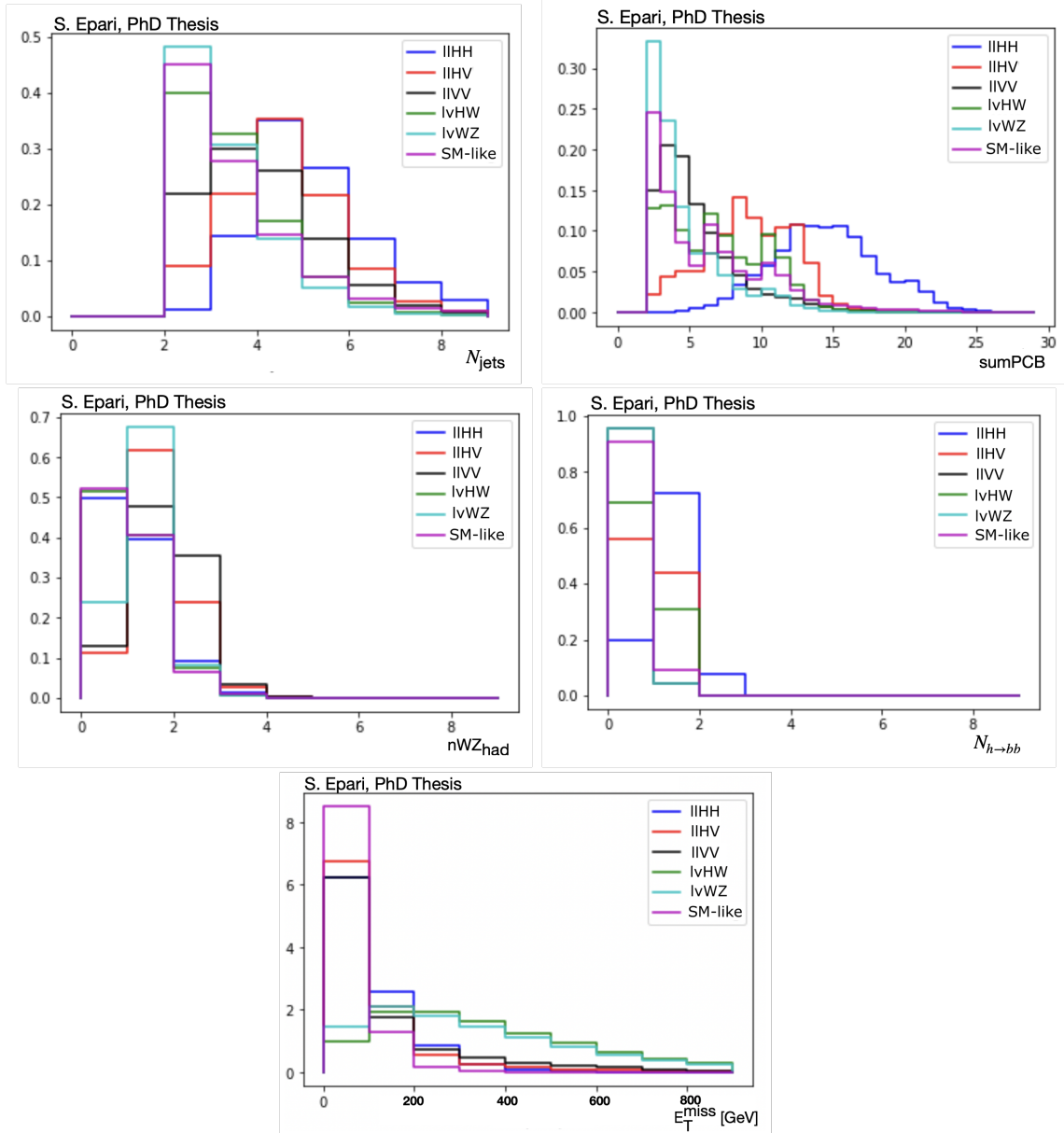


Figure 10.4: DNN training variables for the $2\ell\text{OS}$ channel, defined in Table 10.1. All distributions are normalised to unity except for the E_T^{miss} distribution.

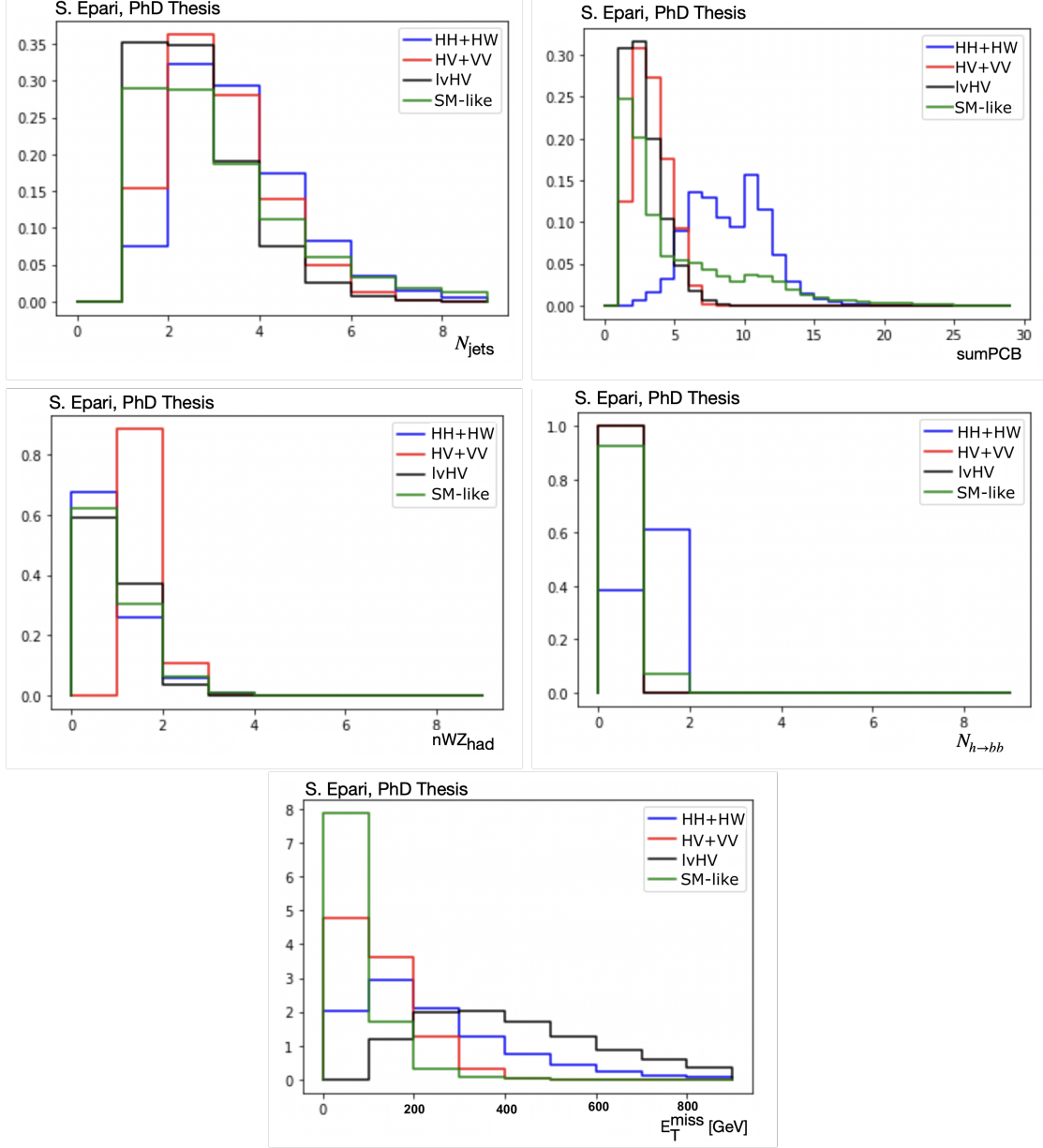


Figure 10.5: DNN training variables for the 3ℓ channel, defined in Table 10.1. All distributions are normalised to unity except for the E_T^{miss} distribution.

The training of the DNN classifiers is done using the KERAS library [137] with TENSORFLOW as a backend [138], combining all signal masses from both models. A similar architecture is used for both $2\ell\text{OS}$ and 3ℓ channels, differing in the number of output categories, shown in Figure 10.6. SM backgrounds are weighted according to their production cross-section. The output categories of the classifier correspond to the six (four) modes relevant to $2\ell\text{OS}$ (3ℓ) channel and the predicted class for each event is interpreted as the highest amongst the class probability assigned to it. The network is trained with batch size of 2000 and up to 100 epochs, using all the available signal mass points using cross-training.

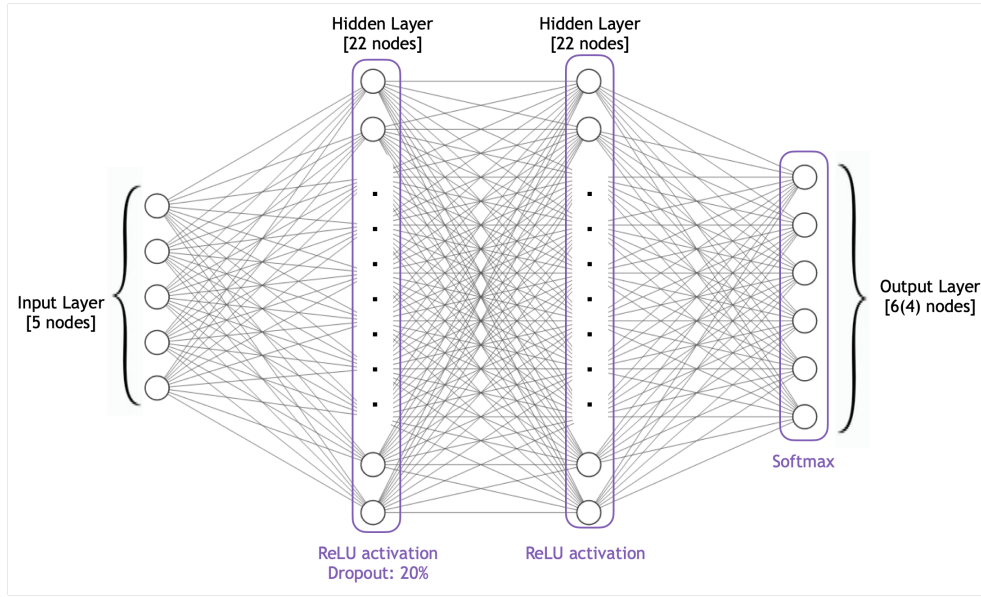


Figure 10.6: DNN architectures.

The performance of the neural network classifiers is presented as a confusion matrix: each row of the matrix represents the instances in an actual class while each column represents the instances in a predicted class. The diagonal entries can be interpreted as the probability of correctly classifying a labelled event. Figure 10.7 shows the performance of the network in validation data for $2\ell\text{OS}$ and 3ℓ channels, respectively.

In the $2\ell\text{OS}$ channel, the confusion between the two categories with a high number of heavy flavor (b -, c -) jets, namely $\ell\ell\text{HH}$ and $\ell\ell\text{HV}$, is limited by the efficiency for correctly identifying such jets. In the 3ℓ channel, confusion between the $\ell\nu\text{HV}$ and $\ell\ell\text{HV} + \text{VV}$ topology is expected to arise due to roughly similar $E_{\text{T}}^{\text{miss}}$ (a peak difference of about 200 GeV between the two categories), in addition to the requirement of a hadronically decaying Higgs and similar jet multiplicities in both topologies. Both classifiers have about

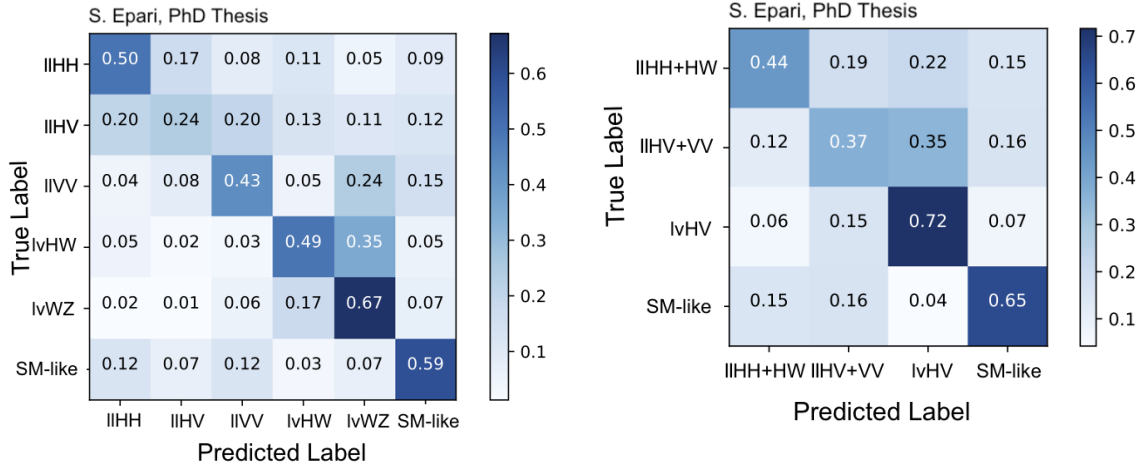


Figure 10.7: Normalised confusion matrices for 2ℓ OS (left) and 3ℓ (right). Each row of the matrix represents the instances in an actual class while each column represents the instances in a predicted class. Along the diagonal is the percentage of events predicted into the correct class by the NN. About 60% (65%) of SM background is correctly removed into the *SM-like* class in the 2ℓ OS (3ℓ) NNs.

60% efficiency in correctly classifying the SM background, with about 15% probability of confusing a signal event with that from the SM.

In the 4ℓ channel, a simple cut-and-count analysis is performed, looking for signal topologies with up to a single leptonically decaying Z candidate (Z_{lep}). The algorithm for identifying such candidates is designed to look for two leptons with an invariant mass in the Z window, i.e. in 60–100 GeV. For final states with more than two leptons, the number of such pairs are counted.

The selections used to define SRs in the 2ℓ OS, 3ℓ and 4ℓ channels is summarised in Table 10.2. A total of 10 SRs (5 in 2ℓ OS, 3 in 3ℓ and 2 in 4ℓ) are defined in each of the VLe and $VLL\mu$ channels. The sum of transverse momentum of the leptons ($H_{T,\text{lep}}$) and missing transverse energy ($E_{\text{T}}^{\text{miss}}$) is expected to be sensitive to the mass of the VLL and is chosen as the discriminating variable in each signal region, to extract the signal strength separately for each mass point.

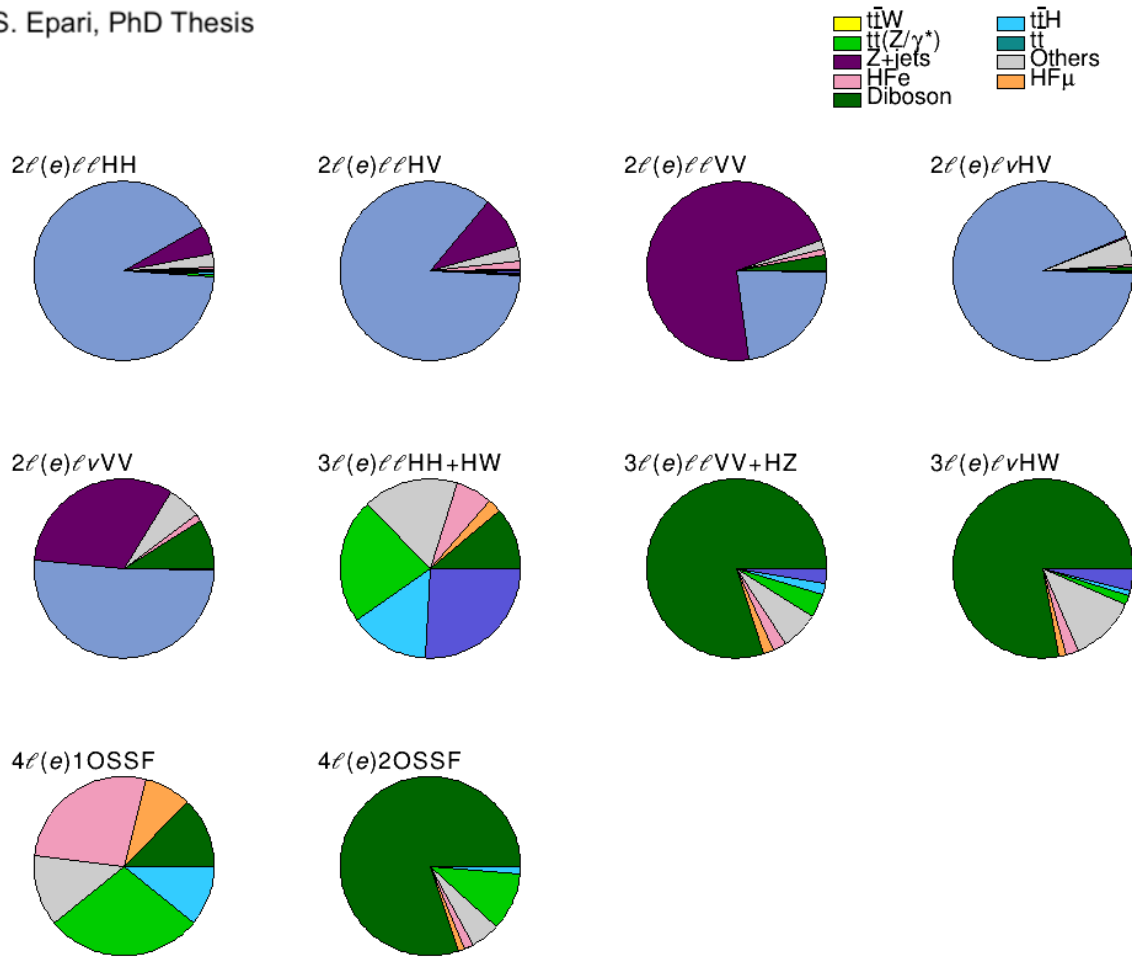
Lepton category	$2\ell\text{OS}$	3ℓ	4ℓ
Lepton flavour	$e: (ee)$ $\mu: (\mu\mu)$	$e: (2e1\mu + 3e)$ $\mu: (2\mu1e + 3\mu)$	$e: (2e2\mu + 3e1\mu + 4e)$ $\mu: (2\mu2e + 3\mu1e + 4\mu)$
Lepton definition	(L^*, L^*)	(L^*, M, M)	(L^*, L^*, L^*, L^*)
Lepton p_T [GeV]	(20, 20)	(10, 20, 20)	(10, 10, 10, 10)
$m_{\ell^+\ell^-}^{\text{OS-SF}}$ [GeV]	> 15	–	–
$ m_{\ell^+\ell^-}^{\text{OS-SF}} - m_Z $ [GeV]	> 10	> 10	< 10 (1OSSF or 2OSSF)
N_{jets}	≥ 2	≥ 1	≥ 0 (1OSSF) ≥ 1 (2OSSF)
Other	$\Delta R(\ell, \ell) > 1$	Total lepton charge = ± 1	Total lepton charge = 0
Region split	$(\ell\ell HH, \ell\ell HV, \ell\ell VV, \ell\nu HW, \ell\nu WZ) \times (e, \mu)$	$(\ell\ell HH + HV, \ell\ell HV + VV, \ell\nu HV) \times (e, \mu)$	$(1\text{OSSF}, 2\text{OSSF}) \times (e, \mu)$
Region naming	$2\ell(e)\ell\ell HH, 2\ell(\mu)\ell\ell HH$ $2\ell(e)\ell\ell HV, 2\ell(\mu)\ell\ell HV$ $2\ell(e)\ell\ell VV, 2\ell(\mu)\ell\ell VV$ $2\ell(e)\ell\nu HW, 2\ell(\mu)\ell\nu HW$ $2\ell(e)\ell\nu WZ, 2\ell(\mu)\ell\nu WZ$	$3\ell(e)\ell\ell HH + HW, 3\ell(\mu)\ell\ell HH + HW$ $3\ell(e)\ell\ell HV + VV, 3\ell(\mu)\ell\ell HV + VV$ $3\ell(e)\ell\nu HV, 3\ell(\mu)\ell\nu HV$	$4\ell(e)1\text{OSSF}, 4\ell(\mu)1\text{OSSF}$ $4\ell(e)2\text{OSSF}, 4\ell(\mu)2\text{OSSF}$

Table 10.2: Event selection summary in the SRs. Light leptons definitions from Table 8.6 are used. Leptons are ordered by p_T in the $2\ell\text{OS}$ and 4ℓ regions. In the 3ℓ regions the lepton with opposite-sign charge is taken first, followed by the two same-sign leptons in p_T order.

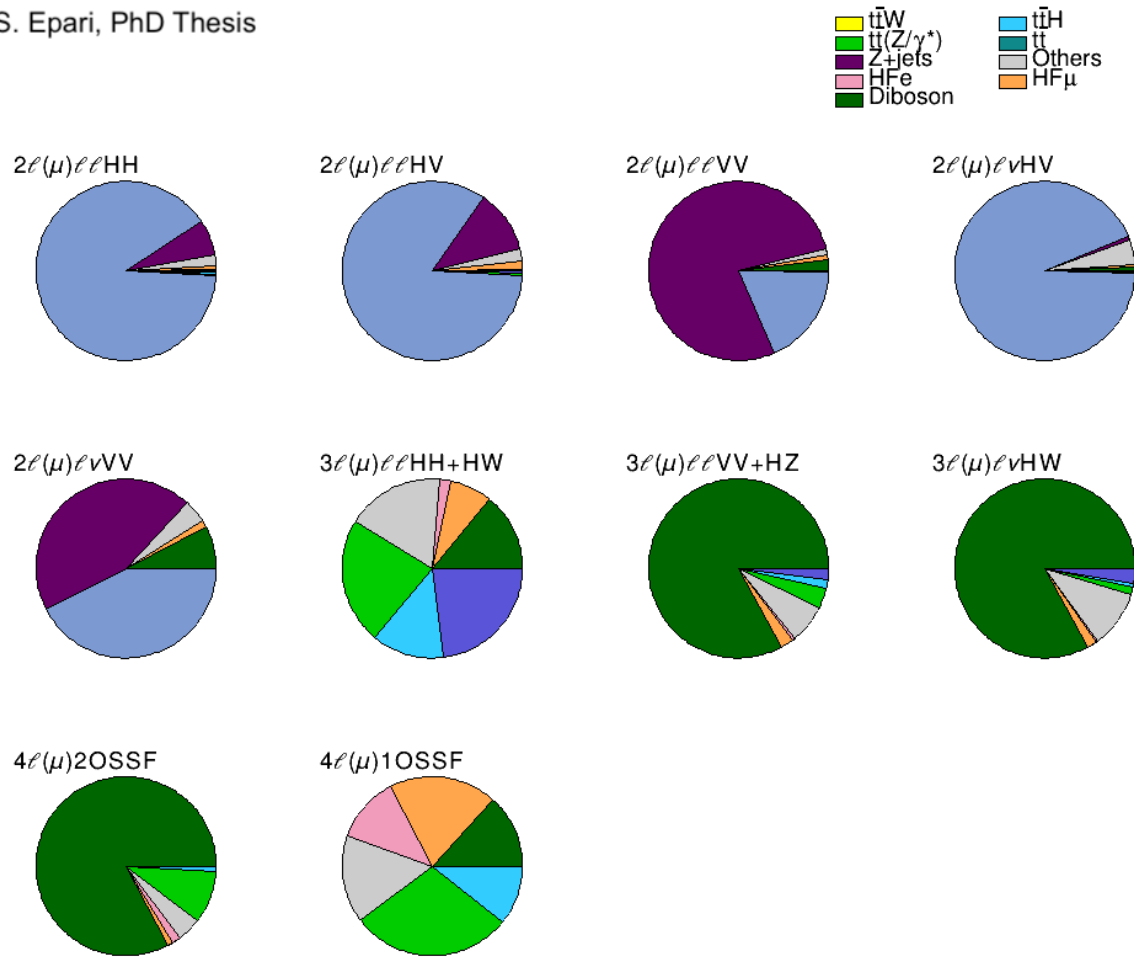
10.3.2 Control regions

Figure 10.8 (10.9) summarises the main SM backgrounds expected in the $\text{VLL}e$ ($\text{VLL}\mu$) SRs. The main prompt backgrounds originate from $t\bar{t}$ and Z +jets in the $2\ell\text{OS}$ and from VV and $t\bar{t}Z$ in the 3ℓ and 4ℓ SRs. Backgrounds from semi-leptonic b -decays are sub-leading in all SRs. Fake leptons from material or internal conversions form a negligible fraction of the total background.

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Figure 10.8: Background composition in the $VLLe$ SRs.

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Figure 10.9: Background composition in the $VLL\mu$ SRs.

The normalisation of major backgrounds common to the SRs is estimated in the likelihood fit to data from dedicated CRs, summarised in Table 10.3. A single 3ℓ CR requiring with at least one Z_{lep} candidate is used to estimate the WZ and $t\bar{t}Z$ background in the 3ℓ SRs. A separate 4ℓ CR requiring exactly two Z_{lep} candidates is defined to model the ZZ background in the 4ℓ SRs. The $t\bar{t}W$ CR is introduced because this is a leading background in the $2\ell\text{SS}$ CRs that aid in estimation of backgrounds with leptons from semi-leptonic b -decays.

Control regions	$t\bar{t}W$	WZ and $t\bar{t}Z$	ZZ	Conversions	HF non-prompt
N_{jets}	≥ 2	≥ 0			≥ 2
$N_{b\text{-jets}}$	≥ 2 $b^{77\%}$	≥ 1 $b^{77\%}$	≥ 0 $b^{77\%}$	0 $b^{77\%}$	1 $b^{77\%}$
Lepton requirement	$2\ell\text{SS}$	3ℓ	$2e2\mu, 4e, 4\mu$	$\mu\mu e^*$	$2\ell\text{SS}$
Lepton definition	(T, T)	(L^*, M, M)	(L^*, L^*, L^*, L^*)	(L^*, M, M)	$(T, M_{\text{ex}}), (T, L^*)$
Lepton p_T [GeV]	$(20, 20)$	$(10, 20, 20)$	$(10, 10, 10, 10)$	$(10, 20, 20)$	$(20, 20)$
$m_{\ell^+\ell^-}^{\text{OS-SF}}$ [GeV]	> 15	–			–
$ m_{\ell^+\ell^-}^{\text{OS-SF}} - m_Z $ [GeV]	–	< 10			–
$ m_{\ell\ell} - m_Z $ [GeV]	–			< 10	–
Region split	–	–	–	internal / material	subleading $e/\mu \times (T, M_{\text{ex}})$
Region naming	$2\ell\text{tt}W$	$3\ell\text{VV}+\text{tt}Z$	$4\ell\text{ZZ}$	$3\ell\text{IntC}$ $3\ell\text{MatC}$	$2\ell\text{tt}(e)_{(T, M_{\text{ex}})}, 2\ell\text{tt}(e)_{(T, L^*)}$ $2\ell\text{tt}(\mu)_{(T, M_{\text{ex}})}, 2\ell\text{tt}(\mu)_{(T, L^*)}$

Table 10.3: Event selection summary in the CRs. Light leptons definitions from Table 8.6 are used. The notation e^* is used to denote material conversion or internal conversion candidates. In the HF non-prompt lepton region naming, “ $2\ell\text{SS}t\bar{t}(e)$ ” (“ $2\ell\text{SS}t\bar{t}(\mu)$ ”) refers to the control region enriched in non-prompt electrons (muons) from semileptonic b -decays originating mostly from $t\bar{t}$.

Theory and data-driven corrections are introduced or estimated for the $t\bar{t}$, Z +jets and WZ (with additional light flavor jets) in inclusive validation regions (VRs), summarised in Table 10.4. These corrections are described in greater detail in this section. Normalisation factors are introduced for these backgrounds in the likelihood fit to data to account for possible normalisation effects introduced while categorising events using classifiers.

Validation / correction regions	$t\bar{t}$	$Z+\text{jets}$	$W^\pm Z$
Lepton flavour	$2\ell\text{OS } e\mu$	$2\ell\text{OS } ee, \mu\mu$	3ℓ
Lepton definition	(L^*, L^*)	(L^*, L^*)	(L^*, T, T)
Lepton p_T [GeV]	$(20, 20)$		$(10, 20, 20)$
$m_{\ell+\ell^-}$ [GeV]	> 15 (OS)	> 15 (OSSF)	–
$ m_{\ell+\ell^-} - m_Z $ [GeV]	> 10 (OS)	< 10 (OSSF)	
N_{jets}	≥ 2		≥ 1
$N_{b-\text{jets}}$	≥ 0 $b^{77\%}$		0 $b^{85\%}$

Table 10.4: Event selection summary in the regions used for deriving data-driven corrections and for validation of the $t\bar{t}$, $Z+\text{jets}$ and WZ background processes. Light leptons definitions from Table 8.6 are used. Leptons are ordered by p_T in the $2\ell\text{OS}$ and 4ℓ regions. In the 3ℓ regions the lepton with opposite-sign charge is taken first, followed by the two same-sign leptons in p_T order.

Diboson background

The known mis-modelling in the jet multiplicity of the WZ MC (with additional light flavor jets) is corrected to data in a similar procedure to that described in Section 9.3.2. The $t\bar{t}Z$ background is suppressed by requiring events with no b -tagged jets at the 85% working point. Instead of a polynomial fit, the MC in each jet multiplicity bin is re-scaled to match data, in a dedicated VR defined in Table 10.4. The magnitude of this re-scaling factor ranges from about 20% at 0 jets and up to 30% at 6 jets. This correction is applied to the VV MC prediction in the entire phase space and assumed to be equally applicable to the MC with additional heavy flavor jets. The effect of this correction on the number of b -jets in the $3\ell VV+t\bar{t}Z$ CR is shown in Figure 10.10. The first bin of this distribution, enriched in WZ with additional light flavor jets, is the bin that shows the maximum improvement upon application of the correction. Up to 25% disagreement remains in the 3 b -jet bin of this distribution, driven by the modelling of the $t\bar{t}Z$ background, to be controlled using a dedicated normalisation factor in the maximum likelihood fit. A systematic uncertainty in the VV correction is derived using a polynomial fit to data which accounts for the effect of any bin-to-bin migration of events, described in Section 10.4.

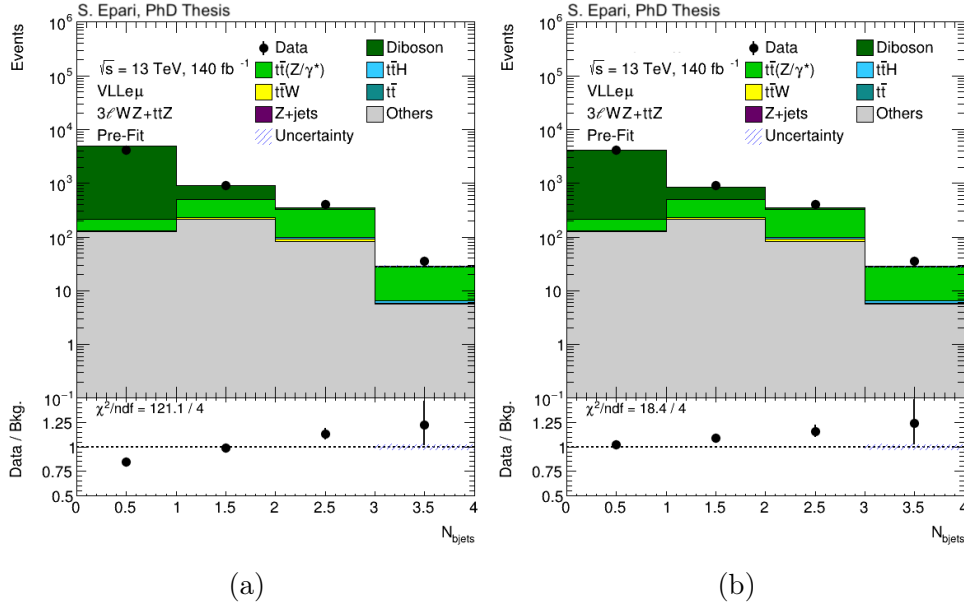


Figure 10.10: Distribution of b -jet multiplicity in the $3\ell VV + ttZ$ control region defined in Table 10.3 (a) before and (b) after the jet multiplicity correction to the diboson MC prediction.

$t\bar{t}$ background

The $t\bar{t}$ background dominates in the $2\ell OS$ SRs, with up to a million events in many regions after categorisation using the deep neural network classifiers. To check and correct the modelling of this background, a $t\bar{t}$ VR was created using $e\mu$ events passing the $2\ell OS$ signal region selection, as described in Table 10.4. The modelling of variables related to the top p_T , jet multiplicity and multiplicity of additional heavy flavor jets is shown in Figure 10.11.

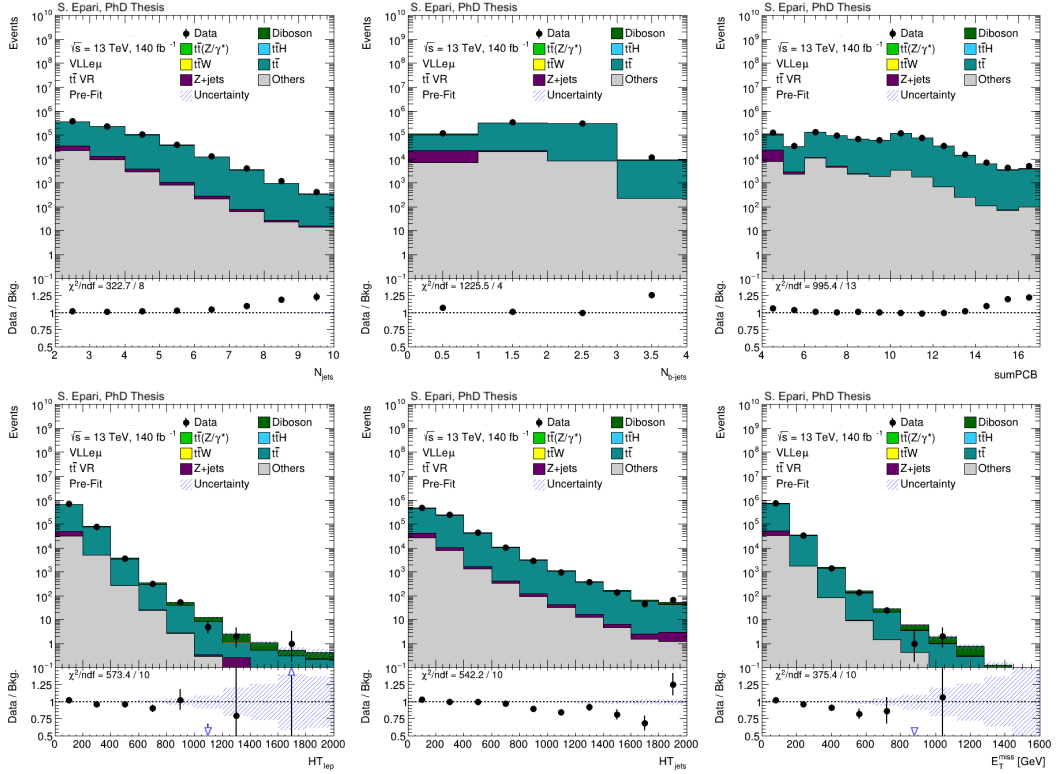


Figure 10.11: Pre-fit agreement in distributions of kinematic variables in the $t\bar{t}$ VR before any corrections are applied.

The modelling of these variables is corrected using a sequence of theory-based and data-driven corrections. Previous studies have shown that the top-quark pair p_T and differential distributions predicted from the latest theoretical predictions at next-to-next-to-leading order in QCD (NNLO-QCD) and next-to-leading order in electroweak (NLO-EW) are significantly softer than the spectrum from the nominal and alternative MC samples considered in this analysis. An iterative recursive re-weighting procedure [142] was used to correct the parton level distributions of top- p_T , anti-top p_T , $m(t\bar{t})$ and $p_T(t\bar{t})$ in each of the MC samples. The corrections improve the modelling of kinematic variables related to the top p_T , in-particular for the sum of the jet p_T in the event (HT_{jets}), sum of total lepton p_T (HT_{lep}) and E_T^{miss} .

Next, a series of iterative data-driven corrections are derived to correct the modelling of the inclusive jet multiplicity and fractions of additional light or heavy flavor jets in the $t\bar{t}$ MC to ensure good modelling in all SRs, which cover different multiplicities and admixtures of jet flavors. These steps are illustrated in Figure 10.12.

First, corrections to the fractions of additional light or heavy flavor jets in the $t\bar{t}$ MC are

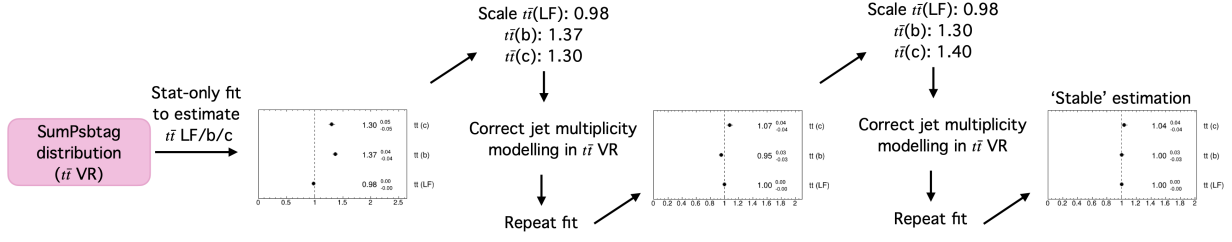


Figure 10.12: Sequential steps for data-driven corrections to the multiplicity of additional light flavor, b - or c - jets and inclusive jet multiplicity in $t\bar{t}$.

estimated by fitting the sumPCB distribution to data with dedicated NFs. These factors are used to correct the $t\bar{t}$ MC. Next, an inclusive correction to the total jet multiplicity of $t\bar{t}$ is derived as a bin-by-bin re-scaling factor. While the jet multiplicity in bulk of the $t\bar{t}$ MC is well-modelled, disagreements of up to 30% have been observed at high jet multiplicities in events with high E_T^{miss} . This mis-modelling has the potential to affect sensitivity to the high E_T^{miss} VLL signal topologies. Thus, an elaborate correction is warranted to ensure good modelling of the MC in all SRs. These bin-to-bin scaling factors for the jet multiplicity distribution are derived in coarse E_T^{miss} bins, namely 0–100 GeV, 100–200 GeV, 200–300 GeV, > 300 GeV, ensuring enough statistics in each bin. After correcting for the number of jets, a fit to the sumPCB is repeated to check that the best-fit values are not affected. These steps are repeated till a *stable* estimation for the fractions of additional light or heavy flavor jets in the $t\bar{t}$ MC. These numbers are determined to be: $t\bar{t} + \text{LF}$: 0.98 (± 0.01); $t\bar{t} + b$: 1.3 (± 0.04) and $t\bar{t} + c$: 1.4 (± 0.05). Kinematic distributions in the $t\bar{t}$ VR, after applying all corrections mentioned above is shown in Figure 10.13. Good agreement is observed across all distributions.

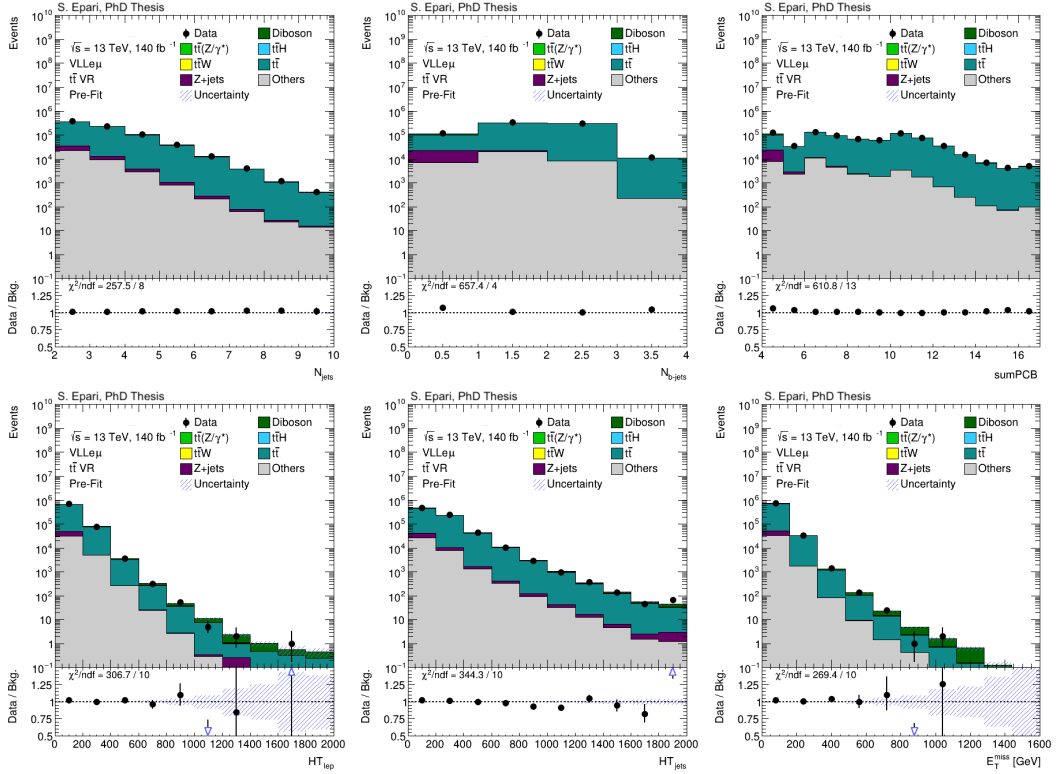


Figure 10.13: Pre-fit agreement in distributions of kinematic variables in the $t\bar{t}$ VR after all $t\bar{t}$ corrections are applied.

Z +jets background

Z +jets is the other dominant background in the 2ℓ OS SRs. To check and correct the modelling of this background, a Z +jets VR was created using events passing the 2ℓ OS signal region selection but with dilepton invariant mass around the Z boson window, described in Table 10.4. Leptons are required to have an angular separation (ΔR_{ll}) greater than unity to suppress boosted Z/γ^* +jets. Kinematic distributions of events in the Z +jets VR is shown in Figure 10.14.

While the jet multiplicity is well-modelled in the bulk of the distribution, disagreements with data of up to 25% are seen at high jet multiplicities. To improve this, a data-driven correction is derived per bin in the distribution of the number of jets. Further, the distribution of ΔR_{ll} shows up to 25% disagreement in the highest bin. To correct this, a bin-by-bin correction is derived to the ΔR_{ll} distribution, as a function of jet multiplicity. Since this is an ad-hoc correction, a systematic uncertainty of the size of the correction is introduced as an additional degree of freedom in the fit, correlated among all regions,

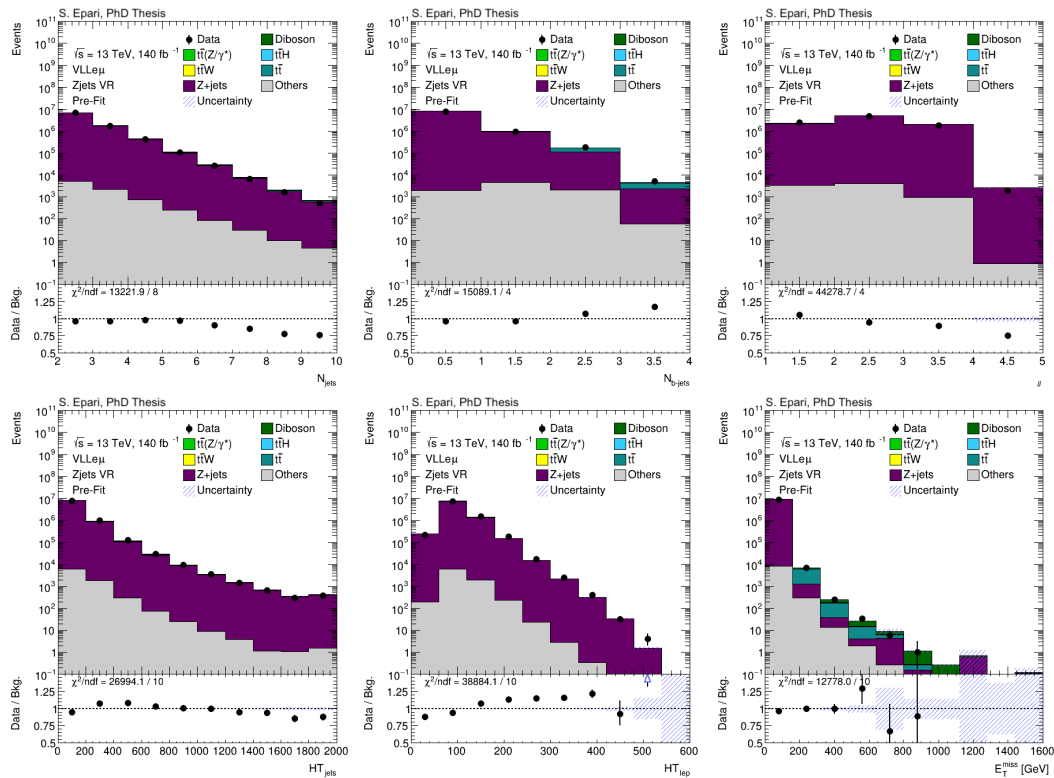


Figure 10.14: Pre-fit agreement in distributions of kinematic variables in the Z +jets VR prior to the application of any corrections. Leptons are required to have an angular separation (ΔR_{ll}) greater than unity to suppress boosted Z/γ^* +jets.

allowing the fit to *undo* the correction if warranted.

Kinematic distributions in the Z +jets VR, after applying all corrections mentioned above is shown in Figure 10.15. Good agreement is observed across all distributions.

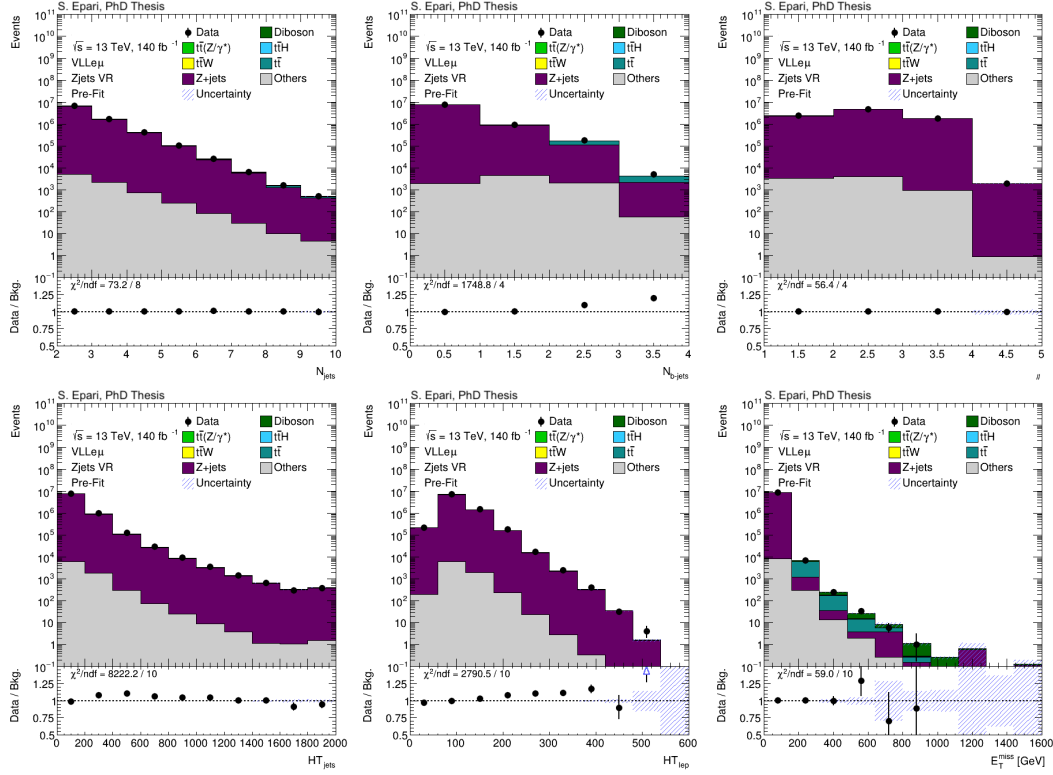


Figure 10.15: Pre-fit agreement in distributions of kinematic variables in the Z +jets VR after all corrections are applied. Leptons are required to have an angular separation (ΔR_{ll}) greater than unity to suppress boosted Z/γ^* +jets.

Fake-lepton estimation

Various sources of fake-leptons in the SRs are classified using an *Isolation and Fakes Forum* (IFF)-based scheme, based on MC truth information. There are eleven truth categories defined in the IFF scheme:

1. Prompt electrons and muons are identified from truth information for the respective lepton. These correspond to IFF class 2. In the case of electrons, converted electrons originating from an FSR photon or bremsstrahlung are also included. Electrons and muons from leptonic τ decays are included in this category.
2. Charge-flip electrons belong to IFF class 3 and are identified if the charge of the first non-parent particle is different from the reconstruction-level charge of the electron. Electrons originating from FSR are excluded from this category.
3. Photon conversions correspond to IFF class 5 and are identified as electrons originating from a photon conversion or an electromagnetic process. Additionally, electrons with a truth type of an isolated/background photon ($= 14/16$) and an origin as a prompt photon conversion or an unhadronized photon also fall into this category. Background electrons from photon conversions with a PDG ID of a photon or an electron are included in this category as well.
4. Electrons from muons belong to IFF class 6 and are identified if the truth type of the electron corresponds to a non-isolated electron or photon and its truth origin is a muon. The contribution of this category is expected to be negligible as an overlap removal between electrons and muons is applied.
5. Tau decays are counted in IFF class 7, and consider non-isolated electrons or muons from hadronic τ decays. τ leptons radiating a photon which subsequently converts into an electron-positron pair also enters this category.
6. b -hadron (IFF class 8) and c -hadron (IFF class 9) decays consists of electrons and muons originating from heavy-flavour decays, and are identified using their truth origin.
7. Light-flavour decays are counted in IFF class 10 and correspond to leptons having the truth type of a hadron ($= 17$). Background electrons with an intermediate photon conversion (e.g. $\pi \rightarrow \gamma\gamma$, $\gamma \rightarrow ee$) and Dalitz decays are also included in this category.

8. Charge-flip muons correspond to IFF class 11 and are identified as muons with a mis-match between their reconstruction level and truth. charge. This effect is expected to be extremely small compared to electrons and is not expected to have a sizable impact on physics analyses.
9. KnownUnknown leptons are those that cannot be classified in to any of the above classes due to missing truth information. These are counted under IFF class 1. Further, leptons failing the selection criteria of the above categories are called *Unknown leptons* and are counted under IFF class 0.

Events with at least two fake leptons in which the individual fake-leptons are identified as having a different source according to the above scheme will be excluded from the individual categories and instead categorised in the *multiple fakes* category. The proportion of events falling into this category is less than 1% in the regions considered in the analysis. Using information from the IFF classes, dedicated CRs are identified for estimating fake-leptons from different non-prompt sources, shown in Table 10.3. The normalisation of these fake-leptons is estimated together with those from dominant prompt backgrounds in a template fit to data:

1. λ^{ExtCO} (λ^{IntCO}), applied to events with at least one electron from material (internal) photon conversion.
2. λ_e^{HF} , applied to events with at least one non-prompt electron from b - or c -hadron decay, dominated by the former. λ_e^{HF} is further de-correlated in to two separate normalisation factors, termed $HF_e^{2l/3l}$ and HF_e^{3l} . $HF_e^{2l/3l}$ targets heavy flavor non-prompt leptons in $2l$ OS and $4l$ SR, where leptons are required to pass just the FCLoose isolation selection. HF_e^{3l} , on the other hand, targets heavy flavor non-prompt leptons in $3l$ regions where additional PLIV cuts are imposed.
3. λ_μ^{HF} , applied to events with at least one non-prompt muon from b - or c -hadron decay, dominated by the former. λ_μ^{HF} is further de-correlated in to two separate normalisation factors, termed $HF_\mu^{2l/3l}$ and HF_μ^{3l} , targeting the $2l$ OS/ $4l$ and $3l$ SRs respectively.

The background contribution from charge-misidentified electrons is negligible in the $2l$ OS and $4l$ channels and estimated through MC simulation. The background contribution from light flavor decays is also negligible in the phase space of the analysis and is estimated from MC simulation. Pre-fit distributions of the template fit regions are shown in Figure 10.16.

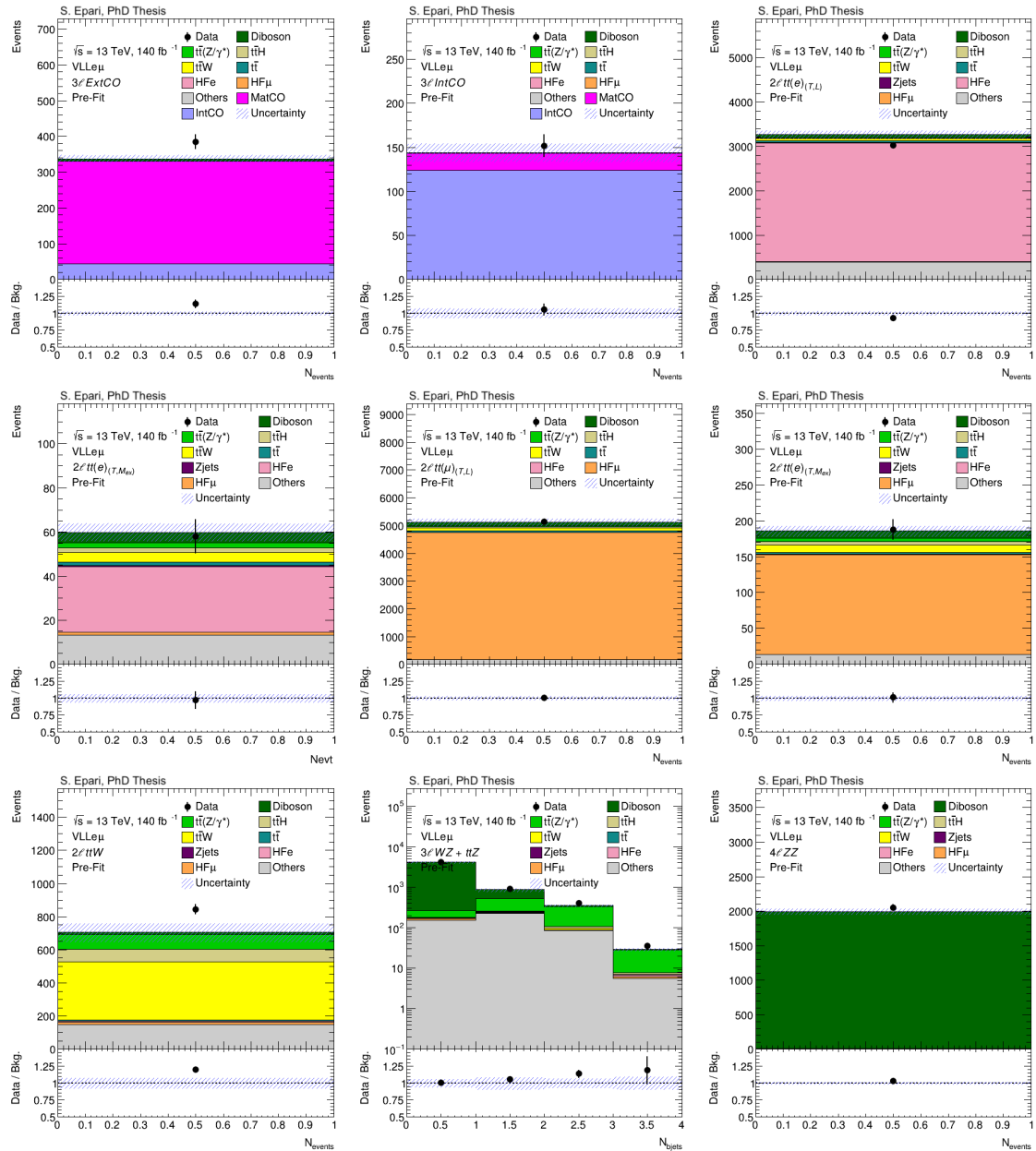


Figure 10.16: Pre-fit agreement in the template fit regions. The blue hashed band includes statistical and systematic uncertainties.

10.3.3 Summary of analysis regions

The summary of regions defined in Tables 10.2, 10.3 and 10.4 is illustrated in Figure 10.17. Orthogonality is maintained between the CRs/VRs and SRs by inverting either the flavor or quality requirements of the leptons or the number of leptonically decaying $Z \rightarrow ll$ candidates. A total of 10 VLL_e SRs, 10 VLL_μ SRs and 9 CRs are defined in the analysis.

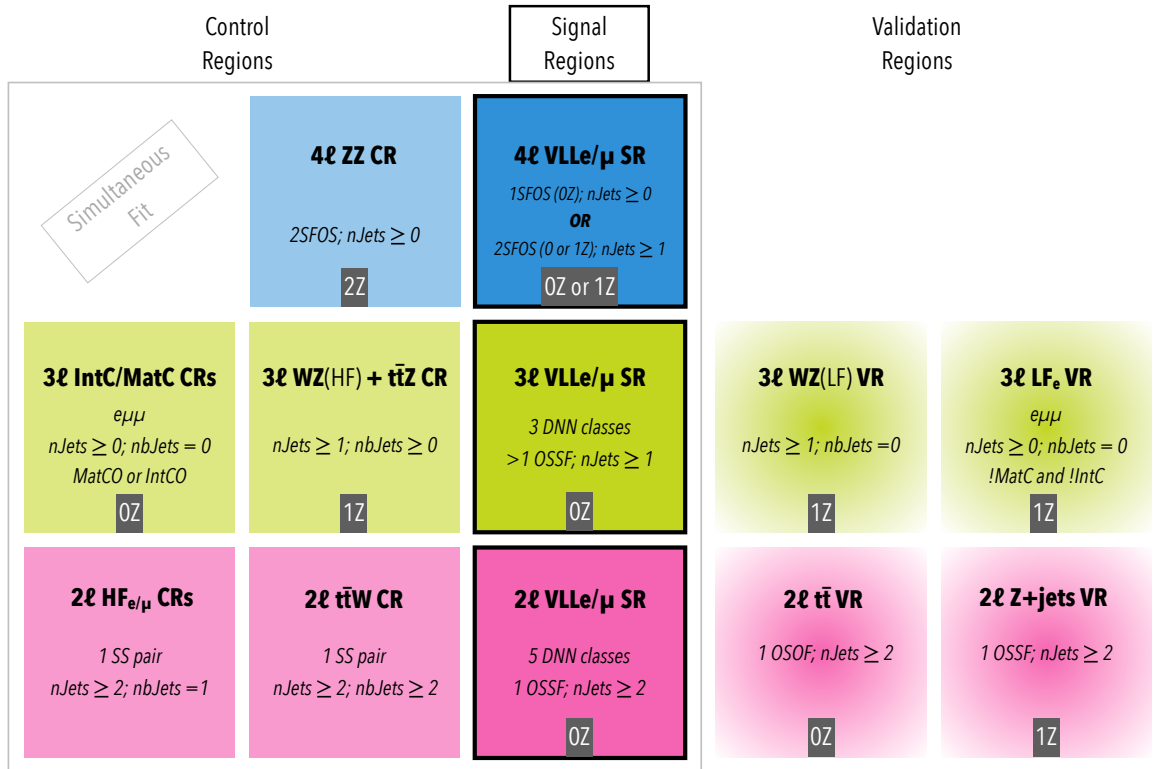


Figure 10.17: Illustrative sketch of the definition of the signal, control and validation regions in the analysis.

10.4 Systematic uncertainties

Systematics considered in the fit in addition to the experimental and theoretical ones defined in Section 8, are described in this section.

Signal modelling uncertainties

The uncertainties in the modelling of the signal samples are evaluated through independent variations of the factorisation and renormalisation scales by a factor two. Additional uncertainties due to PDF effects are estimated taking the difference of the nominal (NNPDF30_nlo_as_0118) to alternative PDF sets (MMHT2014nlo68clas118 and NNPDF30_nlo_as_0119, taken from internal weights “25200” and “266000” respectively).

Modelling systematics for $t\bar{t}$

A systematic model for $t\bar{t}$ is developed following recommendations from the ATLAS Physics Modelling Group, described in this section.

- Parton Shower (PS) and Hadronisation: this uncertainty affects the choice of PS and hadronisation model and is estimated by comparing the nominal POWHEG+PYTHIA8 prediction with POWHEG+HERWIG7.
- Matrix Element(ME)-PS matching: this uncertainty is used to asses the effect of the choice of matching scheme between the ME and PS. It is estimated by comparing the nominal POWHEG+PYTHIA8 prediction with aMCNLO+PYTHIA8.
- Initial State Radiation (ISR) h_{damp} : this uncertainty controls the amount of ISR handled by the ME or PS part of the simulation and is derived by comparing the nominal sample with one that doubles the h_{damp} in POWHEG.
- μ_R and μ_F : these uncertainties are accessed via internal weights in POWHEG+PYTHIA8 and are derived by varying the QCD renormalisation and factorisation scales in the ME calculation by a factor of two up and down relative to the nominal value.
- ISR A14: this uncertainty is accessed by internal weights in POWHEG+PYTHIA8 and corresponds to a variation of the A14 tune (Var3c), which affects the renormalisation scale variations in the ISR parton shower.

- Final State Radiation (FSR): this uncertainty is accessed by internal weights in POWHEG+PYTHIA8 and corresponds to a factor two up and down variations of the renormalisation scale in the FSR parton shower.
- Additional uncertainties due to PDF effects are estimated taking the difference of the nominal (NNPDF30_nlo_as_0118) to alternative PDF sets (MMHT2014nlo68clas118 and NNPDF30_nlo_as_0119, taken from internal weights “25200” and “266000” respectively).

Uncertainties related to the NNLO theory re-weighting are also included as recommended [142], including QCD scale variations on parton level kinematics, effects of additional electroweak corrections, comparison between nominal reweighting and reweighting with inverted order between variables and additional QCD emissions. The effect of these uncertainties is seen to be around 0.1% or less.

Dedicated NNLO theory re-weighting is applied and data-driven corrections derived for the alternative $t\bar{t}$ samples, rescaling them to that of the corrected nominal sample. The scaling factors for the additional light or heavy flavor jets are summarised in Table 10.5 and are seen to vary up to 20% relative to those required by the nominal sample. Corrections to the inclusive jet multiplicity distributions are summarised in Table 10.6 and are <1% for at low jet multiplicities and go up to 16% at 6 jets. No jet multiplicity corrections are derived for the ISR and FSR uncertainties: for these samples, the nominal rescaling is used as a conservative estimate of the uncertainty. All uncertainties are taken to be shape-only, correlated amongst the fit regions. Statistical uncertainty related to re-weighting the jet multiplicity distribution is expected to be very small due to the large statistics of $t\bar{t}$ in the region and is not considered.

Modelling systematics for Z +jets

Systematic uncertainties derived from variations of the re-normalisation and factorisation scale available via internal weights is considered in the search, together with dedicated corrections jet multiplicity and ΔR_{ll} corrections. The magnitude of these corrections is summarised in Tables 10.7 and 10.8 respectively.

Systematic	LF	LF (%)	b	b (%)	c	c (%)
PS & Hadronisation	0.99	-2.94%	1.46	11.54%	2.05	20.59%
ME-PS matching	1.006	-1.37%	1.34	3.08%	1.72	1.18%
ISR hdamp	1.021	-0.1%	1.29	-0.77%	1.68	-1.18%
ISR A14 (up variation)	1.023	0.29%	1.26	-2.77%	1.66	-2.94%
ISR A14 (down variation)	1.021	-0.1%	1.32	1.54%	1.72	1.18%
ISR muR (up variation)	1.137	11.47%	1.44	10.77%	1.89	11.76%
ISR muR (down variation)	0.92	-9.8%	1.16	11.08%	1.52	-10.59%
ISR muF (up variation)	1.04	1.96%	1.31	0.77%	1.72	1.18%
ISR muF (down variation)	0.998	-2.16%	1.27	2.31%	1.65	-2.94%
FSR (up variation)	1.006	-1.37%	1.425	9.62%	1.92	11.76%
FSR (down variation)	1.05	2.94%	1.16	-10.77%	1.42	-16.47%

Table 10.5: The magnitude of the correction for multiplicity of extra jets of light flavor, b- and c-tagged jets for the alternative $t\bar{t}$ samples used in the analysis. The first column for each flavor shows the absolute scaling required. The percentage in the following column is calculated with respect to the scaling applied to the nominal $t\bar{t}$ sample (LF: 0.98; b :1.3; c :1.4).

Systematic	1 jet	2 jets	3 jets	4 jets	5 jets	6 jets	7 jets	8 jets	≥ 9 jets
PS & Hadronisation	-0.58%	+6.76%	-2.04%	-9.26%	-12.36%	-11.73%	-5.31%	+10.21%	+47.91%
ME-PS matching	+0.59%	-2.10%	-4.28%	+2.66%	+11.65%	+16.72%	+19.84%	+22.07%	+45.47%
ISR hdamp	-0.49%	+0.60%	-0.49%	-0.42%	-0.20%	+0.72%	+5.51%	+15.09%	+43.13%

Table 10.6: The magnitude of the correction for each jet multiplicity for the alternative $t\bar{t}$ samples used in the analysis. A x% correction means that the sample needs to be reweighted up by x% with respect to the nominal $t\bar{t}$ sample.

In addition, the following set of systematic uncertainties are assigned to the Z +jets MC:

- Uncertainties based on the difference between re-weighted and un-reweighted ΔR_{ll} distributions (binned in ΔR_{ll}). The size of this uncertainty is equal to the size of the correction. It is correlated amongst the regions, allowing the fit an additional degree of freedom to *undo* the applied correction.
- Uncertainty related to the upper cut-off of perturbative calculations for parton shower evolution is known as the re-summation scale (QSF). This uncertainty is evaluated at truth level by varying the nominal value of 2 GeV by a factor of 4 up and 1/4 down, denoted as QSF4 and QSF025, in a phase space close to that used at reconstruction level in the SRs where Z +jets is a dominant background. Finally, the jet multiplicity distribution of the uncertainty is reweighted to match that of the nominal and

Systematic	2 jets	3 jets	4 jets	5 jets	6 jets	7 jets	8 jets	
varR (up variation)	11.67%	19.07%	28.362%	34.525%	29.622%	22.21%	10.422%	8.587%
varR (down variation)	-13.39%	-19.60%	-24.63%	-30.24%	-38.83%	-45.13%	-51.91%	-52.52%
varF (up variation)	0.729%	2.477%	5.136%	5.124%	-2.34%	-10.12%	-20.51%	-22.31%
varF (down variation)	0.093%	-3.10%	-4.57%	-7.96%	-16.79%	-24.61%	-33.62%	-36.39%

Table 10.7: The magnitude of the correction for each jet multiplicity for the alternative Z +jets samples used in the analysis. A x% correction means that the sample needs to be reweighted up by x% with respect to the nominal sample.

Systematic	N_{jets}	$\Delta R_{ll}:[1,2)$	$\Delta R_{ll}:[2,3)$	$\Delta R_{ll}:[3,4)$	$\Delta R_{ll}:\geq 4$
varR (up variation)	2	14.38%	-1.21%	-9.51%	-29.33%
	3	7.59%	-1.42%	-9.32%	-40.89%
	4	4.18%	-1.21%	-7.667%	-
	≥ 5	4.18%	-1.21%	-7.67%	-
varR (down variation)	2	9.61%	-2.01%	-4.19%	-17.49%
	3	4.05%	-1.83%	-2.30%	-15.34%
	4	1.55%	-1.37%	0.09%	-
	≥ 5	1.55%	-1.37%	0.08%	-
varF (up variation)	2	10.79%	-1.34%	-6.66%	-24.42%
	3	5.25%	-1.35%	-5.81%	-31.71%
	4	2.56%	-1.04%	-4.03%	-
	≥ 5	2.56%	-1.04%	-4.03%	-
varF (down variation)	2	12.44%	-2.19%	-5.97%	-16.25%
	3	5.87%	-2.14%	-4.58%	-22.74%
	4	2.61%	-1.77%	-1.64%	-
	≥ 5	0.65%	-0.83%	0.51%	-

Table 10.8: The magnitude of the ΔR_{ll} correction for each jet multiplicity for the alternative Z +jets samples used in the analysis. A x% correction means that the sample needs to be reweighted up by x% with respect to the nominal Z +jets sample.

parameterized as a function of $H_{T,\text{lep}} + E_T^{\text{miss}}$

- Uncertainty related to the choice of the scale for calculating the overlap between jets from the matrix element and the parton shower, called the CKKW merging scale, is derived similarly. The nominal value of 20 GeV is varied down to 15 GeV (CKKW15) and up to 30 GeV (CKKW30) and differences with respect to the nominal distribution are evaluated at truth level. Finally, the jet multiplicity distribution of the uncertainty is reweighted to match that of the nominal and parameterized as a function of $H_{T,\text{lep}} + E_T^{\text{miss}}$. These effect of the QSF and CKKW uncertainties evaluated as a function of the fitting variable are summarised in Table 10.9.
- A 30% uncertainty is assigned to the Z +jets background in the $\ell\ell\text{HH}$, $\ell\ell\text{HV}$ and $\ell\nu\text{HW}$ SRs.

The statistical uncertainty related to re-weighting the jet multiplicity distribution is expected to be very small due to the large statistics of Z +jets in the region, and is not considered.

Re-summation and merging scale systematic uncertainties						
Variation	$H_{T,\text{lep}} + E_T^{\text{miss}}$ [GeV]					
	0-200	200-400	400-600	600-800	800-1000	1000-2000
CKKW15 [%]	0.13	0.10	2.54	9.60	8.94	44.76
CKKW30 [%]	0.35	2.55	8.35	6.39	28.40	0.52
QSF025 [%]	0.17	0.87	3.00	17.95	5.29	30.50
QSF4 [%]	0.42	0.23	0.21	4.16	4.22	40.32

Table 10.9: Theoretical uncertainties (shown in %) on the Z +jets yields calculated using dedicated variation samples related to the choice of re-summation and merging scales (QSF & CKKW).

Diboson reweighting uncertainty

A systematic uncertainty in the bin-by-bin re-weighting of the jet multiplicity in the VV MC is calculated by fitting the data to MC ratio to a polynomial, to account for correlations between the different jet multiplicity bins:

$$f(x) = a + \frac{b}{x^c} \quad (10.1)$$

This fit is performed starting at one jet because the polynomial has a pole at zero jets. Further, the large statistics in the 0th bin ensures a low uncertainty in this bin and thus, this uncertainty is not considered. The fit parameters are determined to be $a = -0.604$, $b = -0.469$, $c = 0.265$.

Systematic variations around the nominal values are determined by adjusting the eigenfunction parameterizations in Equation 10.1. This accounts for correlations between the fit parameters. Figure 10.18 shows the polynomial fit to the data to MC ratio (red), a 1σ variation of the largest eigen function about the nominal (brown) and the 3σ effect of the same (green). The 3σ variation covers fluctuations in the nominal data to MC ratio at high jet multiplicity, and is taken as the final uncertainty in this fit. This shape effect of this uncertainty is applied to the VV sample, correlated amongst all the regions.

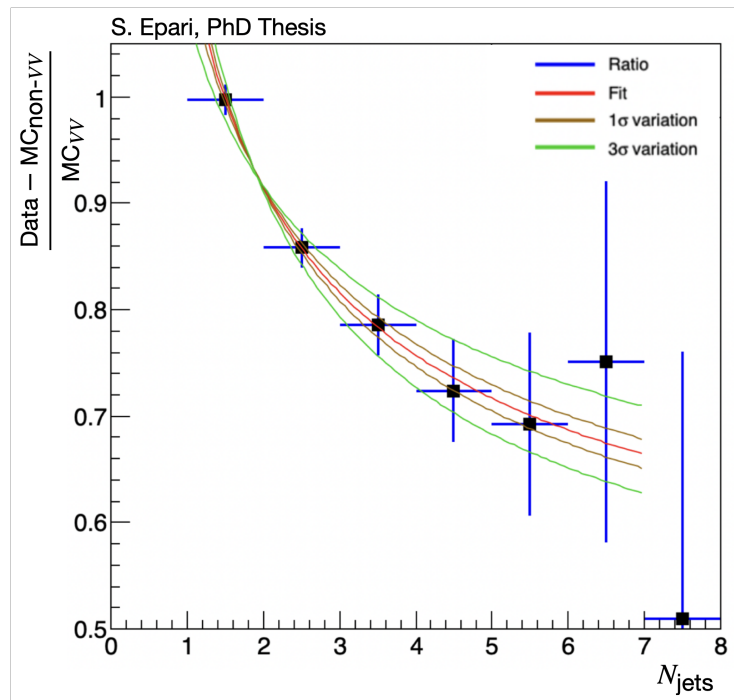


Figure 10.18: Data to MC ratio in the jet multiplicity bins of the $W^\pm Z$ VR, fitted with a polynomial (red). The 1σ variation of the largest eigenfunction is shown in brown, while the corresponding 3σ variation is shown in green. The 3σ variation is chosen as the systematic uncertainty because it covers the variations at high jet multiplicity.

Non-prompt lepton modelling uncertainties

Backgrounds related to charge mis-identified electrons are below 1% in the phase space of this analysis and estimated through MC simulation. These backgrounds are assigned a flat 20% uncertainty in their measurement. Further, backgrounds from fake leptons from light-flavor hadrons are also sub-leading in the search and assigned a 30% prior uncertainty.

Summary of systematic uncertainties

A summary of all systematic uncertainties included in the analysis is given in Table 10.10. A total of 120 systematic uncertainties, including experimental and theoretical uncertainties are considered in the analysis.

Systematic uncertainty	Components	Systematic uncertainty	Components
Luminosity	1	VLL modelling	
Pileup re-weighting	1	QCD scale (μ_F, μ_R)	1
Physics Objects		Parton shower	1
Electron	5	α_s +PDFs	1
Muon	10	$t\bar{t}H$ modelling	
Jet energy scale and resolution	31	Cross section (N)	1
Jet vertex fraction	1	Parton shower and hadronisation model	1
Jet flavour tagging	15	$t\bar{t}W$ modelling	
E_T^{miss}	3	Generator	1
Total (Experimental)	67	QCD scale	1
Data-driven background estimates		$t\bar{t}Z$ modelling	
$t\bar{t}$ modelling	14	Cross section (N)	1
Z +jets modelling	7	Matrix-element MC generator	1
VV modelling	1	$t\bar{t}$ modelling	
Total (Data-driven reducible background)	22	Radiation	2
		Parton shower and hadronisation model	1
		Generator	1
		WZ modelling	
		Cross section (N)	1
		Heavy flavour composition (N)	1
		Other background modelling	
		Cross section (N)	16
		Total (Signal and background modelling)	31
		Total (Overall)	120

Table 10.10: Sources of systematic uncertainty considered in the analysis. N means that the uncertainty is taken as normalisation-only for all processes and channels affected. Some of the systematic uncertainties are split into several components, as indicated by the number in the rightmost column.

10.5 Results

Separate maximum likelihood fits are performed for the VLL e and VLL μ models, introducing either the 10 VLL e SRs or 10 VLL μ SRs described in Table 10.2, fitted simultaneously with the 9 CRs (Table 10.3) to data. Background-only (*B-only*) fits measure normalisation for $t\bar{t}W$, $t\bar{t}Z$, WZ (separately for light flavor and heavy flavor), ZZ , conversions (internal and material) and non-prompt leptons (HFe, HF μ), assuming there is no BSM processes in the regions. For the 2 ℓ OS regions populated with unique ad-mixtures of light and heavy flavor jets from $t\bar{t}$ with varying amounts of E_T^{miss} , namely $\ell\ell\text{HH}$, $\ell\ell\text{HV}$ and $\ell\nu\text{HW}$, are assigned dedicated normalisation factors. Similarly, the Z +jets background in 2 ℓ OS regions where this is a dominant background, namely $\ell\nu\text{VV}$ and $\ell\ell\text{VV}$, are assigned two separate NFs in the fit. These target the modelling of Z +jets events with high E_T^{miss} and low E_T^{miss} respectively. In these regions, $t\bar{t}$ is a sub-leading background and is measured with a single NF.

Maximum likelihood fits performed by free-floating the VLL signal strength in addition to the background NFs of the *B-only* fit are termed signal-plus-background fits (*S+B* fits). These fits are performed for each VLL e or VLL μ model considering all mass points, to test the presence of a BSM signal. The results from the *B-only* and *S+B* fits for the VLL e (VLL μ) models are discussed in Section 10.5.1 (Section 10.5.2).

10.5.1 Template fit to data (VLL e models)

Figure 10.19 shows the fitted NFs for the *B-only* fit to CRs and VLL e SRs, *S+B* fit considering a VLL e signal of 600 GeV from the doublet model and *S+B* fit considering a VLL e signal of 200 GeV from the singlet model.

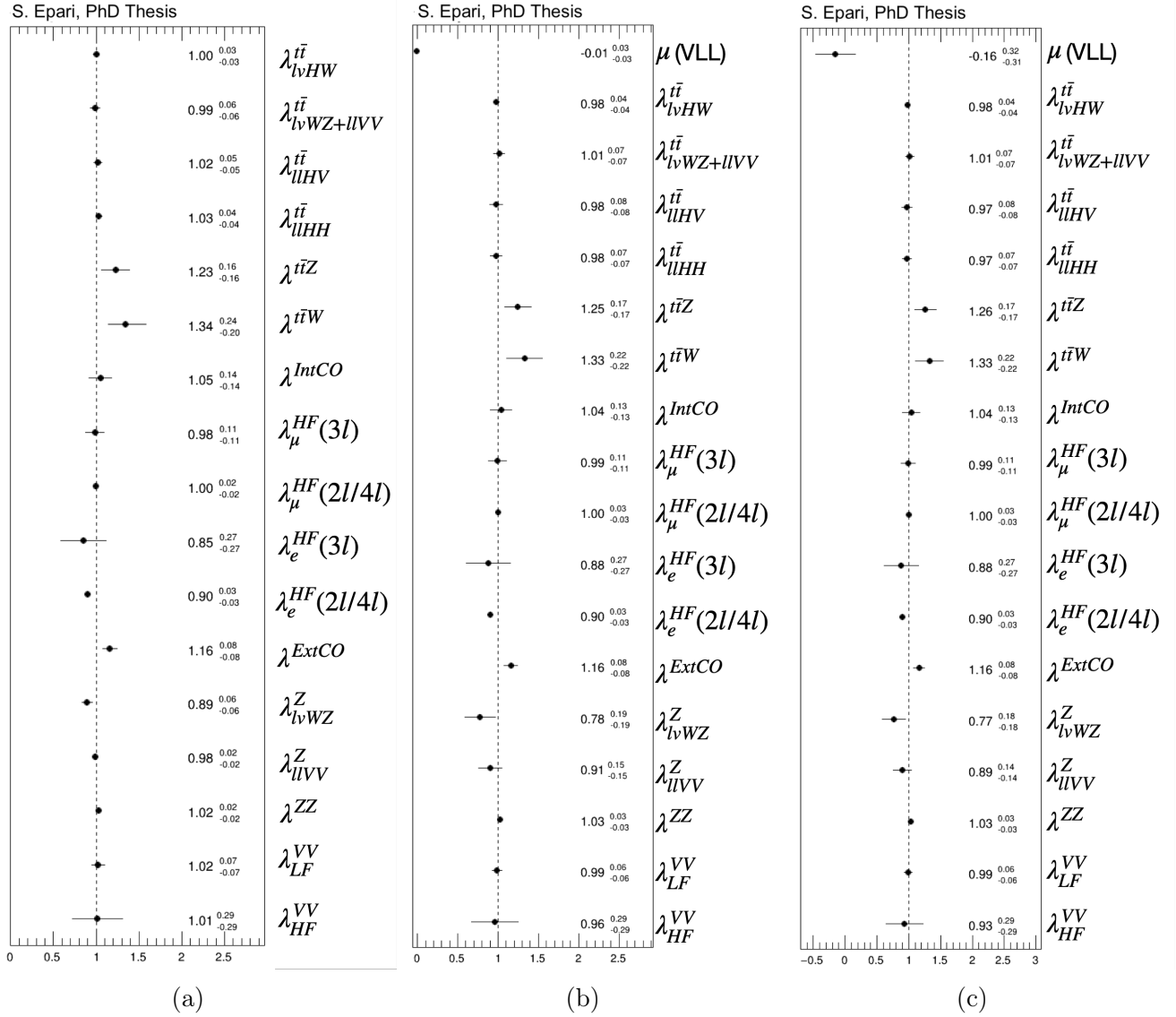


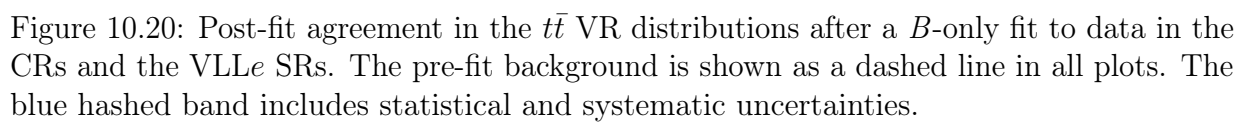
Figure 10.19: Fitted normalisation factors from the (a) B -only fit to CRs and VLL μ SRs, (b) $S+B$ fit considering a VLL e signal of 600 GeV from the doublet model and, (c) $S+B$ fit considering a VLL e signal of 200 GeV from the singlet model.

In all fits, the $t\bar{t}$ and Z +jets NFs show good compatibility with unity, indicating that the inclusive calibrations made to the respective backgrounds are preserved after categorisation by the DNN classifier. A powerful validation of the $t\bar{t}$ background is done by checking the post-fit distributions of the $t\bar{t}$ VR selected by the 2 ℓ OS DNN classifier, in $H_{T,\text{lep}} + E_T^{\text{miss}}$, shown in Figure 10.20 for the B -only fit.

The normalisation of $t\bar{t}Z$ and $t\bar{t}W$ backgrounds are measured higher than unity, compatible with the measurement from other analyses in similar phase space. All other NFs are measured compatible with unity. The fitted signal strength for VLLe signals across all mass hypotheses from both the doublet and singlet models is measured to be compatible with zero. This means that the analyses fails to reject the B -only hypothesis for this set of couplings and masses. The nuisance parameters from the B -only fit, together with the measured correlations between various NFs and NPs is shown in Figure 10.21.

Correlations between the NFs measuring the $t\bar{t}$ background in the 2 ℓ OS regions is introduced by the PDF (var 252) uncertainty. This uncertainty is of the order of 3-4%. The uncertainties in the re-summation and merging scales of Z +jets (CKKW and QSF), estimated at truth level, introduce further correlations between the Z +jets NFs. Systematics on E_T^{miss} affect the normalisation of the ZZ process. The behaviour of NPs from the three fits is consistent. The local significance from similar $S+B$ fits performed for the other mass points from both models is found to be lower than unity. Figure 10.22 shows the post-fit SR distributions of the VLLe SRs, showing the 600 GeV signal from the doublet model. No significant excess is seen in any of the SR bins, with large statistical errors in the extreme ends of the distributions expected to be populated by signal events from either model.

Table 10.11 shows the summary of yields in the 10 VLLe SRs after the B -only fit. Figures 10.23a and 10.23b and show the summary of the regions after the profile likelihood fit, together with the pre-fit background expectation.



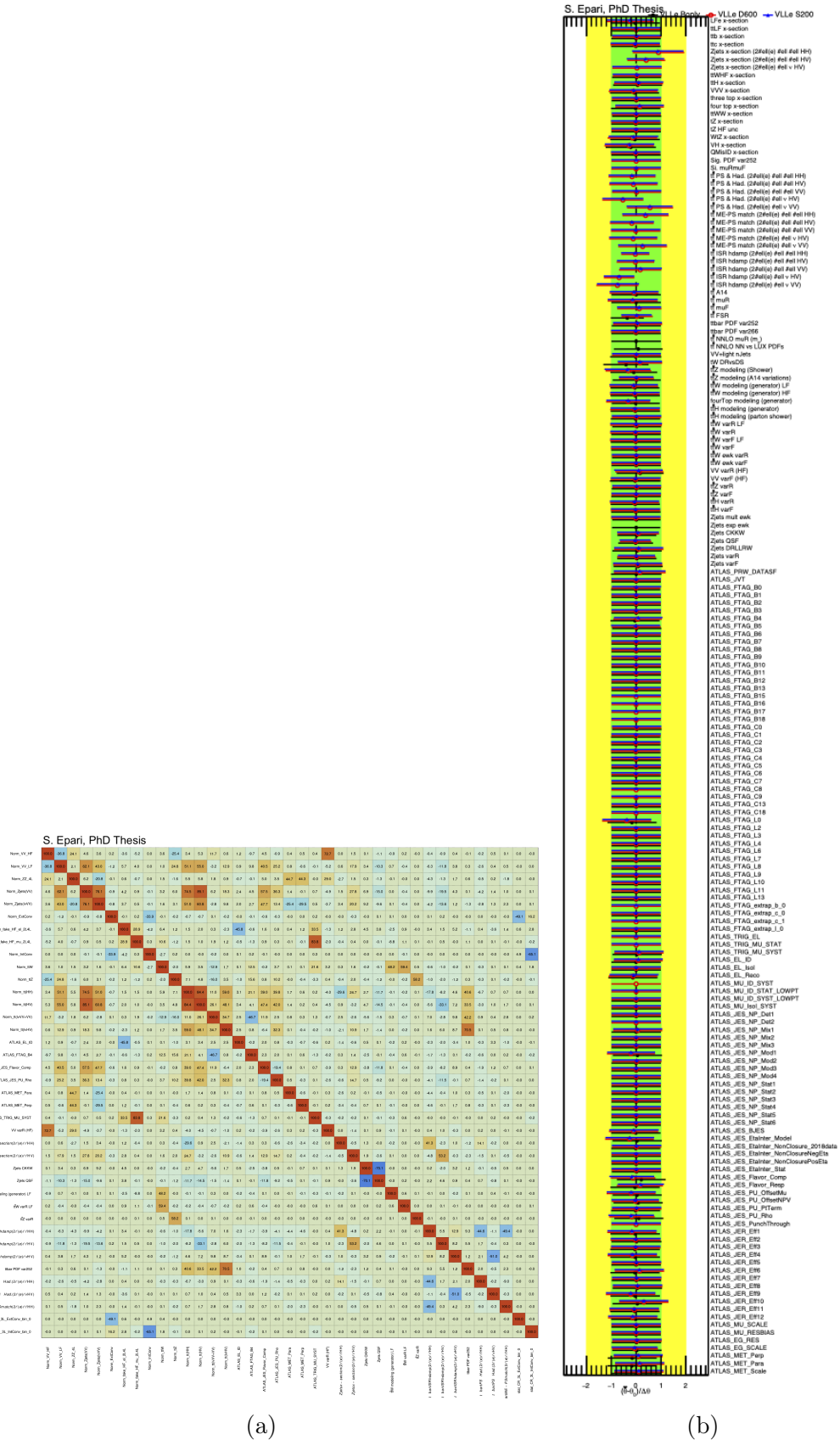


Figure 10.21: (a) The correlation matrix corresponding to a fit under the B -only hypothesis to the CRs and VLLe SRs. (b) Overlay of pulls and constraints on the nuisance parameters from the B -only fit, $S+B$ fit considering a VLLe signal of 600 GeV from the doublet model and $S+B$ fit considering a VLLe signal of 200 GeV from the singlet model.

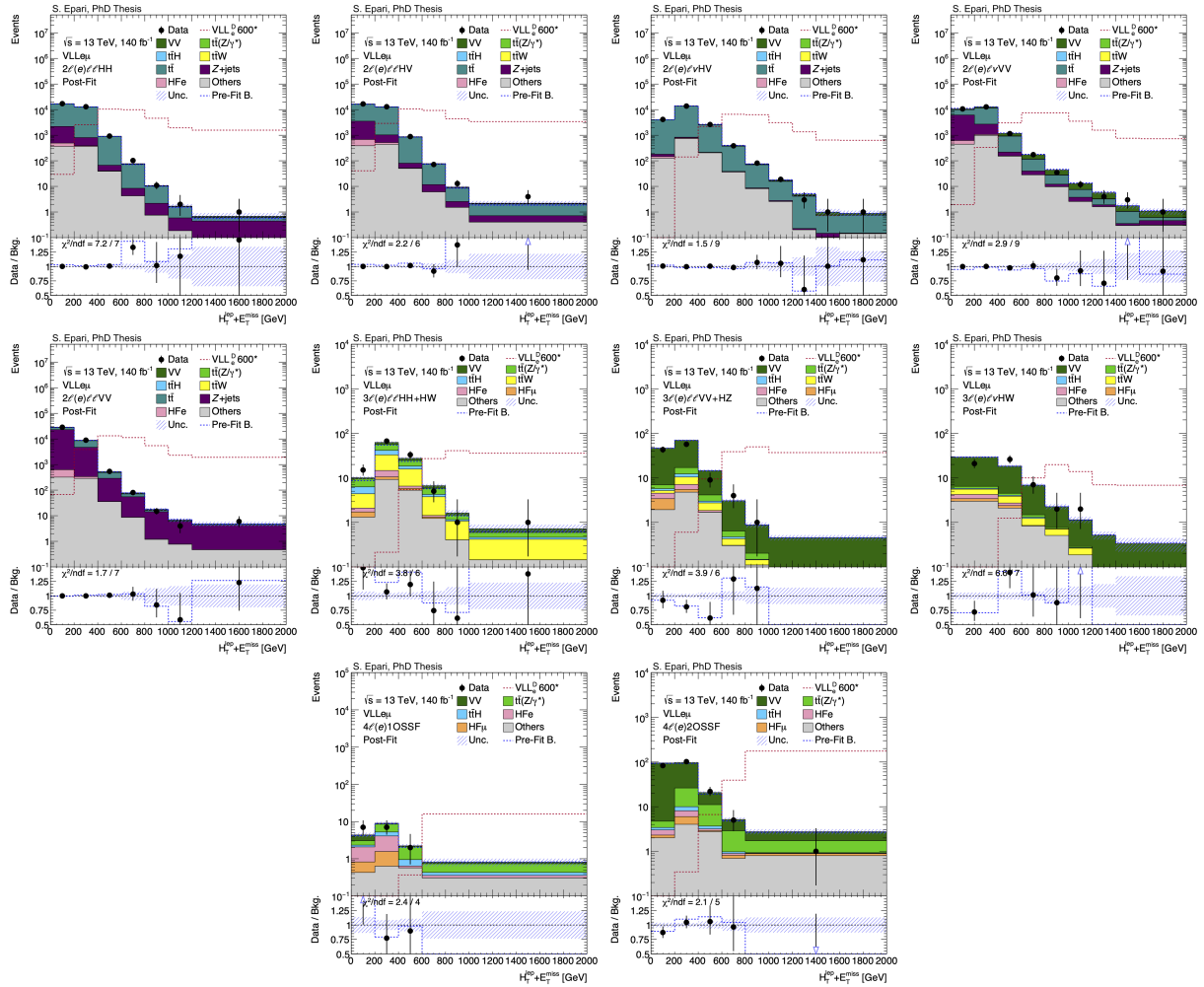


Figure 10.22: Post-fit agreement in the VLLe SR distributions used in a $S+B$ fit to data in the CRs and the VLLe SRs, considering a VLLe signal of mass 600 GeV from the doublet model. The signal is shown as a red dashed line, normalised to the total background yield. The pre-fit background is shown as a blue dashed line in all plots. The blue hashed band includes statistical and systematic uncertainties.

	$2\ell(e)\ell\ell HH$	$2\ell(e)\ell\ell HV$	$2\ell(e)\ell\ell VV$	$2\ell(e)\ell\nu HW$	$2\ell(e)\ell\nu VV$
VV	53.5 ± 8.4	98 ± 18	1124 ± 72	148 ± 11	2336 ± 54
$t\bar{t}Z$	165 ± 93	182 ± 92	54 ± 26	59 ± 42	30 ± 21
$t\bar{t}H$	106 ± 15	56.5 ± 8.4	12.41 ± 2.07	14.9 ± 1.9	5.49 ± 0.85
$t\bar{t}W$	119 ± 16	140 ± 17	39.6 ± 6.3	57.5 ± 5.9	29.8 ± 4.3
$t\bar{t}$	27629 ± 678	25527 ± 724	8971 ± 510	19458 ± 344	13356 ± 377
Z +jets	2158 ± 639	3410 ± 722	27070 ± 558	101 ± 34	7259 ± 355
HFe	156.6 ± 6.0	377 ± 14	356 ± 14	77.7 ± 3.0	269 ± 10
HF μ	—	—	—	—	—
Others	770 ± 167	885 ± 168	654 ± 69	1105 ± 321	1618 ± 177
Total	31157 ± 179	30674 ± 187	38277 ± 210	21022 ± 146	24901 ± 159
Data	31162	30677	38279	21022	24890

	$3\ell(e)\ell\ell HH+HW$	$3\ell(e)\ell\ell VV+HZ$	$3\ell(e)\ell\nu HW$	$4\ell(e)1OSSF$	$4\ell(e)2OSSF$
VV	10.65 ± 1.06	106.8 ± 3.3	45.2 ± 2.5	$2.1-.19$	174.8 ± 6.9
$t\bar{t}Z$	26.8 ± 3.2	7.4 ± 1.5	1.28 ± 0.19	5.47 ± 0.60	27.7 ± 2.8
$t\bar{t}H$	13.8 ± 1.9	$2.7-.49$	0.578 ± 0.087	1.75 ± 0.24	2.95 ± 0.42
$t\bar{t}W$	32.9 ± 3.1	4.99 ± 0.71	$3.1-.37$	—	—
$t\bar{t}$	—	—	—	—	—
Z +jets	—	—	—	—	—
HFe	5.4 ± 1.7	2.871 ± 0.902	1.18 ± 0.37	3.89 ± 0.29	3.11 ± 0.13
HF μ	2.33 ± 0.27	2.25 ± 0.26	0.727 ± 0.084	$1.33-.096$	2.641 ± 0.089
Others	17.6 ± 4.9	8.9 ± 1.9	6.7 ± 1.4	1.94 ± 0.35	10.3 ± 2.3
Total	109.2 ± 5.3	135.4 ± 4.2	58.46 ± 3.05	16.42 ± 1.09	221.2 ± 7.3
Data	122	114	58	16	213

Table 10.11: Summary of observed and predicted yields in the 10 VLLe SRs. The background prediction is shown after the combined likelihood fit to data under the B -only hypothesis across all CR and SR categories. The uncertainties correspond to the combined statistical and systematic uncertainties in the predicted yields. Dashes refer to components that are negligible or not applicable.

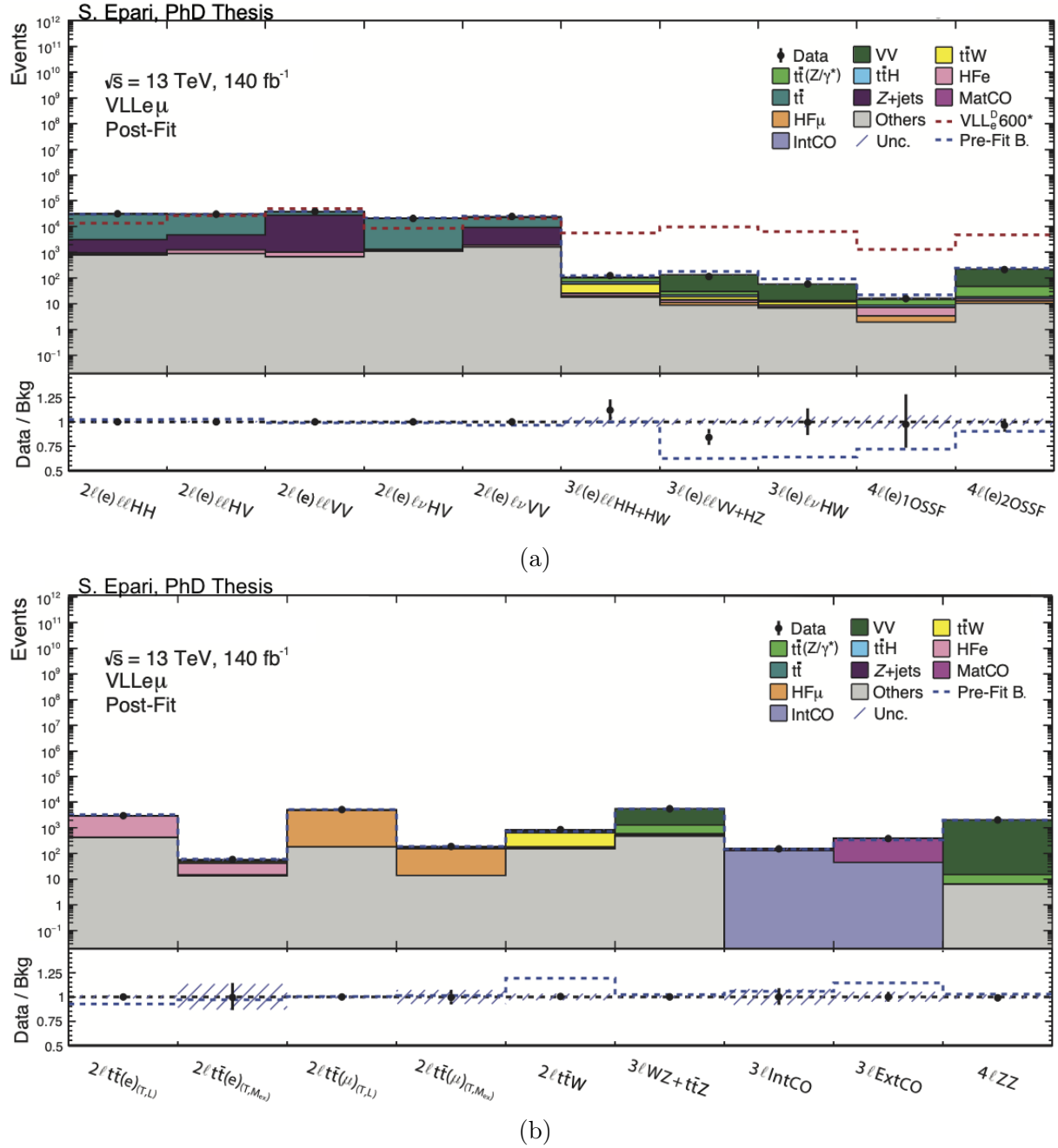


Figure 10.23: Comparison between data and the background prediction for the event yields in the (a) 10 VLL e SRs and the (b) 9 CRs. The expected signal from a VLL e of mass 600 GeV from the doublet model (normalised to the total background) as well as the background contributions are shown after the likelihood fit to data under the $S+B$ hypothesis. The total background prediction before the likelihood fit to data is shown as a dashed blue histogram in the upper panel. The blue hatched band includes both statistical and systematic uncertainties.

10.5.2 Template fit to data (VLL μ models)

Figure 10.24 shows the fitted NFs for the B -only fit to CRs and VLL μ SRs, $S+B$ fit considering a VLL μ signal of 600 GeV from the doublet model and $S+B$ fit considering a VLL μ signal of 200 GeV from the singlet model.

In all fits, the $t\bar{t}$ and Z +jets NFs show good compatibility with unity, indicating that the inclusive calibrations made to the respective backgrounds are preserved after categorisation by the DNN classifier. A powerful validation of the $t\bar{t}$ background is done by checking the post-fit distributions of the $t\bar{t}$ VR selected by the 2ℓ OS DNN classifier, in $H_{T,\text{lep}} + E_T^{\text{miss}}$, shown in Figure 10.25 for the B -only fit.

The normalisation of $t\bar{t}Z$ and $t\bar{t}W$ backgrounds are measured higher than unity, compatible with the measurement from other analyses in similar phase space. All other NFs are measured compatible with unity. Compared to the VLL e fit, the normalisation of VV (HF) is measured to be slightly different, but compatible with unity. The fitted signal strength for VLL μ signals across all mass hypotheses from both the doublet and singlet models is measured to be compatible with zero. This means that the analyses fails to reject the B -only hypothesis for this set of couplings and masses. The nuisance parameters from the B -only fit, together with the measured correlations between various NFs and NPs is shown in Figure 10.26. Correlations between the NFs measuring the $t\bar{t}$ background in the 2ℓ OS regions is introduced by the PDF (var 252) uncertainty as in the VLL e fits. This uncertainty is of the order of 3-4%. Additional correlations between these parameters, unique to this fit, arise from the $t\bar{t}$ FSR uncertainty. Further, an anti-correlation of about 50% is seen between the Z +jets cross-section in the $\ell\ell$ HH SR and the $t\bar{t}$ ME-PS matching systematic. A possible source of this anti-correlation comes from the large statistical uncertainty in the last bin of this region, populated by both $t\bar{t}$ and Z +jets. The uncertainties in the re-summation and merging scales of Z +jets (CKKW and QSF), estimated at truth level, introduce further correlations between the Z +jets NFs. Systematics on E_T^{miss} affect the normalisation of the ZZ process. The behaviour of NPs from the three fits is consistent. The local significance from similar $S+B$ fits performed for the other mass points from both models is found to be lower than unity. Figure 10.27 show the post-fit SR distributions of the VLL μ SRs, showing the 600 GeV signal from the doublet model. No significant excess is seen in any of the SR bins, with large statistical errors in the extreme ends of the distributions expected to be populated by signal events from either model.

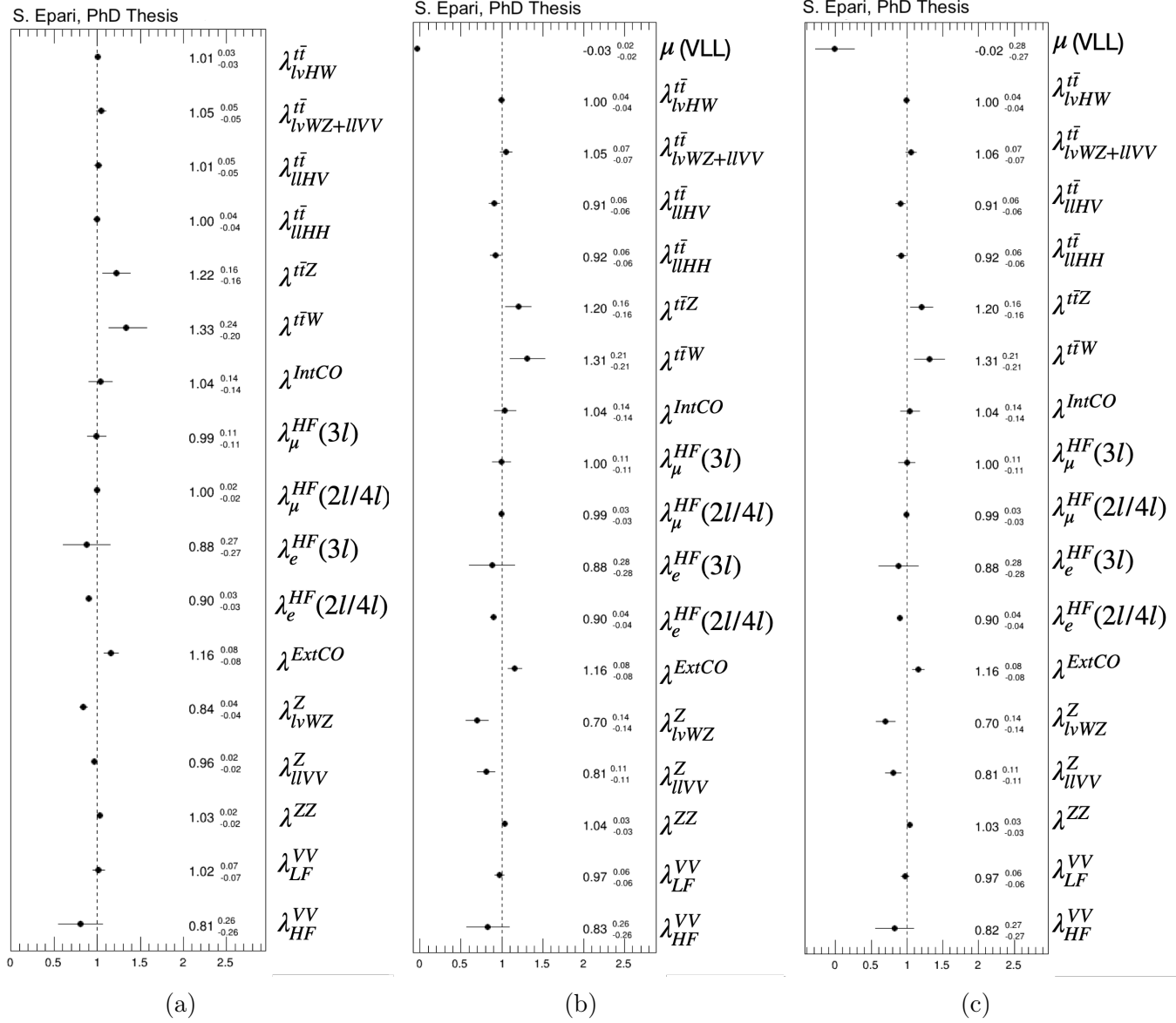


Figure 10.24: Fitted normalisation factors from the (a) B -only fit to CRs and VLL μ SRs, (b) $S+B$ fit considering a VLL μ signal of 600 GeV from the doublet model and, (c) $S+B$ fit considering a VLL μ signal of 200 GeV from the singlet model.

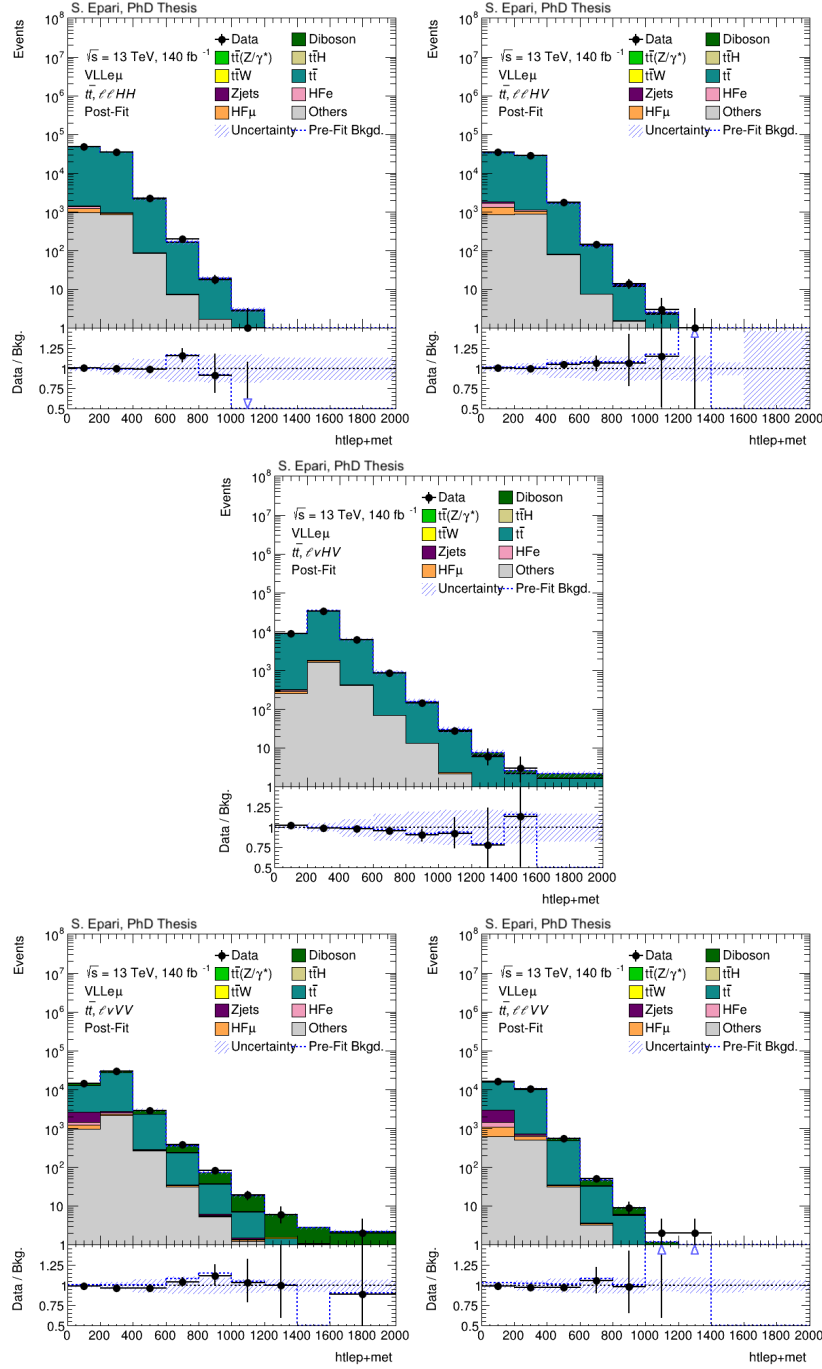


Figure 10.25: Post-fit agreement in the $t\bar{t}$ VR distributions after a B -only fit to data in the CRs and the $VLL\mu$ SRs. The pre-fit background is shown as a dashed line in all plots. The blue hashed band includes statistical and systematic uncertainties.

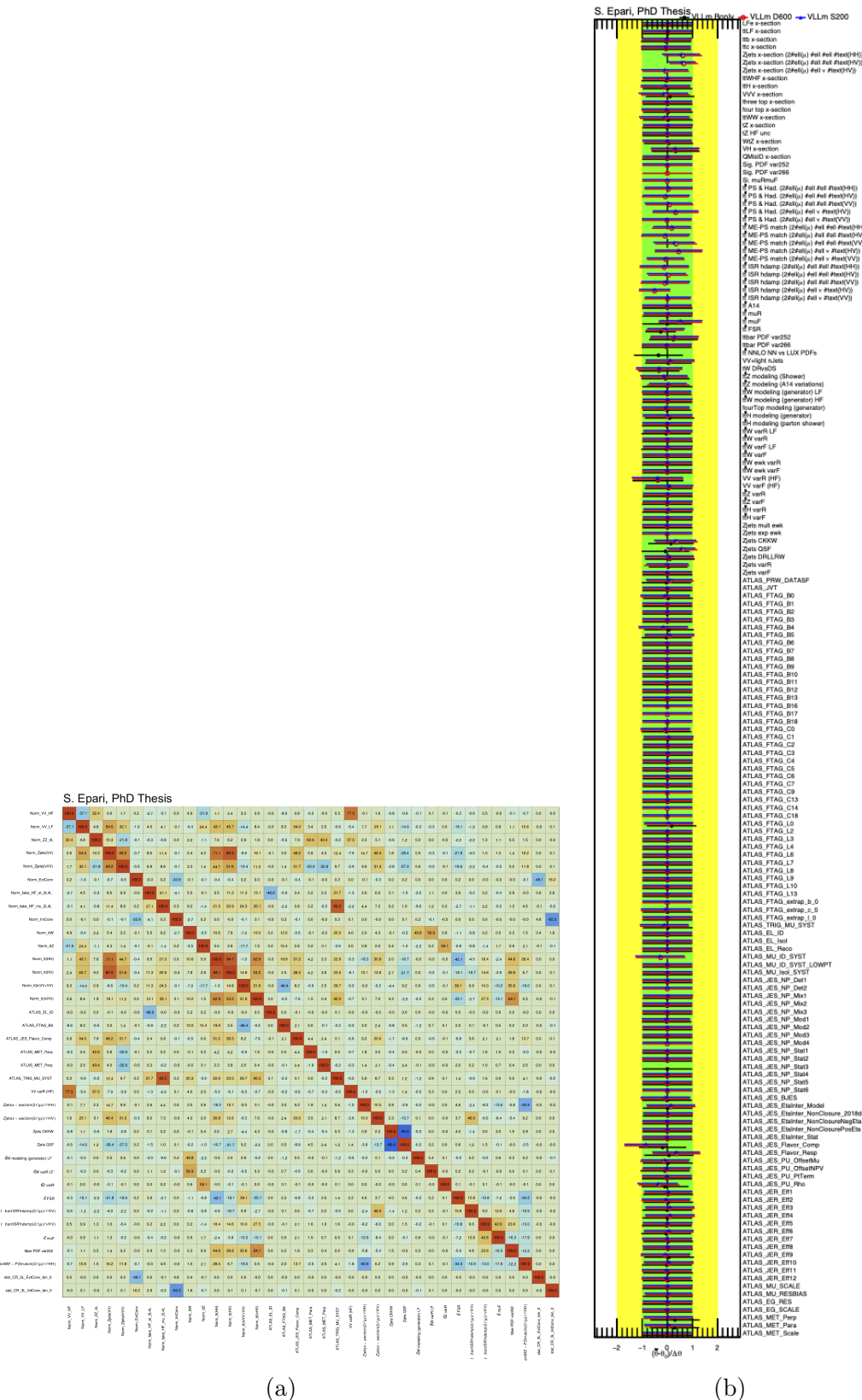


Figure 10.26: (a) The correlation matrix corresponding to a fit under the B -only hypothesis to the CRs and VLL μ SRs. (b) Overlay of pulls and constraints on the nuisance parameters from the B -only fit, $S+B$ fit considering a VLL μ signal of 600 GeV from the doublet model and $S+B$ fit considering a VLL μ signal of 200 GeV from the singlet model.

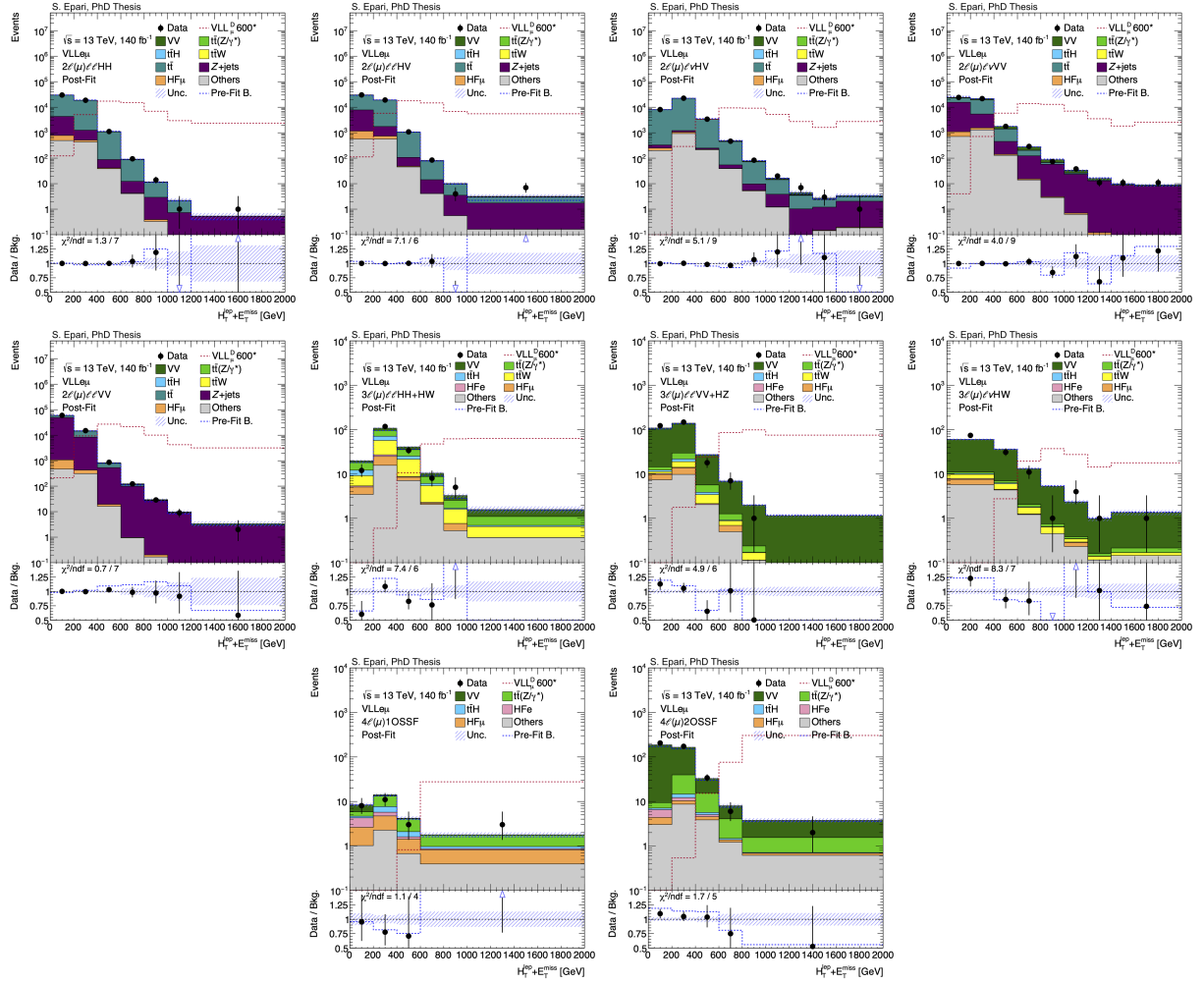


Figure 10.27: Post-fit agreement in the $VLL\mu$ SR distributions used in a $S+B$ fit to data in the CRs and the $VLL\mu$ SRs, considering a $VLL\mu$ signal of mass 600 GeV from the doublet model. The signal is shown as a red dashed line, normalised to the total background yield. The pre-fit background is shown as a blue dashed line in all plots. The blue hashed band includes statistical and systematic uncertainties.

Table 10.12 shows the summary of yields in the 10 VLL μ SRs after the B -only fit. Figures 10.28a and 10.28b and show the summary of the regions after the profile likelihood fit, together with the pre-fit background expectation.

	$2\ell(\mu)\ell\ell HH$	$2\ell(\mu)\ell\ell HV$	$2\ell(\mu)\ell\ell VV$	$2\ell(\mu)\ell\nu HW$	$2\ell(\mu)\ell\nu VV$
VV	69 ± 10	124 ± 22	1578 ± 114	230 ± 17	3941 ± 115
$t\bar{t}Z$	245 ± 159	248 ± 137	75 ± 43	77 ± 60	39 ± 29
$t\bar{t}H$	159 ± 21	86 ± 12	18.47 ± 3.07	19.9 ± 2.5	7.4 ± 1.1
$t\bar{t}W$	178 ± 25	215 ± 28	58 ± 11	77.0 ± 8.1	40.2 ± 6.4
$t\bar{t}$	43844 ± 922	40598 ± 1013	15741 ± 742	32351 ± 539	22525 ± 506
Z +jets	4339 ± 911	7755 ± 1002	57003 ± 802	282 ± 88	18913 ± 476
HFe	—	—	—	—	—
HFm	377 ± 11	765 ± 23	725 ± 21	181.4 ± 5.4	637 ± 19
Others	968 ± 229	1179 ± 249	801 ± 113	1392 ± 455	2162 ± 260
Total	50175 ± 240	50966 ± 256	75990 ± 325	34607 ± 193	48260 ± 227
Data	50178	50968	75976	34605	48276
	$3\ell(\mu)\ell\ell HH+HW$	$3\ell(\mu)\ell\ell VV+HZ$	$3\ell(\mu)\ell\nu HW$	$4\ell(\mu)2OSSF$	$4\ell(\mu)1OSSF$
VV	23.0 ± 1.9	235.0 ± 6.8	97.9 ± 4.2	326 ± 11	3.75 ± 0.27
$t\bar{t}Z$	45.2 ± 4.6	12.5 ± 2.2	1.88 ± 0.27	40.7 ± 4.0	9.45 ± 1.04
$t\bar{t}H$	21.4 ± 2.8	4.2 ± 0.89	0.77 ± 0.11	3.73 ± 0.49	$2.9-4.4$
$t\bar{t}W$	50.5 ± 4.7	7.4 ± 1.3	4.22 ± 0.69	—	—
$t\bar{t}$	—	—	—	—	—
Z +jets	—	—	—	—	—
HFe	2.76 ± 0.88	0.94 ± 0.30	0.39 ± 0.13	4.39 ± 0.17	2.87 ± 0.20
HFm	12.6 ± 1.4	6.61 ± 0.75	1.97 ± 0.23	3.98 ± 0.12	5.24 ± 0.27
Others	29.2 ± 3.3	19.9 ± 3.2	12.3 ± 2.3	17.4 ± 3.8	4.35 ± 0.51
Total	183.0 ± 6.0	283.9 ± 7.2	117.5 ± 5.0	395 ± 11	28 ± 1.6
Data	177	297	123	420	25

Table 10.12: Summary of observed and predicted yields in the 10 VLL μ SRs. The background prediction is shown after the combined likelihood fit to data under the B -only hypothesis across all CR and SR categories. The uncertainties correspond to the combined statistical and systematic uncertainties in the predicted yields. Dashes refer to components that are negligible or not applicable.

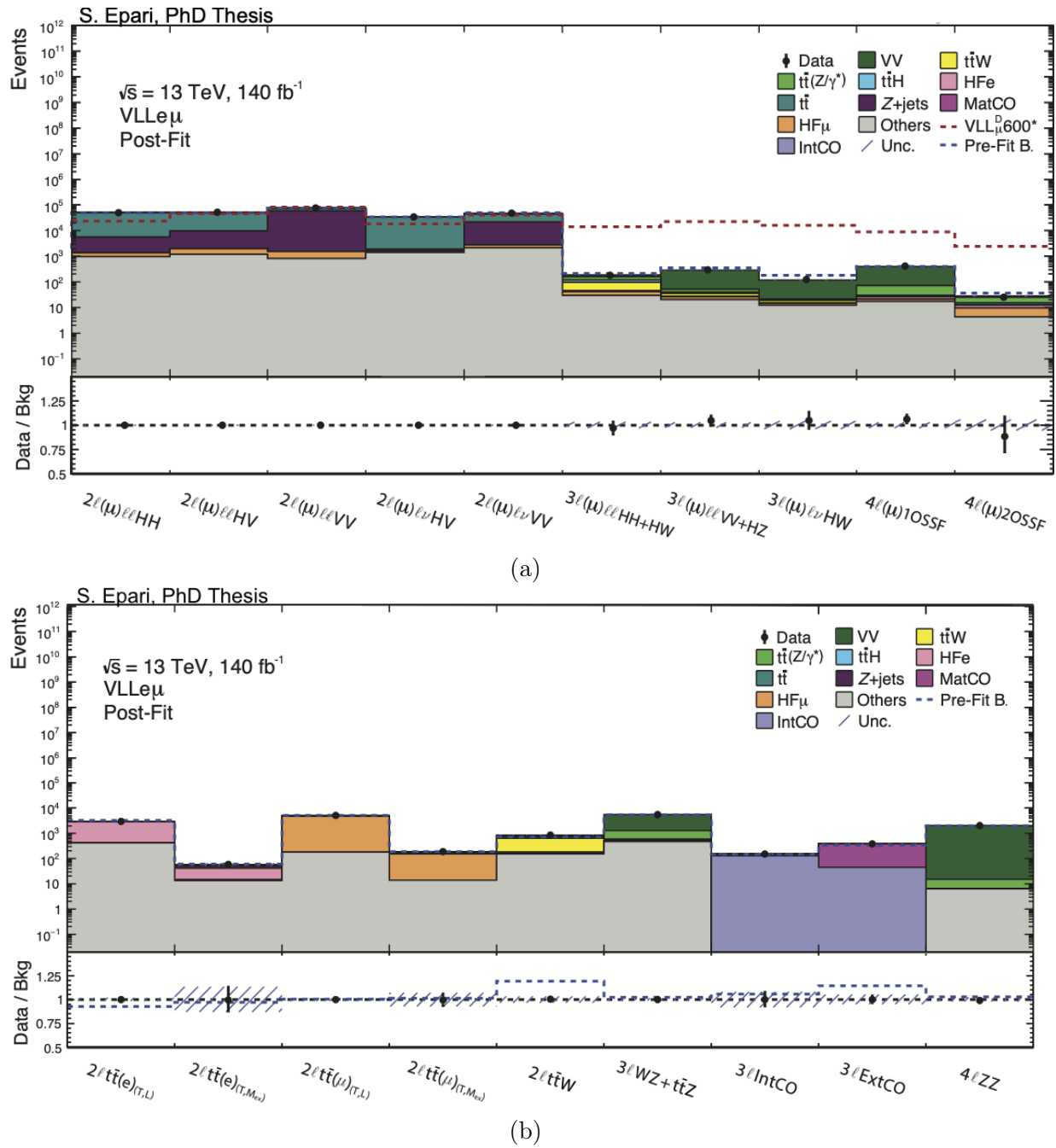


Figure 10.28: Comparison between data and the background prediction for the event yields in the (a) 10 VLL_{μ} SRs and the (b) 9 CRs. The expected signal from a VLL_{μ} of mass 600 GeV from the doublet model (normalised to the total background) as well as the background contributions are shown after the likelihood fit to data under the $S+B$ hypothesis. The total background prediction before the likelihood fit to data is shown as a dashed blue histogram in the upper panel. The blue hatched band includes both statistical and systematic uncertainties.

10.5.3 Expected and observed upper limits

No significant excess is observed over the SM expectation value after the likelihood fit to data in any of the SRs, for any of the models under study. Figure 10.29 (10.30) show the 95% confidence level (CL) expected limits on the cross-section of both the VLL_e (VLL_μ) singlet and doublet as a function of the mass of the VLL, calculated using a $S+B$ fit to data in all the CRs and VLL_e (VLL_μ) SRs. The VLL_e singlet is observed (expected) to be excluded at 95% confidence level for masses up to 320 (300) GeV while the VLL_e doublet is observed (expected) to be excluded at 95% confidence level for masses up to 1220 (1230) GeV. The VLL_μ singlet is observed (expected) to be excluded at 95% confidence level for masses up to 400 (330) GeV while the VLL_μ doublet is observed (expected) to be excluded at 95% confidence level for masses up to 1270 (1250) GeV.

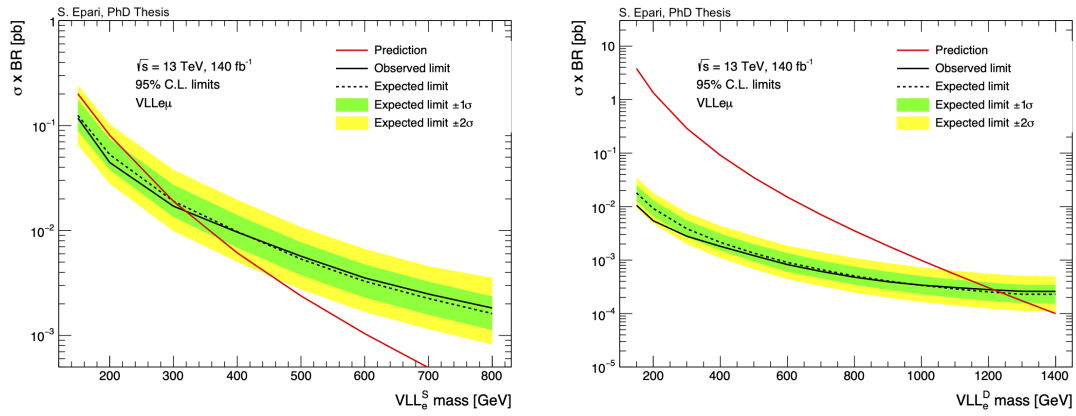


Figure 10.29: 95% CL expected and observed limits on the cross-section of a VLL_e singlet and doublet as a function of the mass of the VLL.

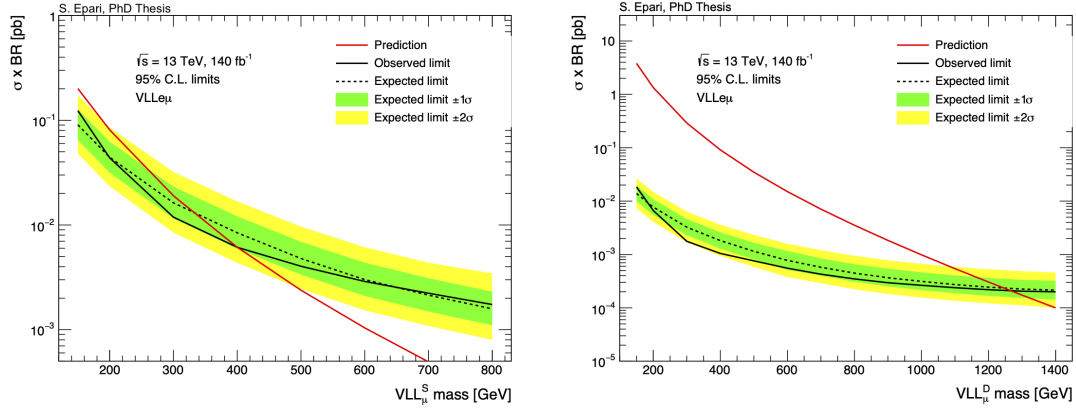


Figure 10.30: 95% CL expected and observed limits on the cross-section of a $VLL\mu$ singlet and doublet as a function of the mass of the VLL.

Figures 10.31 and 10.32 show the contributions of individual analysis channels ($2\ell OS$, 3ℓ , 4ℓ) to the 95% CL expected limits on the cross-section of a $VLL\mu$ doublet and singlet respectively, as a function of the mass of the $VLL\mu$. In the singlet models, the main sensitivity at low masses comes from 4ℓ channel and from the $2\ell OS$ channel at high masses. In the doublet models, the 3ℓ channel is most sensitive to the VLL signal, expected due to a larger signal yield from additional the neutral VLL modes present in the model. The $2\ell OS$ channel providing better sensitivity for VLLs with masses greater than 1 TeV. Overall, the exclusion on the singlet cross-sections are expected to be worse than that from the doublet due to much lower signal production cross-sections, in addition to more challenging signal topologies from the large E_T^{miss} expected from the signal.

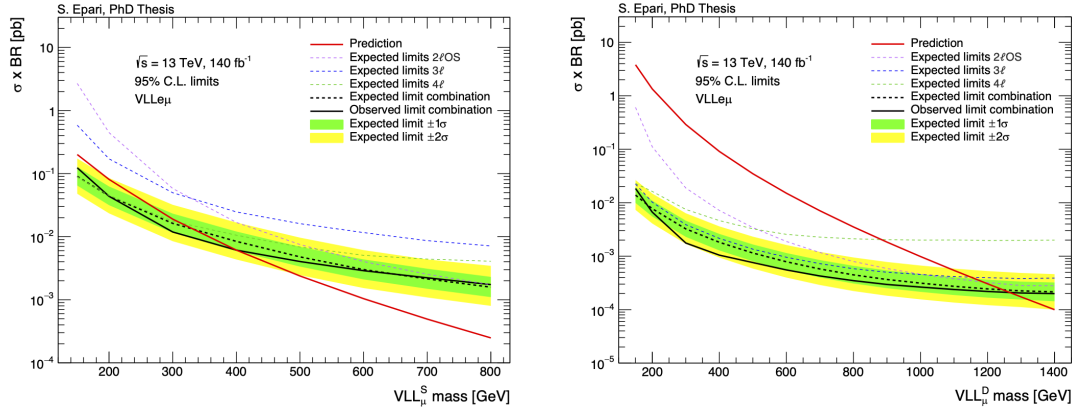


Figure 10.31: 95% CL expected and observed limits on the cross-section of a $VLL\mu$ singlet and doublet as a function of the mass of the VLL, overlaid with the contribution from each analysis channel ($2\ell OS$, 3ℓ , 4ℓ), along with the combination.

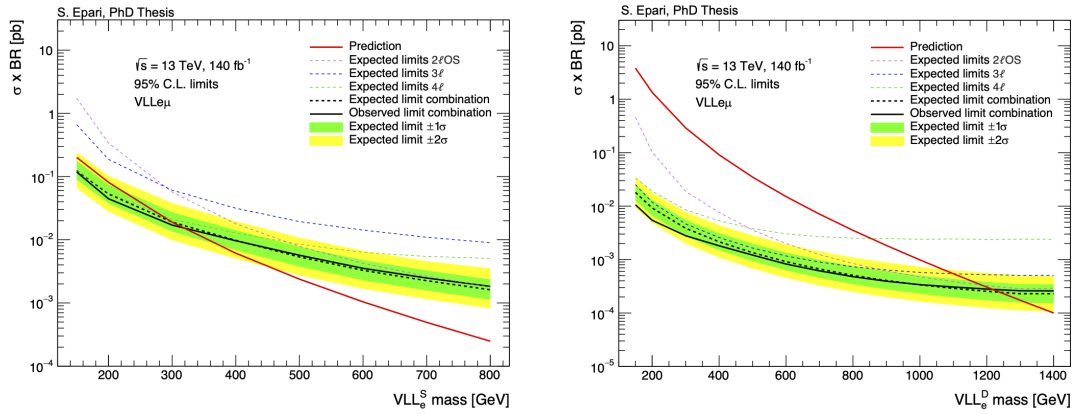


Figure 10.32: 95% CL expected and observed limits on the cross-section of a $VLLe$ singlet and doublet as a function of the mass of the VLL, overlaid with the contribution from each analysis channel ($2\ell OS$, 3ℓ , 4ℓ), along with the combination.

10.6 Conclusions

This chapter presented the first direct LHC search for a doublet or singlet vector-like lepton coupling to first and second generation Standard Model leptons. The search is based on a dataset of proton-proton collisions at $\sqrt{s} = 13$ TeV recorded with the ATLAS detector during Run 2 of the LHC, corresponding to an integrated luminosity of 140 fb^{-1} . The search is performed in the multilepton (two, three, and four light leptons) final state. A deep-neural-network-based categorisation is performed to enhance the purity of the various signal types and to discriminate signal against the SM background. The dominant backgrounds originate from $t\bar{t}$, Z +jets, $t\bar{t}W$, $t\bar{t}Z$, and VV , and are estimated from MC simulation and normalised to data in a simultaneous fit of the signal and control regions. No significant excess is observed over the SM expectation value for any of the models under study. The VLL_e singlet is observed (expected) to be excluded at 95% confidence level for masses up to 320 (300) GeV while the VLL_e doublet is observed (expected) to be excluded at 95% confidence level for masses up to 1220 (1230) GeV. The VLL_μ singlet is observed (expected) to be excluded at 95% confidence level for masses up to 400 (330) GeV while the VLL_μ doublet is observed (expected) to be excluded at 95% confidence level for masses up to 1270 (1250) GeV. A paper summarising the results presented in this chapter is in the process of publication.

Search for vector-like leptons from the 4321 model in multilepton plus b -jets final states

This chapter presents a search for pair-produced vector-like leptons (VLL) from a 4321 model [231], preferentially coupling to third generation SM fermions. The search is structured in two complementary sets of channels: the first set of channels target VLLs in final states with multiple light leptons, b -jets and hadronically decaying τ -leptons (τ_{had}), while the second set of channels targets VLLs in final states with only τ_{had} and no light leptons. The focus of this chapter is the former, presenting a preliminary study not yet unblinded by ATLAS. The chapter concludes with a brief discussion on public results from the latter channels in Section 11.8.

11.1 Simplified model

The 4321 model is a UV-complete model built from the larger gauge group $\text{SU}(4) \times \text{SU}(3) \times \text{SU}(2) \times \text{U}(1)$. This model has three heavy gauge bosons: a color octet (G'), a weak isospin-singlet vector leptoquark (U_1 , electric charge $2/3e$) and a color singlet Z' . Additionally, the model features generations of vector-like fermions: vector-like quarks (VLQ), U/D , C/S , T/B and VLLs, N_1/E_1 , N_2/E_2 , N_3/E_3 . While the model allows for all three generations of VLLs, for simplicity, the search assumes the presence of only one generation of VLLs. These VLLs are assumed to couple preferentially to SM τ -leptons and are considered to be from an $\text{SU}(2)$ doublet, with the charged and neutral VLLs being mass-degenerate.

This search targets electroweak pair-production of VLLs via off-shell decays of the SM W boson or Z/γ . Production modes mediated by Z' are suppressed by decoupling this particle from the model and setting its mass to 100 TeV. Similarly, processes mediated by G' exchange are suppressed by setting its mass to 5 TeV. Finally, masses of the VLQs are set to 3.5 TeV. As shown in Ref. [232], to accommodate flavor anomalies, the model favors VLLs decays to the vector leptoquark U_1 and SM τ -leptons. Thus, to ensure a realistic model, the decay width of U_1 is constrained to 500 GeV, while the mass is set to 3.5 TeV to allow for off-shell decays. Two scenarios, without and with right-handed currents are possible, leading to similar kinematics and the former is chosen for this study. The VLLs are normalised to the next-to-leading order production cross-sections shown in Figure 10.2. The various production and decay modes for these VLLs are shown in Figure 11.1, producing final states with multiple τ , b -jets and missing transverse energy.

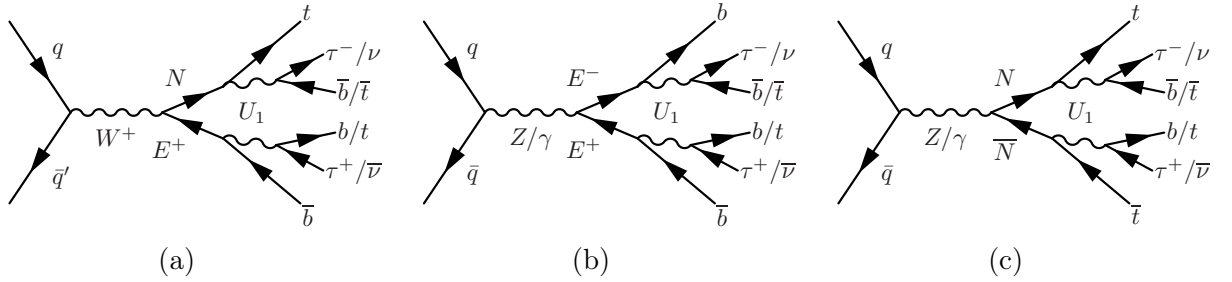


Figure 11.1: Feynman diagrams for production and decay of vector-like leptons from the 4321 model (a) $pp \rightarrow E N$, (b) $pp \rightarrow E^+ E^-$, (c) $pp \rightarrow N N$.

The 4321 model can accommodate for current experimental anomalies in low energy fermionic processes like B -meson decays and $(g - 2)_\mu$, while remaining consistent with electroweak precision measurements [232–234]. A search for VLLs from the 4321 model was performed by the CMS collaboration using the 96.5 fb^{-1} dataset collected in 2017 and 2018, and a 2.8σ local deviation between fit to the signal+background model as compared to background-only model, almost irrespective of the VLL mass (in targeted range 500 - 1050 GeV), was reported [235]. Final states with ≥ 3 b -jets, split according to the multiplicity of τ_{had} were considered and the highest excluded observed (expected) VLL mass is around 500 (650) GeV, as shown in Figure 11.2.

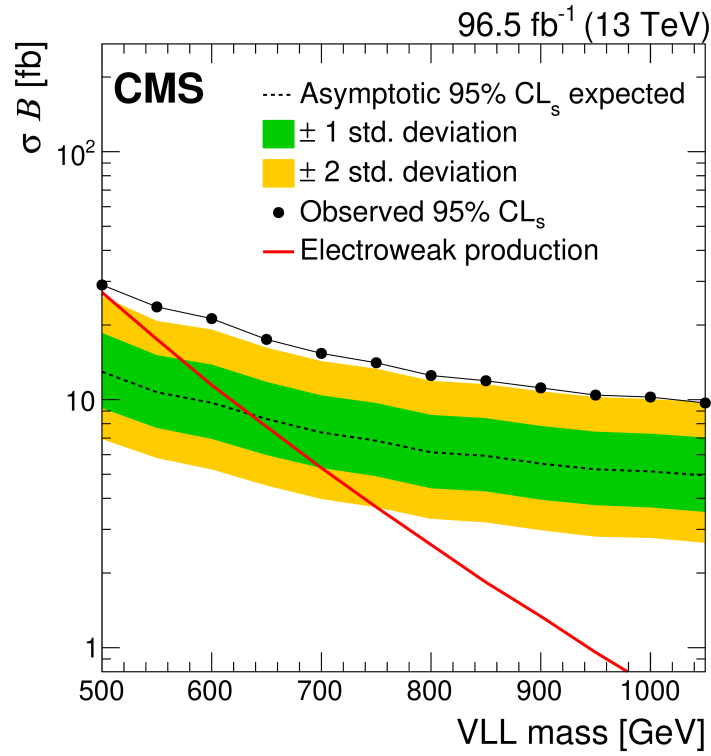


Figure 11.2: Expected and observed 95% CL upper limits on the product of the VLL pair production cross section and the branching fraction to third generation quarks and leptons, combining the 2017 and 2018 data and all τ_{had} channels. The theoretical prediction from the 4321 model for electroweak production of VLLs at leading order is shown in the red line. Figure taken from Ref. [235].

11.2 Datasets, triggers and object definitions

The full Run 2 dataset, corresponding to an integrated luminosity of 140 fb^{-1} with an uncertainty of 0.83%, at the centre-of-mass energy $\sqrt{s} = 13 \text{ TeV}$ is used for this search.

Events with two or more light leptons and $E_T^{\text{miss}} < 200 \text{ GeV}$ are pre-selected using a logical OR of single and di-lepton triggers (SLT OR DLT). To allow full trigger efficiency, events with $E_T^{\text{miss}} < 200 \text{ GeV}$ are pre-selected using the E_T^{miss} trigger. Details about these triggers are summarised in Tables 8.2 and 8.3 respectively.

Physics objects are reconstructed using the definitions established in Chapter 8. Events are separated into channels with two same-sign ($2\ell\text{SS}$), opposite-sign ($2\ell\text{OS}$) and $3\ell/4\ell$ leptons with various τ_{had} multiplicities using the loose light lepton definitions established in Chapter 8. For electrons (muons), the TightLH (Medium) ID and FCLoose isolation WP is used to pre-select events. However, PLIV isolation cuts for both electrons and muons are dropped to improve signal acceptance in these channels. This strategy is discussed in more detail in Section 11.3. B -jets are tagged at the 85% DL1r WP. τ_{had} candidates are reconstructed using the Loose RNN WP, as described in Table 8.9.

Signal samples were generated at next-to-leading order using MADGRAPH5_AMC@NLO [85] with NNPDF23LO. PYTHIA8.186 with the A14 tune was used as the showering algorithm. The matrix element was calculated at LO in QCD, with emission of up to two additional partons. Detector level effects were incorporated using ATLAS *Fast Simulation*, as described in Chapter 6. Signal events were generated for VLL masses in the range of 200 GeV to 1500 GeV with the 100 GeV spacing. The NLO generator cross-section was used for the normalisation of the signals.

11.3 Analysis strategy

The search considers two sets of complementary channels to search for VLLs from the 4321 model:

- τ_{had} -only channels, consisting of at least one τ_{had} candidate. These channels are split according to the multiplicity of τ_{had} as in the CMS search, except the $0\tau_{\text{had}}$ plus multi b -jet channel is not considered in the search due to low sensitivity because of the large multi-jet background.
- Channels with at least two light leptons including both hadronic and leptonic τ

decays. These channels are termed *multilepton (ML) channels* and serve as a powerful validation to the observations from the τ_{had} -only channels.

In both cases, all channels are required to have at least three b -jets and are split into signal regions (SRs) depending on the number of light-leptons and τ_{had} to maximise the signal sensitivity. Dedicated mass-parameterised signal versus background neural networks (NNs) are trained against the standard model background in each SR and output score of the NNs are considered as discriminating variables for the SRs in the simultaneous profile-likelihood fit for the signal and background. Data-driven techniques to estimate the major backgrounds, such as $t\bar{t}$ +jets with real or fake τ_{had} , VV , W/Z +jets and QCD multi-jets (τ_{had} -only channels).

The work detailed in this dissertation is a preliminary study of the ML channels. The work on the τ_{had} -only channels is now a public result [236] and is discussed briefly in Section 11.8.

11.3.1 Signal regions

The ML channel is divided into four SRs depending on the multiplicity of light leptons and τ_{had} , defined in Table 11.1.

Dedicated mass-parameterised deep neural network (DNN) classifiers are trained against the total background, separately for the sum of the $2\ell\text{SS}+0\tau_{\text{had}}$, $2\ell\text{SS}+\geq 1\tau_{\text{had}}$ and $3\ell/4\ell+\geq 0\tau_{\text{had}}$ regions, as well as for the $2\ell\text{OS}+\geq 1\tau_{\text{had}}$ region. A single training for the $2\ell\text{SS}/3\ell/4\ell$ channels is preferred because these channels have similar background compositions, different from those in the $2\ell\text{OS}$ channel. This strategy, thus, ensures optimal background discrimination in all channels. The score of the DNN classifiers is used as discriminating variables in the likelihood fit. The DNN classifiers are trained using the MVAtoolkit [237, 238] that interfaces to the KERAS library [137] with TENSORFLOW as a backend [138]. The same architecture was used for both classifiers, differing only in the training variables shown in Table 11.2, optimised to target the expected backgrounds in the respective channels. A sketch of the architecture of the classifiers is shown in Figure 11.3. Binary cross-entropy is used as the loss metric and the Adam optimization algorithm [136] is used for training optimisation. The DNN classifier is trained with batch size of 1000 and learning rate 0.0001, with a maximum number of epochs set to a large number of $\mathcal{O}(120)$, and the model evaluated in the last epoch is chosen.

	$2\ell\text{SS}+0\tau_{\text{had}}$	$2\ell\text{SS}+\geq 1\tau_{\text{had}}$	$2\ell\text{OS}+\geq 1\tau_{\text{had}}$	$3\ell/4\ell + \geq 0\tau_{\text{had}}$
Number of e/μ	2		2	≥ 3
Total e/μ charge	± 2		0	3ℓ : ± 1 4ℓ : 0
e charge mis-ID veto	yes		—	yes
Minimum $p_{\text{T}}^{e/\mu}$ [GeV]	(20,20,20)			3ℓ : (10, 20, 20) 4ℓ : (10, 10, 10, 10)
Minimum p_{T}^{τ} [GeV]			≥ 20	
$m_{\ell\ell}(\text{OSSF pair})$ [GeV]	—		> 12	3ℓ : > 12
$ m_{\ell\ell} - m_Z $ [GeV]	—		< 10	—

Table 11.1: Summary of SRs defined in the multilepton (ML) channels. Light leptons definitions from Table 8.6 are used. All channels are required to have at least three b -jets tagged at the 85% DL1r working point. Electrons (muons) are selected using the TightLH (Medium) identification and FCLoose isolation working points. The Loose RNN working point is used to reconstruct τ_{had} candidates.

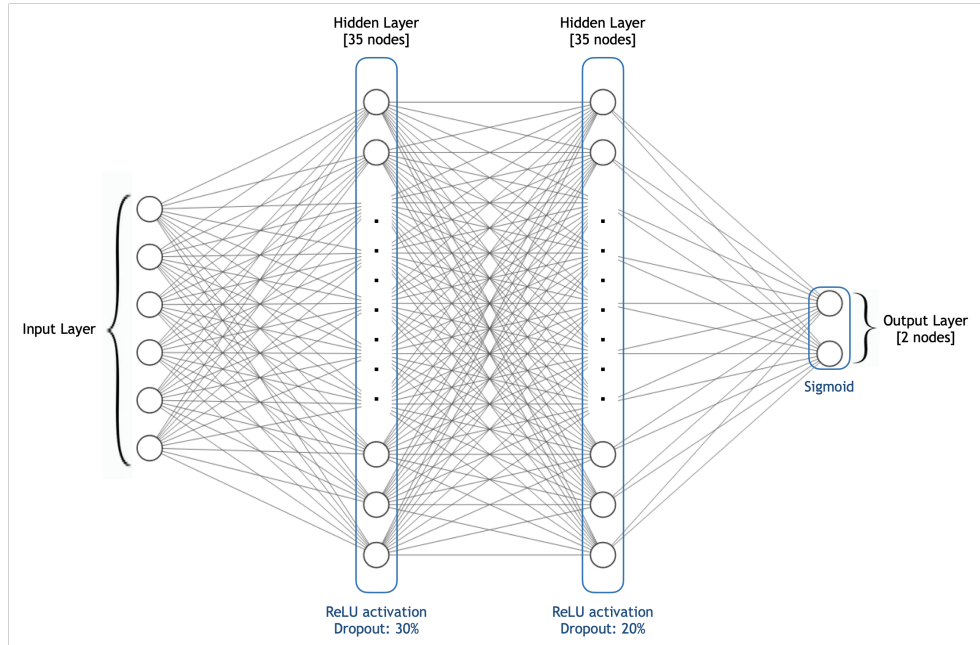


Figure 11.3: Architecture of the mass-parameterised DNN trained against the total background separately for the sum of $2\ell\text{SS}+0\tau_{\text{had}}$, $2\ell\text{SS}+\geq 1\tau_{\text{had}}$ and $3\ell/4\ell + \geq 0\tau_{\text{had}}$ regions and for the $2\ell\text{OS}+\geq 1\tau_{\text{had}}$ region.

Variable	2ℓSS/3ℓ/4ℓ DNN	2ℓOS+≥1τ _{had} DNN
Number of jets (N_{jets})	Y	Y
Number of hadronic tau candidates (N_{τ})	Y	-
Type of di-leptonic event (ee, eμ or μμ)	Y	Y
Type of tri-leptonic event (eee, eeμ, eμμ or μμμ)	Y	-
Total number of light leptons	Y	-
Total charge of all leptons (including hadronic taus) (sumQ)	Y	Y
p_T sum of all light leptons ($H_{T,\text{lep}}$)	Y	Y
p_T sum of all jets ($H_{T,\text{jets}}$)	Y	Y
p_T sum of all hadronically decaying taus ($H_{T,\text{tau}}$)	Y	Y
Missing transverse energy (E_T^{miss})	Y	Y
Sum of pseudo-continuous b-tagging scores of jets (sumPCB)	Y	Y
Sum of pseudo-continuous tau tagging WPs (sumPCT)	Y	Y
Sum of pseudo-continuous PLIV WPs (sumPLIV)	Y	-
Invariant mass of two closest b -jets in ΔR ($m_{bb}^{\text{min}\Delta R}$)	-	Y
Average ΔR between two b -jets (ΔR_{bb})	-	Y
Minimum of invariant mass of light-lepton and τ _{had} pairs ($m_{\ell\tau}^{\text{min}}$)	-	Y

Table 11.2: Input variables for mass-parameterized signal versus background neural networks.

In contrast to the g2HDM and VLLe/μ analyses, PLIV cuts on light leptons are dropped in this analysis to increase signal acceptance. Instead, powerful fake light lepton rejection is provided by constructing a new variable called the *sum of pseudo-continuous PLIV* (*sumPLIV*). This variable is constructed using the PLIV working point (WP) passed by each light lepton in the event:

- A weight of 2 is assigned to a light lepton if it passes both the *Tight* and *VeryTight* PLIV WP.
- A light lepton receives a weight of 1 if it passes the *Tight* PLIV WP but not the *VeryTight* WP.
- No weight is assigned to the light lepton if it passes only the *Medium* PLIV WP.

These weights are then scaled by predefined factors to emphasize the contribution of light lepton in different positions: the first light lepton is scaled by 27, the second by 9, the third by 3, and the fourth by 1. Similarly, the RNN WPs for τ_{had} identification are used to create the *sum of pseudo-continuous tau tagging* (sumPCT). Figure 11.4 shows the difference in shape of these variables for the signal and background, in an inclusive region used for training the NN against the sum of backgrounds in the 2ℓSS+0τ_{had}, 2ℓSS+≥1τ_{had} and 3ℓ/4ℓ + ≥0τ_{had} SRs. The signal MC peaks towards the higher (lower) end of the sumPLIV

(sumPCT) distributions. This approach ensures optimal separation of fake light leptons from the signal without the need to exclude these from the phase space, which may have a non-negligible impact on signal acceptance in the region.

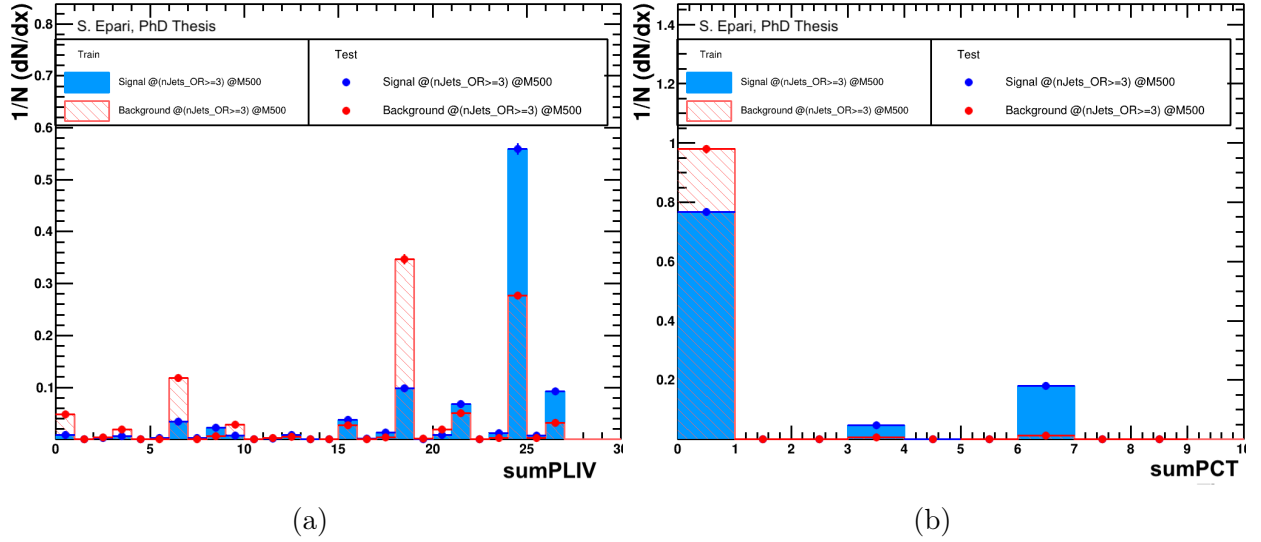


Figure 11.4: Scaled distributions of (a) Sum of pseudo-continuous PLIV WPs (sumPLIV) and (b) Sum of pseudo-continuous τ tagging WPs (sumPCT) in an inclusive region used for training the DNN against the sum of the events passing the $2\ell\text{SS}+0\tau_{\text{had}}$, $2\ell\text{SS}+\geq 1\tau_{\text{had}}$ and $3\ell/4\ell+\geq 0\tau_{\text{had}}$ selections. The signal MC corresponds to a VLL of 500 GeV and is shown in blue, while the sum of backgrounds is indicated in red.

The distributions of the score of the DNN classifiers for a 500 GeV VLL, shown in Figure 11.5, show good discrimination between the signal and background distributions.

The performance of the DNN classifiers is evaluated using *Receiver Operating Characteristic* (ROC) curves, shown in Figure 11.6. The distributions of the signal and background shapes in the training variables used in the NNs is shown in Appendix B, for a 500 GeV VLL.

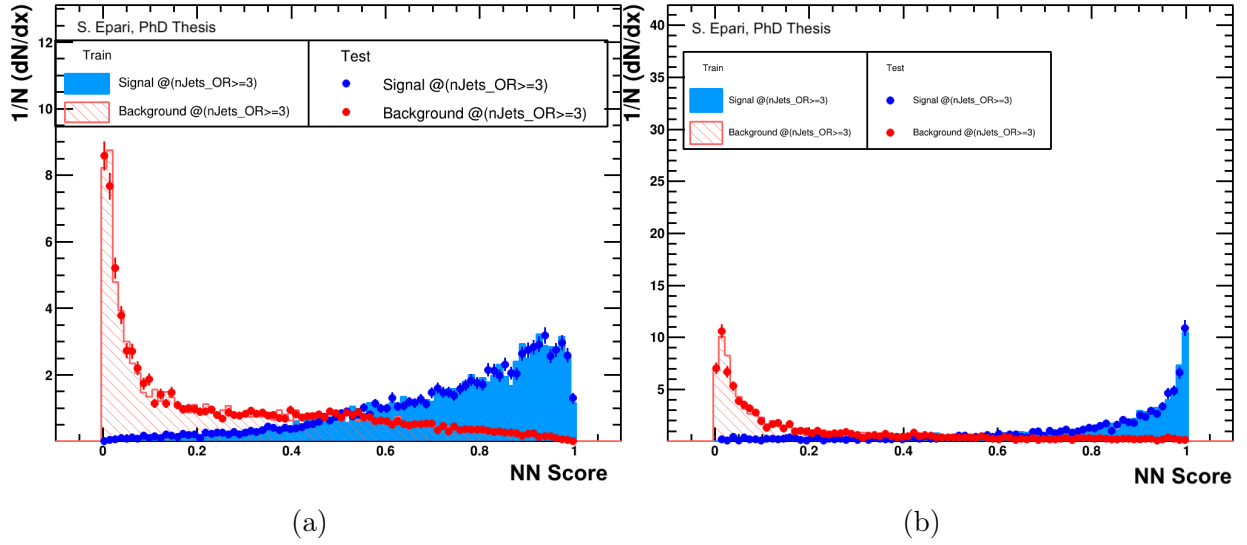


Figure 11.5: Scaled distributions of DNN classifier scores for (a) the sum of the events passing the $2\ell\text{SS}+0\tau_{\text{had}}$, $2\ell\text{SS}+\geq 1\tau_{\text{had}}$ and $3\ell/4\ell+\geq 0\tau_{\text{had}}$ selections and (b) events passing the $2\ell\text{OS}+\geq 1\tau_{\text{had}}$ selection. The signal MC corresponds to a VLL of 500 GeV and is shown in blue while the sum of backgrounds is indicated in red.

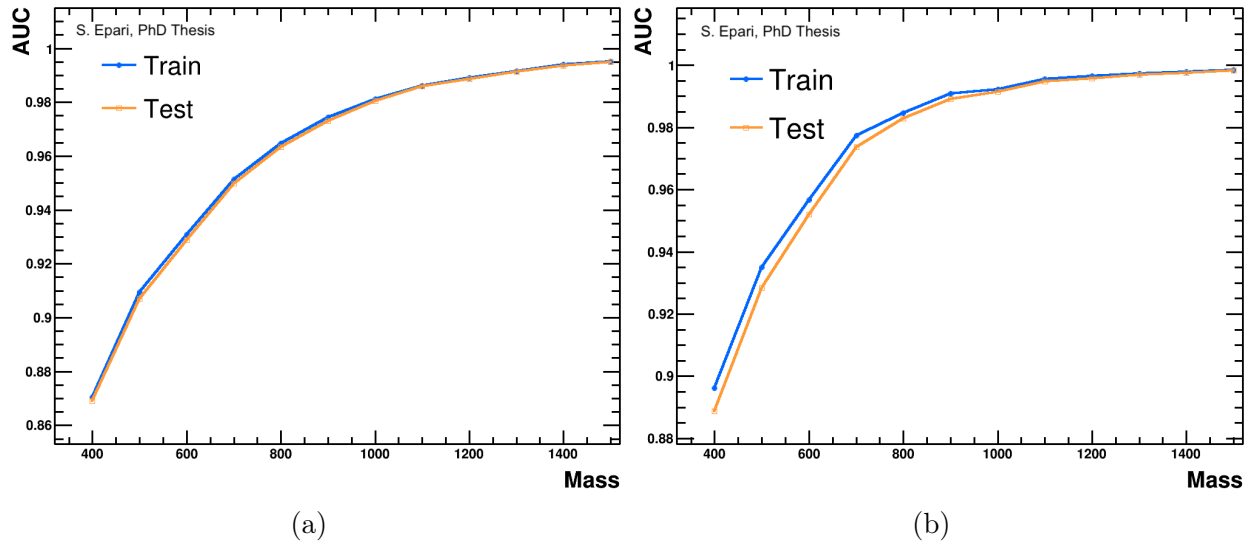


Figure 11.6: Area under the receiver operating characteristic (ROC) curve for the NN performance for various mass points. The training is performed for (a) the sum of the events passing the $2\ell\text{SS}+0\tau_{\text{had}}$, $2\ell\text{SS}+\geq 1\tau_{\text{had}}$ and $3\ell/4\ell+\geq 0\tau_{\text{had}}$ selections and (b) events passing the $2\ell\text{OS}+\geq 1\tau_{\text{had}}$ selection.

11.3.2 Blinding strategy

The lowest excluded VLL mass from the CMS search is at 500 GeV. The event yield from this signal is used for *blinding* bins with signal over background over 5% to avoid bias while estimated SM backgrounds in a background-only fit.

11.3.3 Control regions

Figure 11.7 highlights the main SM backgrounds expected in the SRs. Major prompt backgrounds originate from $t\bar{t}W$, $t\bar{t}t\bar{t}$ and $t\bar{t}\gamma^*$ production, with smaller contributions from VV in the 3ℓ and 4ℓ channels. Non-prompt light lepton backgrounds originate mainly from semi-leptonic b -decays and populate the $2\ell SS$ channels. Backgrounds from mis-identified τ_{had} , mainly from $t\bar{t}$ and $Z + \text{jets}$, dominate in the $2\ell SS + \geq 1\tau_{\text{had}}$ SRs. Dedicated CRs are defined to estimate or correct major backgrounds common to the SRs, summarised in Table 11.3.

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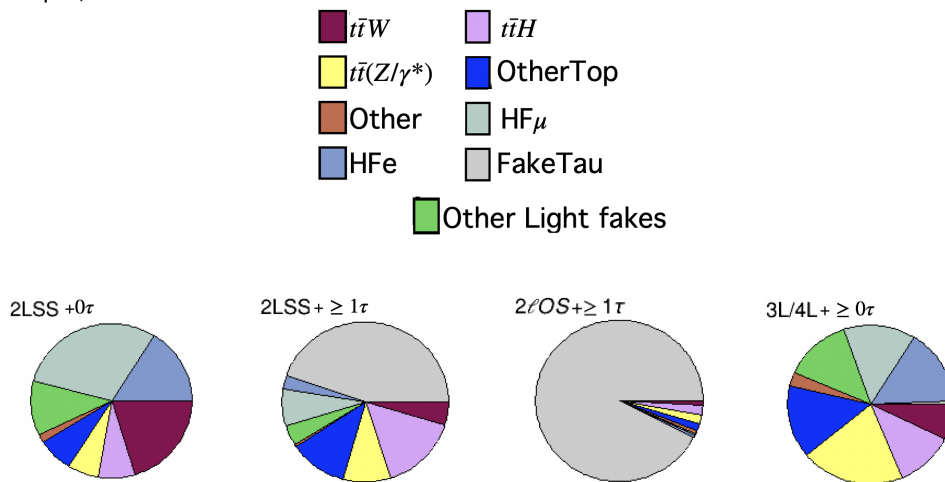


Figure 11.7: Background composition in the SRs.

All backgrounds are estimated using simulated samples described in Section 8.5.2. Event kinematics of the simulated $t\bar{t}$, $Z + \text{jets}$ and VV backgrounds require dedicated corrections to better describe the data, borrowed from Chapter 10. Yields of $t\bar{t}W$, $t\bar{t}Z$, VV and non-prompt-lepton backgrounds from semi-leptonic b -decays, are adjusted via normalisation factors that are determined by performing a likelihood fit to data across all event categories, shown in Section 9.5. Estimation of the fake τ_{had} background from $t\bar{t}$ and $Z + \text{jets}$ is described in Section 11.3.3.

Control regions	WZ+ $t\bar{t}Z$	$t\bar{t}W$	HF non-prompt
N_{jets}		≥ 2	
$N_{b\text{-jets}}$	$\geq 1b^{85\%}$	$2b^{85\%}$	$1b^{85\%}$
Lepton requirement	3ℓ		$2\ell\text{SS}$
Lepton definition	(L, M, M)	(T, T)	(T, M_{ex})
Lepton p_{T} [GeV]	(10, 20, 20)	(20, 20)	(20, 20)
$m_{\ell^+\ell^-}^{\text{OS-SF}}$ [GeV]	> 12		–
$ m_{\ell^+\ell^-}^{\text{OS-SF}} - m_Z $ [GeV]	< 10		–
Region split	–	–	subleading $e/\mu \times [(T, M_{\text{ex}})]$
Region naming	3ℓ WZ+ $t\bar{t}Z$	$2\ell\text{SS}/\text{OS } t\bar{t}W$	$2\ell\text{tt}(e)_{(T, M_{\text{ex}})}$ $2\ell\text{tt}(\mu)_{(T, M_{\text{ex}})}$

Table 11.3: Event selection summary in the CRs. Light leptons definitions from Table 8.6 are used. In the HF non-prompt lepton region naming, “ $2\ell\text{SStt}(e)$ ” (“ $2\ell\text{SStt}(\mu)$ ”) refer to the CRs enriched in non-prompt electrons (muons) from semi-leptonic b -decays originating mostly from $t\bar{t}$ and with the lepton flavours for the leading and subleading leptons corresponding to “ $ee, \mu e$ ” (“ $\mu\mu, e\mu$ ”).

Estimation of fake τ_{had} background

The dominant fake τ_{had} background comes from $t\bar{t}$ or $Z + \text{jets}$ events where a jet is misidentified as a τ_{had} candidate. This background is estimated using a semi-data-driven approach, where the predictions from MC simulations are taken as the baseline and data-to-MC *scale factors* (SFs) are derived as a function of the p_T of the reconstructed τ_{had} and multiplicity of associated charged tracks, using a region enriched in $t\bar{t}$ events with at least one reconstructed (fake) τ_{had} . Uncertainties in the SFs are evaluated in an alternative control region dominated by the $Z + \text{jets}$ events with at least one reconstructed (fake) τ_{had} . The SFs (f_{τ}^{fake}) are determined for three exclusive identification working points: *Loose-not-Medium*, *Medium-not-Tight* and *Tight*, as shown in Equation 11.1.

$$f_{\tau}^{\text{fake}} = \frac{N_{\tau}^{\text{data}} - N_{\text{real}}^{\text{MC}}}{N_{\text{fake}}^{\text{MC}}}, \quad (11.1)$$

where N_{τ}^{data} is the number of τ_{had} reconstructed in data, and $N_{\text{real}}^{\text{MC}}$ and $N_{\text{fake}}^{\text{MC}}$ are the number of real and mis-identified τ_{had} in MC simulation respectively. Figure 11.8 shows the distributions of f_{τ}^{fake} obtained from $t\bar{t} + 1\tau_{\text{had}}$ and $Z + \text{jets} + 1\tau_{\text{had}}$ regions, as a function of τ_{had} p_T and number of tracks. The largest difference between the two estimates is in the case of the *Loose-not-Medium* WP for 3-prong taus. These SFs are applied to fake τ_{had} events in all processes and in each region.

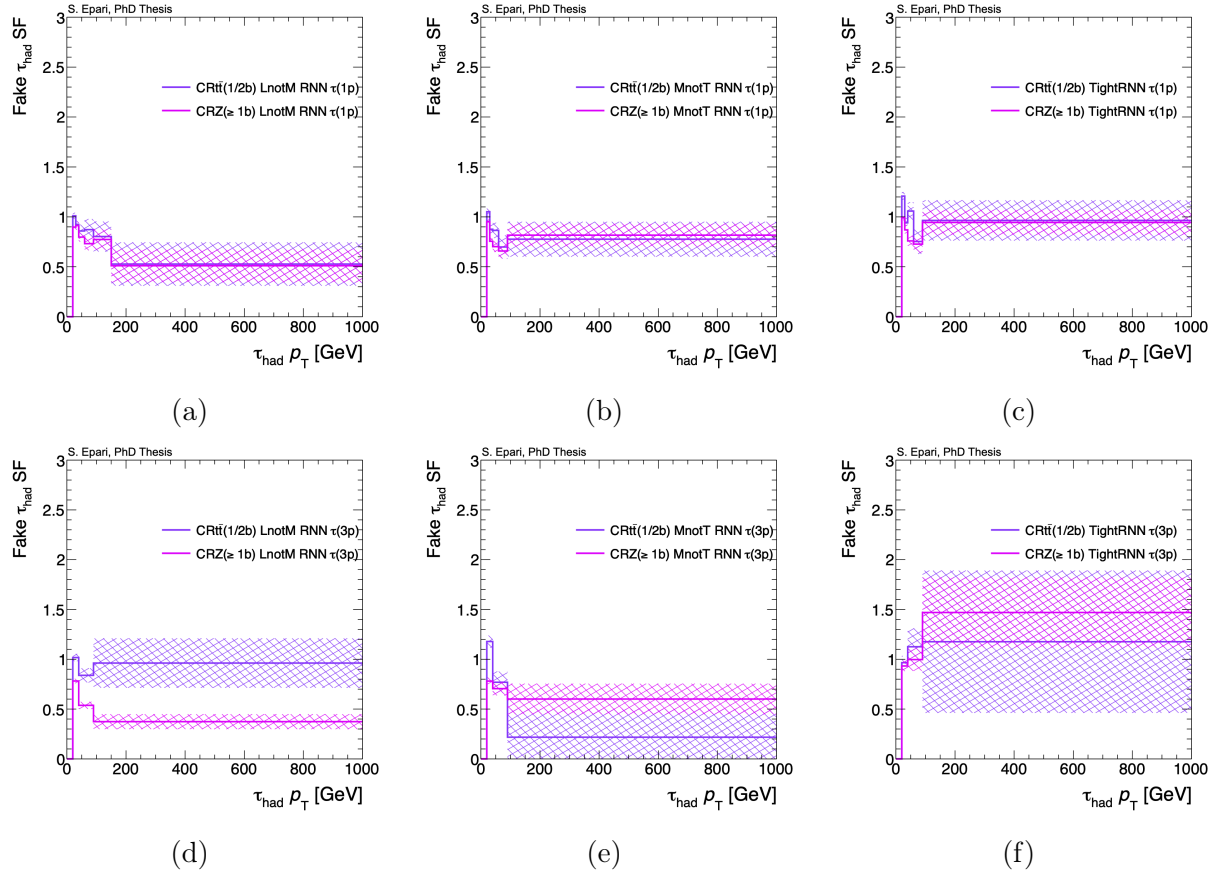
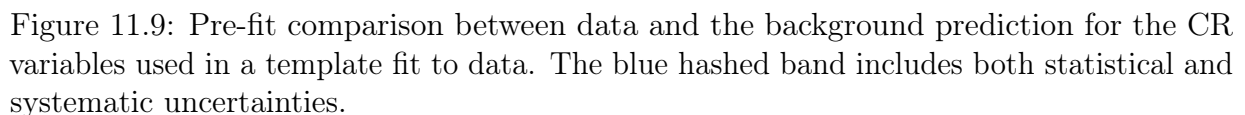


Figure 11.8: The fake τ_{had} scale factors (f_{τ}^{fake}) are derived from $t\bar{t} + 1\tau_{\text{had}}$ (pink) and $Z + \text{jets} + 1\tau_{\text{had}}$ (purple) regions for 1-prong τ_{had} in various working points: (a) Loose-not-Medium WP, (b) Medium-not-Tight WP, and (c) Tight WP. Similarly, for 3-prong τ_{had} , the working points are: (d) Loose-not-Medium WP, (e) Medium-not-Tight WP, and (f) Tight WP. The shaded bands represent the statistical uncertainties.

The template fit method, described in detail in Chapter 10, is used to estimate the normalisation of $t\bar{t}W$, VV (heavy flavor), $t\bar{t}Z$ and non-prompt electrons and muons from semi-leptonic b -decays. These selections used to create these regions are described in Table 11.3. The number of events in the $t\bar{t}W$ and HF non-prompt CRs are used to estimate the normalisation of the respective background. On the other hand, the b -jet multiplicity in the $WZ+t\bar{t}Z$ CR is used to provide a good separation between the WZ (dominant at $N_{\text{bjets}} = 1$) and $t\bar{t}Z$ backgrounds (dominant at $N_{\text{bjets}} > 1$). Pre-fit distributions of these CRs are shown in Figure 11.9.



11.3.4 Summary of analysis regions

The summary of regions defined in analysis is illustrated in Figure 11.10. A total of 4 SRs (Table 11.1) and 4 CRs (Table 11.3) are defined.

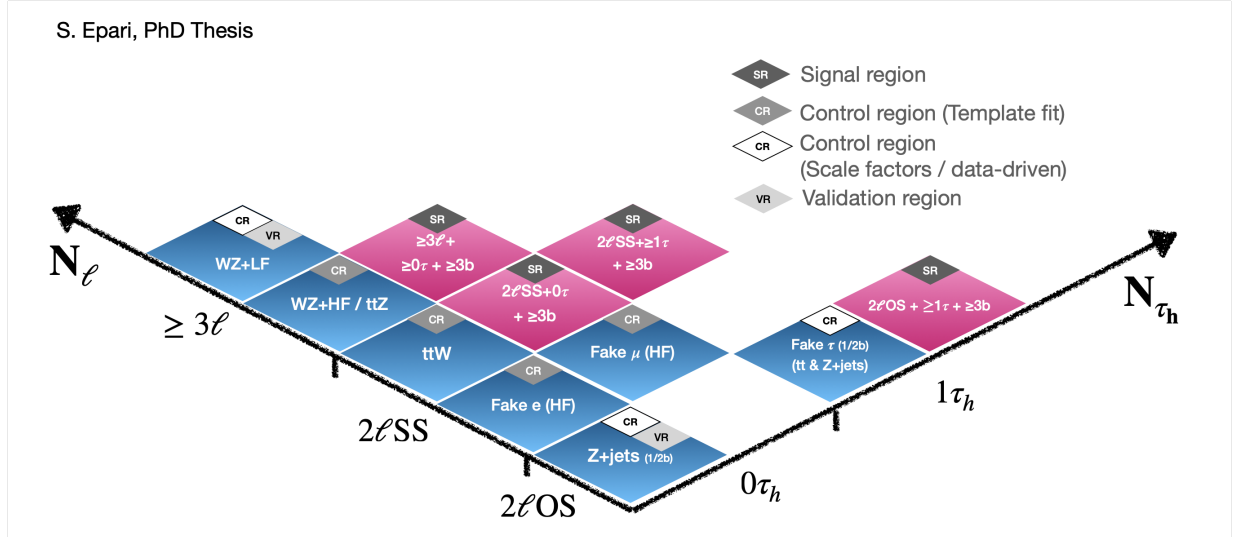


Figure 11.10: Illustrative sketch of multilepton regions defined in the 4321 analysis.

11.4 Systematic uncertainties

All systematic uncertainties listed in Chapter 8, except those on JER, JES, and E_T^{miss} , are included in the systematic model built for the analysis. These missing uncertainties, together with the models built for $t\bar{t}$ and $Z + \text{jets}$ in Chapter 10, and systematic uncertainties in the signal MC and τ_{had} (described in Section 11.3.3) are expected to be included in the fit to data, including the SRs. Table 11.4 shows a summary of the systematic model. The components yet to be included are marked in gray.

Systematic uncertainty	Components	Systematic uncertainty	Components
Luminosity	1	VLL modelling	
Pileup reweighting	1	QCD scale (μ_F, μ_R)	1
Physics Objects		Parton shower	1
Electron	5	α_s +PDFs	1
Muon	10	$t\bar{t}H$ modelling	
Tau	21	Cross section (N)	1
Jet energy scale and resolution	31	Parton shower and hadronisation model	1
Jet vertex fraction	1	$t\bar{t}W$ modelling	
Jet flavour tagging	15	Generator	1
E_T^{miss}	3	QCD scale	1
Total (Experimental)	88	$t\bar{t}Z$ modelling	
Data-driven background estimates		Cross section (N)	1
$t\bar{t}$ NNLO/NNLL(QCD)+NLO(EW) theory reweighting	2	Matrix-element MC generator	1
Fake τ_{had} estimates	14	$t\bar{t}$ modelling	
Mat. Conv. modelling	1	Cross section (N)	1
Int. Conv. modelling	1	Radiation	2
Total (Data-driven reducible background)	18	Parton shower and hadronisation model	1
		Generator	1
		WZ modelling	
		Cross section (N)	1
		Heavy flavour composition (N)	1
		Other background modelling	
		Cross section (N)	10
		Total (Signal and background modelling)	26
		Total (Overall)	134

Table 11.4: Sources of systematic uncertainty considered in the analysis. N means that the uncertainty is taken as normalisation-only for all processes and channels affected. Some of the systematic uncertainties are split into several components, as indicated by the number in the rightmost column.

11.5 Results

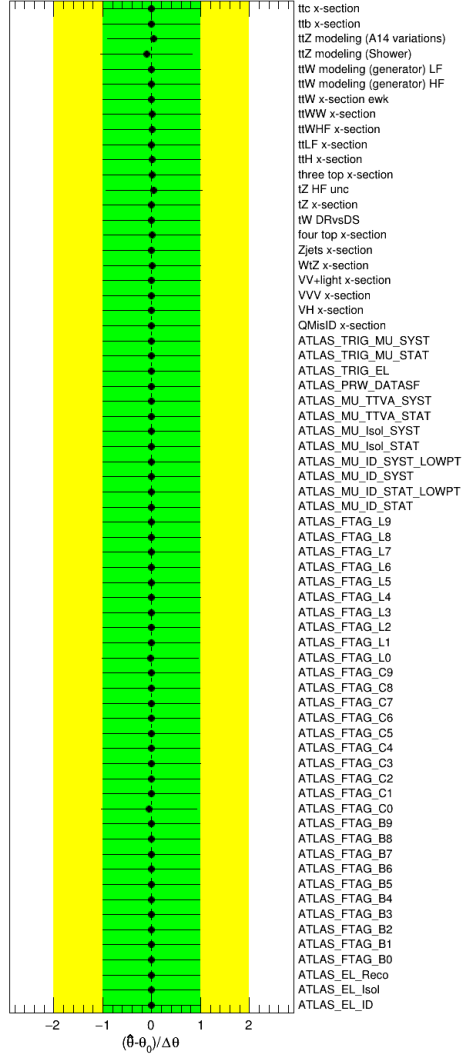
This section discusses the results of a control region only (*CR-only*) fit performed to validate the modelling of all major SM backgrounds. This fit, also called the *template fit*, includes the 4 CRs defined in Table 11.3 and fits normalisation factors for $t\bar{t}W$, $t\bar{t}Z$, VV and non-prompt leptons (HFe , $\text{HF}\mu$). All systematic uncertainties discussed in Section 11.4 are included in the fit except those for $t\bar{t}$ and $Z + \text{jets}$, which are sub-leading backgrounds in these regions.

The results of this fit are discussed in Section 11.6. Preliminary sensitivity of the search estimated including statistical uncertainties from the ML channels is discussed in Section 11.7. This search is expected to be statistically limited and negligible degradation of sensitivity is expected from considering various systematics uncertainties. The section concludes with a brief discussion of the results from the τ_{had} -only channels in Section 11.8.

11.6 Background-only fit to data in control regions

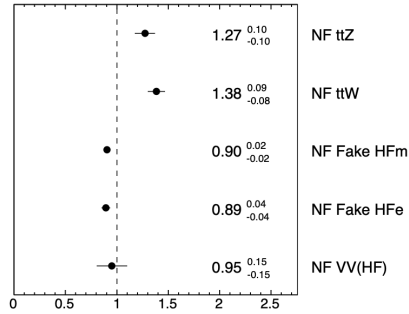
A *CR-only* fit to data, including the 4 CRs defined in Table 11.3, was performed to fits normalisation factors (NFs) for $t\bar{t}W$, $t\bar{t}Z$, VV and non-prompt leptons (HFe , $\text{HF}\mu$), shown in Figure 11.11b. Figure 11.11a shows the pulls and constraints on the nuisance parameters, while figure 11.12 shows the correlation matrix between the nuisance parameters and normalisation factors above a 20% threshold. The NFs for the non-prompt leptons backgrounds are compatible with those measured in the VLLe/μ analysis and slight difference is expected due to a looser b -tagging WP used in this analysis. Further, the NFs for $t\bar{t}Z$, $t\bar{t}W$ and VV are compatible with the VLLe/μ analysis as well. No significant pulls or constraints are seen in the NPs. Correlations between some two-point systematic NPs and respective NFs (for example, between the $t\bar{t}Z$ modelling NP and Norm $t\bar{t}Z$ and similarly for $t\bar{t}W$) are expected because of the acceptance effect of the NP. Post-fit distributions of the CRs are shown in Figures 11.13.

S. Epari, PhD Thesis



(a)

S. Epari, PhD Thesis



(b)

Figure 11.11: Fitted normalisation factors for a *CR-only* fit to data. The normalisation factors for the background components of HF_e and HF_μ as well as WZ (Heavy Flavor), ttZ and ttW are left free-floating.

S. Epari, PhD Thesis

Norm_VV_HF	100.0	-4.7	-6.8	-1.7	-44.6	-20.9	10.4	0.1	46.3	-0.7	0.2	-34.1	0.5	-1.9	30.4	0.2
Norm_fake_HF_el	-4.7	100.0	39.4	9.4	-2.5	-6.3	-26.8	-23.6	3.4	49.9	-44.5	1.5	0.2	-3.5	-0.1	-30.1
Norm_fake_HF_mu	-6.8	39.4	100.0	9.1	1.6	-2.7	2.5	0.1	1.2	76.9	0.2	3.7	0.1	-12.9	-1.3	0.0
μ (ttW)	-1.7	9.4	9.1	100.0	-5.6	18.3	0.9	0.2	3.6	29.6	-3.0	2.6	-38.0	66.0	3.0	0.3
Norm_ttZ	-44.6	-2.5	1.6	-5.6	100.0	22.6	9.1	-0.0	-2.0	-1.4	0.1	-32.0	-0.8	-0.0	-62.7	-0.0
ATLAS_FTAG_B0	-20.9	-6.3	-2.7	18.3	22.6	100.0	-0.2	0.0	-0.1	0.0	0.0	0.0	0.0	0.0	-0.4	-0.0
ATLAS_FTAG_C0	10.4	-26.8	2.5	0.9	9.1	-0.2	100.0	-0.0	-1.5	-0.1	0.0	0.4	0.3	0.1	-6.1	-0.0
ATLAS_FTAG_C5	0.1	-23.6	0.1	0.2	-0.0	0.0	-0.0	100.0	-0.0	0.0	-0.0	0.0	0.0	0.0	-0.0	-0.0
ATLAS_FTAG_L0	46.3	3.4	1.2	3.6	-2.0	-0.1	-1.5	-0.0	100.0	-0.0	0.0	0.2	0.2	0.0	-3.2	-0.0
ATLAS_TRIG_MU_SYST	-0.7	49.9	76.9	29.6	-1.4	0.0	-0.1	0.0	-0.0	100.0	0.0	0.0	0.0	0.0	-0.2	0.0
QMISID x-section	0.2	-44.5	0.2	-3.0	0.1	0.0	0.0	-0.0	0.0	0.0	100.0	0.0	-0.0	0.0	0.0	-0.0
WtZ x-section	-34.1	1.5	3.7	2.6	-32.0	0.0	0.4	0.0	0.2	0.0	0.0	100.0	-0.0	-0.0	0.9	0.0
ttWHF x-section	0.5	0.2	0.1	-38.0	-0.8	0.0	0.3	0.0	0.2	0.0	-0.0	-0.0	100.0	0.0	0.7	0.0
ttW modeling (generator) LF	-1.9	-3.5	-12.9	66.0	-0.0	0.0	0.1	0.0	0.0	0.0	0.0	-0.0	0.0	100.0	0.1	0.0
ttZ modeling (Shower)	30.4	-0.1	-1.3	3.0	-62.7	-0.4	-6.1	-0.0	-3.2	-0.2	0.0	0.9	0.7	0.1	100.0	-0.0
Stat error bin 0 HFe CR	0.2	-30.1	0.0	0.3	-0.0	-0.0	-0.0	-0.0	-0.0	0.0	-0.0	0.0	0.0	0.0	-0.0	100.0
	Norm_VV_HF	Norm_fake_HF_el	Norm_fake_HF_mu	μ (ttW)	Norm_ttZ	ATLAS_FTAG_B0	ATLAS_FTAG_C0	ATLAS_FTAG_C5	ATLAS_FTAG_L0	ATLAS_TRIG_MU_SYST	QMISID x-section	WtZ x-section	ttWHF x-section	ttW modeling (generator) LF	ttZ modeling (Shower)	Stat error bin 0 HFe CR

Figure 11.12: Correlation matrix for a *CR-only* fit to data. Only nuisance parameters and normalisation factors above a 20% threshold are shown.

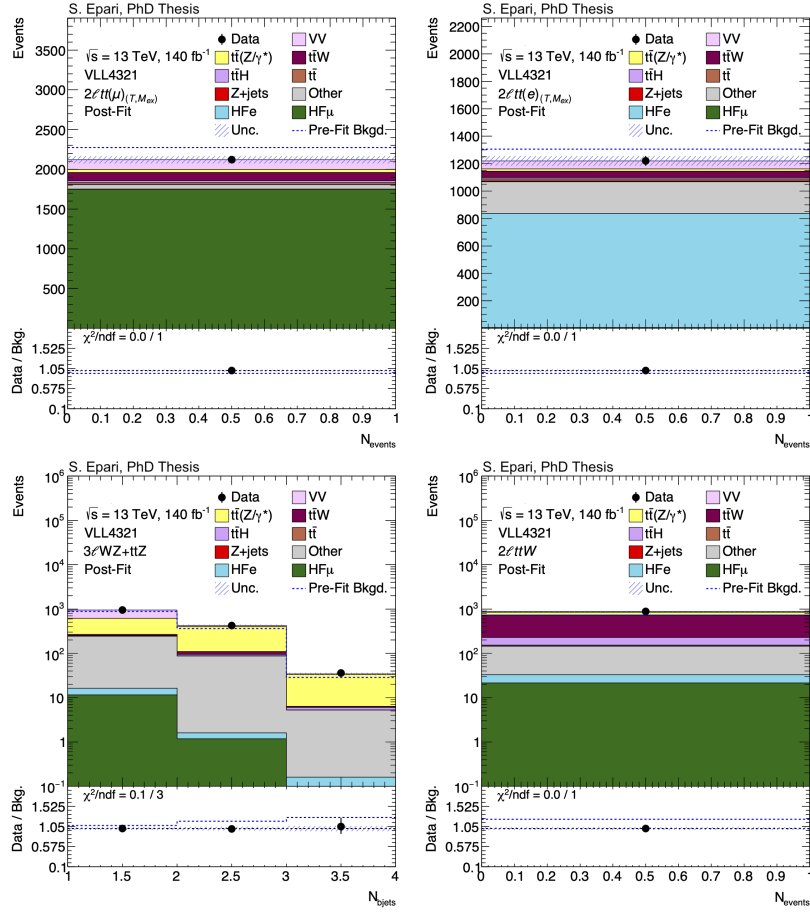


Figure 11.13: Post-fit comparison between data and the background prediction for the control region variables used in the template fit. The blue hashed band includes both statistical and systematic uncertainties.

11.7 Preliminary sensitivity from multilepton channels

Figure 11.14 shows the NN score distributions in the SRs defined in Table 11.1. The $t\bar{t}t\bar{t}$ background dominates at high NN scores in the $2\ell SS+0\tau_{\text{had}}$ SR. The $2\ell SS+\geq 1\tau_{\text{had}}$ and $2\ell OS+\geq 1\tau_{\text{had}}$ SRs are dominated by the fake τ_{had} background.

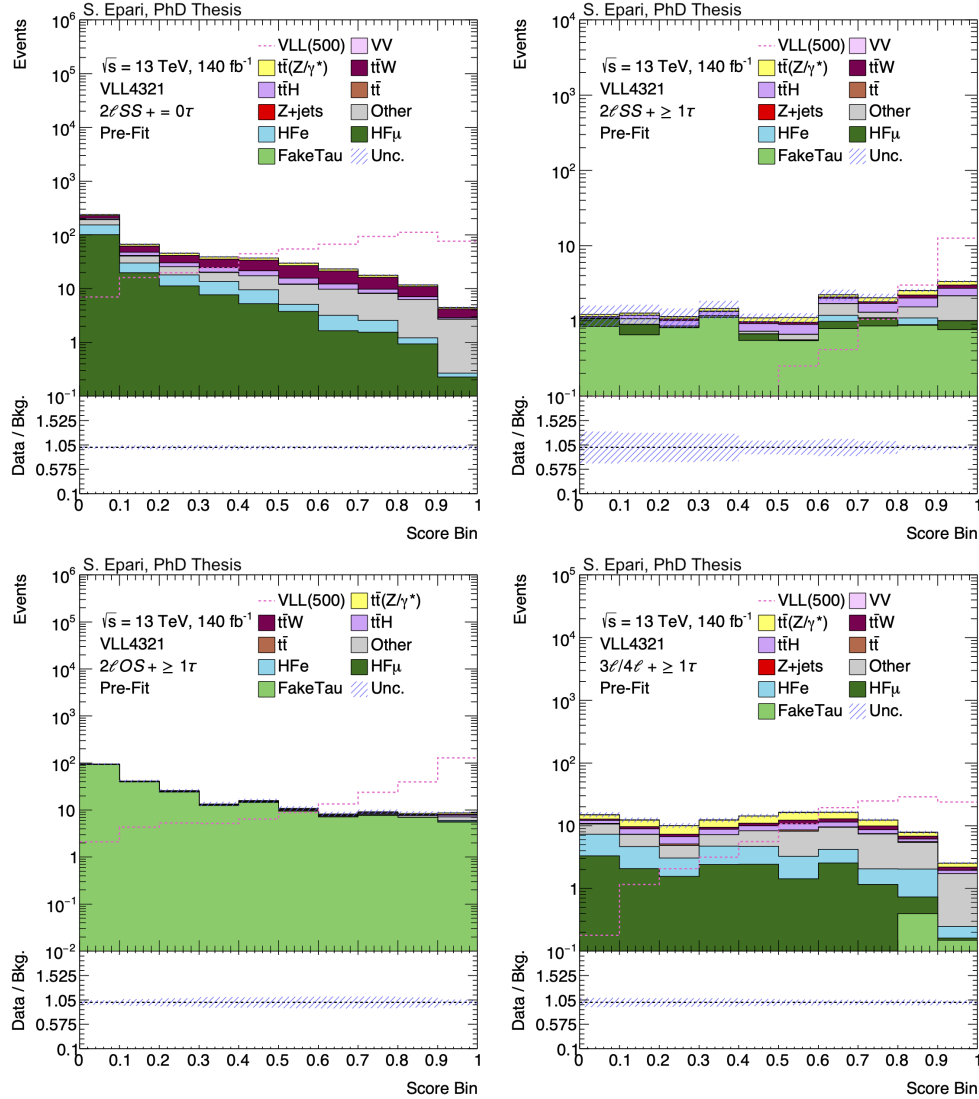
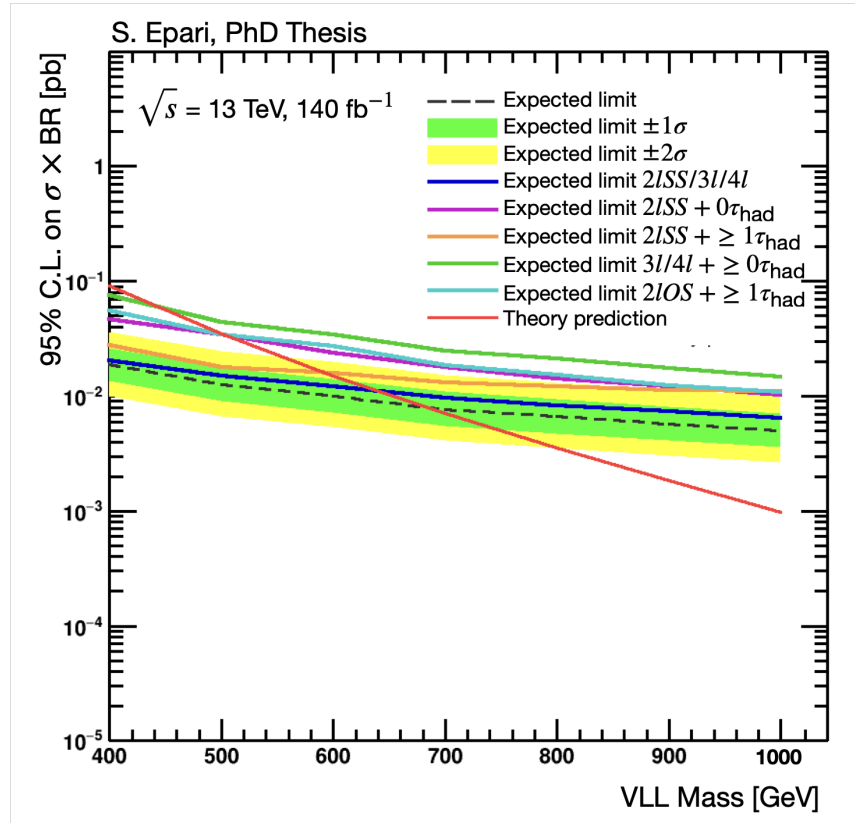


Figure 11.14: NN score distributions for the SRs defined in Table 11.1.

These distributions are used to estimate the 95% CL expected limits on the cross-section of the VLL as a function of the VLL mass considering a fully Asimov fit considering only statistical uncertainties and normalisation factors for the prompt $t\bar{t}Z$, $t\bar{t}W$ and VV and for heavy flavor electron and muon backgrounds. The result is shown in Fig-

ure 11.15. The combined exclusion is around 690 GeV, with maximum sensitivity from the $2\ell\text{SS}+\geq 1\tau_{\text{had}}$ SR at lower masses and competitive sensitivity from the $2\ell\text{SS}+\geq 1\tau_{\text{had}}$, $2\ell\text{SS}+0\tau_{\text{had}}$ and $2\ell\text{OS}+\geq 1\tau_{\text{had}}$ channels at higher masses. This analysis is statistically limited and little to slight degradation is expected from adding systematics to the model. The combined sensitivity at low masses is comparable to that from the CMS analysis (Figure 11.2).



(a)

Figure 11.15: Statistical-only 95% CL expected limits on the cross-section of the VLL as a function of the VLL mass for the ML regions.

11.8 Results from τ_{had} -only channels

Events in the τ_{had} -only channels were selected with at least τ_{had} candidate and at least three b -jets and no light leptons, to complement the effort from the CMS search. To enhance signal acceptance in the phase space, events are selected using a *trigger bucket* strategy, combining acceptances from the missing transverse energy (MET) trigger, single τ_{had} trigger

(STT), di- τ_{had} trigger (DTT) and the b -jet (BJET) trigger in sequential order. Five SRs, depending on the combination of triggers used, number of τ_{had} and b -jets were defined to maximise sensitivity. The selections used to define the SRs is shown in Table 11.5. Dedicated mass parameterised NNs were trained to optimally reject background in each of the SRs.

Signal region	$1\tau 3b$ MST	$1\tau \geq 4b$ MST	$1\tau 3b$ BT	$1\tau \geq 4b$ BT	$\geq 2\tau \geq 3b$		
Trigger bucket	MET $\cup$ STT		BJET		MET	STT	DTT
Number of τ_{had}	1				≥ 2	2 (OS)	≥ 3
τ_{had} ID	Tight				≥ 1 Loose	≥ 1 Medium	≥ 2 Medium
Number of b -tags @77%	3	≥ 4	3	≥ 4		≥ 3	
Number of jets	≥ 4					≥ 3	
NN score category	1τ MST		1τ BT			$\geq 2\tau$	

Table 11.5: Summary of the selection cuts for each of the five SRs. The last row refers to the NN score distributions obtained from the event categories considered for the signal optimization using the neural networks. Table taken from Ref [236].

Major prompt backgrounds in this phase space include $t\bar{t}$ and $Z + \text{jets}$, corrected using the procedure described in Chapter 10. Additionally, the QCD multi-jet background was estimated using a data-driven method. Comparison of data and background Monte Carlo for each of the 5 SRs is shown in Figure 11.16. In general, good agreement between the data and predicted background yields is seen across all SRs.

95% CL upper limits are set on the cross section for the VLL pair production as a function of the assumed m_{VLL} . Figures 11.17 shows the 95% CL upper limits on the VLL pair production cross section as a function of m_{VLL} . The observed and expected 95% CL lower limits on m_{VLL} are 910 GeV and 970 GeV, respectively. This first ATLAS result for VLL search in the final states with the third generation of SM fermions from VLL decays through U_1 rules out the 2.8σ excess reported by the CMS collaboration [235]. The search sensitivity is driven by the $\geq 2\tau \geq 3b$ channel in the targeted mass range. At high mass ($m_{\text{VLL}} > 700$ GeV), the 1τ MST channels also reinforce the sensitivity further.

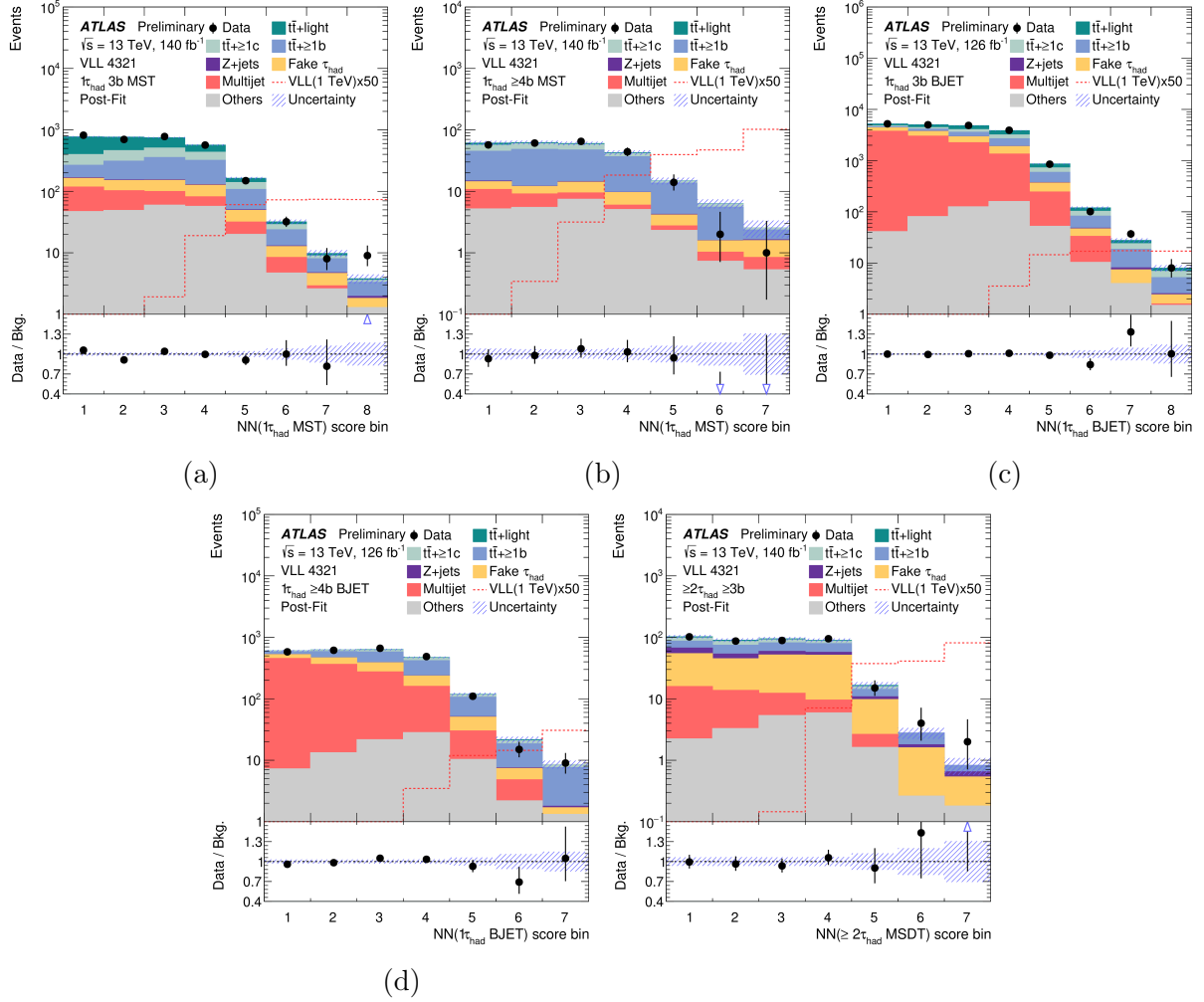


Figure 11.16: Comparison between data and the background prediction in the τ_{had} -only SRs categories. The blue hatched band shows the combined size of the statistical and systematic uncertainty. Figures taken from Ref [236].

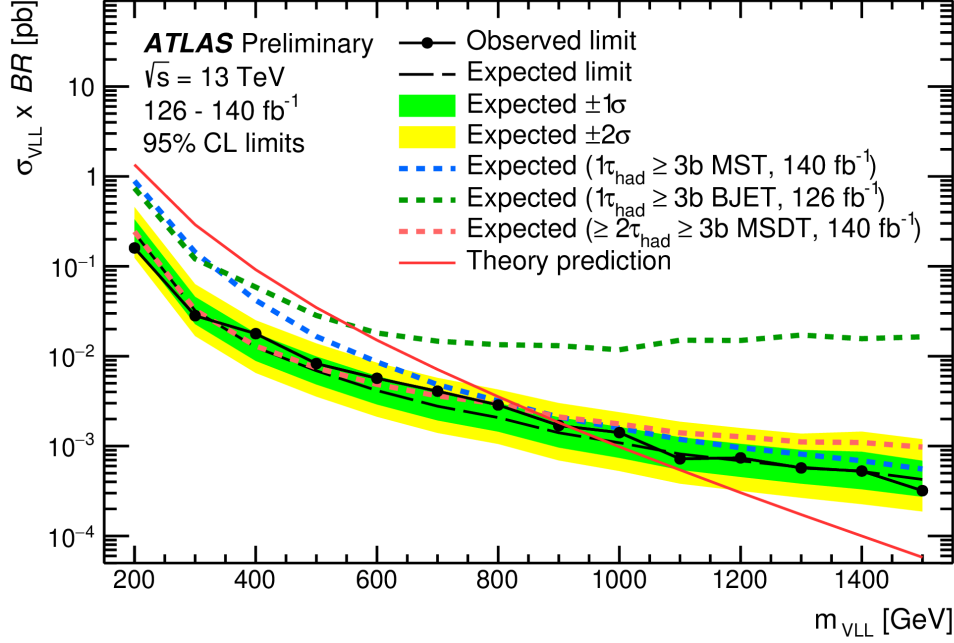


Figure 11.17: 95% CL expected limits on the cross-section of the VLL as a function of the VLL mass for a combination of all 0ℓ signal and control regions. Figure taken from Ref [236].

11.9 Conclusions

This chapter presented the preliminary studies conducted for the search for vector-like leptons preferentially coupling to third generation SM fermions. VLLs from the 4321 model couple to a third generation SM quark by exchanging U_1 , producing final states with multiple τ , b -jets and missing transverse energy. The 4321 model can accommodate anomalies in B -meson decays and $(g - 2)_\mu$. A search for VLLs from the 4321 model was performed by the CMS collaboration using the 96.5 fb^{-1} dataset collected in 2017 and 2018, and a broad 2.8σ local deviation in final states with multiple τ_{had} candidates, while excluding VLLs up to 500 GeV (650 GeV expected). This ATLAS search for VLLs from the 4321 model in the τ_{had} -only channel disfavors the 2.8σ excess reported by the CMS collaboration. Preliminary sensitivity to the model is estimated from the light lepton channels and is competitive with the ATLAS τ_{had} -only channels and the CMS search at low VLL masses. Despite the lack of an excess compatible with the model, these channels are interesting in their own right by being the one of the first analyses to search for new physics in multilepton final states with at least 3 b -tags and high missing transverse energy. The results from these channels

will be finalised and combined with those from the τ_{had} -only channels in the final ATLAS publication. In particular, the strategy of using the sum of pseudo-continuous PLIV as an input to the signal-versus-background neural networks was developed within the context of this search. This approach ensures optimal separation of fake light leptons from the signal without the need to exclude these from the phase space, which may have a non-negligible impact on signal acceptance in the region.

Conclusions and outlook

*Let me tell you a secret.
There is no perfect cookie.*

The Standard Model (SM) of particle physics is, to-date, the most well-known, consistent and well-tested framework for describing matter at its smallest scales. Despite the SM's success in explaining observed phenomena, there remain numerous unresolved questions in particle physics, including the nature of dark matter, the hierarchy problem, and the matter-antimatter asymmetry in the universe, to name a few. Since the energy scale at which new physics might emerge is unknown, the LHC's strategy is to cast a wide net, searching across a diverse set of final states and models.

The work presented in this dissertation covers three diverse but related aspects of the ATLAS experiment at CERN. The central idea of this thesis is structured around searches for new phenomena in final states with two, three or four or more leptons, termed *multilepton final states*. These signatures are particularly promising in searches for Beyond Standard Model (BSM) physics for several reasons. Firstly, they are a feature in decays of particles from many distinct BSM models, such as those predicting new heavy resonances, supersymmetry (SUSY), or models involving extended Higgs sectors, making searches in these states highly versatile. Secondly, multilepton signatures typically have background contributions from SM processes that are well-understood or easily corrected compared to other final states, allowing for enhanced sensitivity to potential new physics. Moreover, these channels often benefit from reduced systematic uncertainties due to their well-understood background composition and lepton identification efficiencies. Consequently, most searches in multilepton final states are statistically dominated and will scale effectively with the

increased integrated luminosity expected in future LHC runs.

Three distinct BSM models, motivated by current experimental tensions, are presented in this dissertation. These searches use data from proton-proton collisions at a center-of-mass energy of $\sqrt{s} = 13$ TeV recorded by the ATLAS detector at the Large Hadron Collider during Run 2 and explore final states involving multiple light leptons, taus, jets, and missing transverse energy (E_T^{miss}), and provide a broad overview of potential new physics scenarios accessible with multilepton searches at the LHC.

The g2HDM search

The first-ever LHC search for a flavorful general two Higgs doublet model (g2HDM) is presented in this dissertation. This model is an extension of the SM with an additional complex Higgs doublet, giving rise to five Higgs bosons: two CP-even scalar fields, one CP-odd pseudo-scalar and two charged Higgs. In the alignment limit, the target model allows FCNCs in the heavy Higgs sector while respecting the SM-like nature of the $h(125)$ particle discovered at the LHC. This model is phenomenologically interesting since it can explain the generation of the baryon asymmetry in the universe.

The g2HDM model considered in this search has four degrees of freedom: the mass of the heavy neutral Higgs m_H and ρ_{tq} (the coupling between the top and up/charm or another top quark). The various g2HDM signals explored lead to final states with same-sign $t\bar{t}$, $t\bar{t}q$, $t\bar{t}tq$, three top and four top quarks, leading to final states with two same-sign, three or four light leptons and multiple b -jets. Deep neural networks are trained to create signal regions targeting these different decay modes since this approach has the potential to allow sensitivity to other BSM models with similar final states. Finally, dedicated DNNs are then trained in each signal region to optimally reject SM backgrounds. The major backgrounds expected in the analyses are from non-prompt leptons from semi-leptonic b -decays from $t\bar{t}$ and prompt $t\bar{t}W$. The former are suppressed with requirements on BDT-based lepton isolation referred to as PLIV. Signal processes initiated by uu or ug interactions are more charge-asymmetric than the $t\bar{t}W$ background. Therefore, categorizing signal regions (SRs) by the total charge of light leptons provides additional separation between the $t\bar{t}W$ background and the signal processes.

A maximum-likelihood fit is performed across categories in order to test for a possible signal and constrain the leading backgrounds simultaneously. A broad excess was observed in the 4-dimensional parameter space of allowed masses and couplings, with the largest local significance being 2.8 standard deviations, for a signal with $m_H = 900$ GeV and $\rho_{tt}=0.32$,

$\rho_{tc}=0.05$ and $\rho_{tu}=0.85$. The largest pre-fit tension between data and the background yields was observed in the sstt, ttq and tttq SRs. The normalisation factor of $t\bar{t}W$ was measured higher than unity, compatible with dedicated measurements of the SM $t\bar{t}W$ cross-section. This search was also used to set limits on RPV SUSY models motivated by flavour and $(g-2)_\mu$ anomalies, featuring multiple light leptons and b -jets in the final state, using the existing DNNs that were trained for the g2HDM model.

This search is dominated by statistical uncertainties and is expected to have a more sophisticated follow-up by adding in data collected in Run 3. Improvements in the signal acceptance are expected from relaxing light lepton selections in the signal regions, like PLIV. This can significantly increasing the signal yield, at the cost of a dramatic increase of background, particularly from non-prompt leptons. This increase can be compensated for by a more advanced neural network to reject this background by taking PLIV as an input training variable (as done in the VLL4321 search Chapter 11), rather than as a per-lepton selection criterion. Further improvements are expected using a dedicated neural network training for each mass hypothesis, to be sensitive to the heavy Higgs boson mass.

The VLL $e\mu$ search

This is the first direct LHC search for pair-produced vector-like electrons and muons, collectively termed vector-like light leptons (VLLs). Compared to the broad LHC search program for vector-like quarks, VLL searches are only recently gaining interest and are challenging because VLLs are expected to be produced via the electroweak interaction and thus, have much lower production cross-sections. Models containing these particles might explain the observed tensions between the measured and predicted values of the anomalous moment of the muon and the electron, and the *Cabibbo angle anomaly*. Simplified models of VLL e and VLL μ , from either an $SU(2)$ doublet or an $SU(2)$ singlet are considered in this search. Depending on the $SU(2)$ representation, VLLs decay to a SM lepton and a $h/W/Z$ boson.

The search is structured in channels with two opposite-sign (2ℓ OS), three (3ℓ) or four (4ℓ) light leptons. Channels with at least two opposite-sign electrons are used to target VLL e while those with at least two opposite-sign muons are used to target VLL μ . Signal regions targeting distinct signal topologies are defined in the 2ℓ OS and 3ℓ lepton channels depending on the number of hadronically or leptonically decaying $h/W/Z$ and leptons using dedicated *signal-vs-signal-vs-background* categorisation deep neural networks. The advantage of defining the above topologies is to design signal regions sensitive to not only

the VLL models, but also any similar non-VLL like topology that falls into one of the above categories. In the absence of an overall excess in the search, this categorisation is valuable to possibly pin-point the features of a different BSM signal by looking at the topologies which show the most disagreement with data, as input to future studies. A single neural network is used to target both singlet and doublet signatures by using E_T^{miss} as an input variable to the neural network. A simple cut-and-count search is done in the 4ℓ channel where distinct signal topologies cannot be defined. Sophisticated corrections are developed for improving the simulation of major backgrounds expected in the $2\ell\text{OS}$ channel, namely $t\bar{t}$ and Z +jets. Further, the normalisation of these backgrounds, separately in signal regions with unique admixtures of light and heavy flavor jets from these processes, is estimated in the statistical fit to data. The normalisation of $t\bar{t}Z$ and $t\bar{t}W$ backgrounds are measured higher than unity, compatible with the measurement from other analyses in a similar phase space, and all other normalisation factors are measured compatible with unity. No significant excess is observed over the SM expectation value after the likelihood fit to data in any of the SRs, for any of the models under study. The VLL_e singlet is observed (expected) to be excluded at 95% confidence level for masses up to 320 (300) GeV while the VLL_e doublet is observed (expected) to be excluded at 95% confidence level for masses up to 1220 (1230) GeV. The VLL_μ singlet is observed (expected) to be excluded at 95% confidence level for masses up to 400 (330) GeV while the VLL_μ doublet is observed (expected) to be excluded at 95% confidence level for masses up to 1270 (1250) GeV. This search is dominated by statistical uncertainties.

In the doublet models, the 3ℓ channel is most sensitive to the VLL signal, with the $2\ell\text{OS}$ channel providing better sensitivity for VLLs with masses greater than 1 TeV. The increased luminosity and higher center-of-mass energy in Run 3 will further enhance the sensitivity, particularly at higher VLL masses. For the singlet models, the main sensitivity at low masses comes from 4ℓ channel and from the $2\ell\text{OS}$ channel at high masses. While this search will also benefit from Run 3 data, additional optimizations are necessary to improve the sensitivity of this search, due to the significantly lower cross-sections of this model. In particular, sophisticated multi-variate techniques are being developed to reject background efficiently at VLL masses, while loosening event selections to improve signal acceptance.

The VLL4321 search

The third search presented in this dissertation aims to search for pair-produced VLLs from a ‘4321’ model, preferentially coupling to third generation SM fermions. The ‘4321’ model

is a UV-complete model built from the larger gauge group $SU(4) \times SU(3) \times SU(2) \times U(1)$, and introduces a host of BSM gauge bosons, VLQs and VLLs. It can accommodate current experimental anomalies in low energy fermionic processes like B -meson decays, while remaining consistent with electroweak precision measurements. A search for VLLs from the 4321 model was performed by the CMS collaboration using the 96.5 fb^{-1} dataset collected in 2017 and 2018, and a 2.8σ local deviation between fit to the signal+background model as compared to background-only model, almost irrespective of the VLL mass was reported, in final states with ≥ 3 b -jets, split according to the multiplicity of τ_{had} . This ATLAS search for VLLs from the 4321 model in similar τ_{had} -only channels disfavors the 2.8σ excess reported by the CMS collaboration.

The work presented in this dissertation estimates preliminary sensitivity to the model from the light lepton channels not explored in either the ATLAS or CMS search. Events are separated into channels with two same-sign ($2\ell\text{SS}$), opposite-sign ($2\ell\text{OS}$) and $3\ell/4\ell$ leptons with various τ_{had} multiplicities. In contrast to the g2HDM and VLL e/μ analyses, PLIV cuts on light leptons are dropped in this search to increase signal acceptance. Instead, powerful fake light lepton rejection is provided by constructing a new variable called the *sum of pseudo-continuous PLIV (sumPLIV)*, constructed using the PLIV working point (WP) passed by each light lepton in the event. This approach ensures optimal separation of fake light leptons from the signal without the need to exclude these from the phase space, which may have a non-negligible impact on signal acceptance in the region. Dedicated mass-parameterised deep neural network (DNN) classifiers are trained against the total background, separately for the sum of the two same-sign and three or more light lepton channels and the channel with two opposite-sign leptons, ensures optimal background discrimination in all channels. The $t\bar{t}t\bar{t}$ background dominates at high NN scores in the $2\ell\text{SS}+0\tau_{\text{had}}$ SR. The $2\ell\text{SS}+\geq 1\tau_{\text{had}}$ and $2\ell\text{OS}+\geq 1\tau_{\text{had}}$ SRs are dominated by the fake τ_{had} background.

The preliminary sensitivity to the model is estimated from these light lepton channels is competitive with the ATLAS τ_{had} -only channels and the CMS search at low VLL masses. The combined exclusion is around 690 GeV, with maximum sensitivity from the $2\ell\text{SS}+\geq 1\tau_{\text{had}}$ at lower masses and competitive sensitivity from the $2\ell\text{SS}+\geq 1\tau_{\text{had}}$, $2\ell\text{SS}+0\tau_{\text{had}}$ and $2\ell\text{OS}+\geq 1\tau_{\text{had}}$ channels at higher masses. This search is statistically limited and little to slight degradation is expected from adding systematics to the model. Despite the lack of an excess compatible with the model, these channels are interesting in their own right by being the one of the first analyses to search for new physics in multilepton final states

with at least 3 b -tags and high missing transverse energy. The results from these channels will be finalised and combined with those from the τ_{had} -only channels in the final ATLAS publication.

Studies with TileCal MinBias data

The work on searching for BSM physics is complemented by the other two topics covered in this dissertation, on studying the TileCal light yield degradation with the data obtained by the integrator read-out of the ATLAS TileCal during Run 2 and deriving TileCal-related uncertainties for the ATLAS luminosity measurement in Run 3.

The former study is the first Run 2 study providing valuable feedback to the TileCal Phase-II upgrade plans, such as the replacement of the E-cells during the Long Shutdown 2, before the start of Run 3. The results from this study are also essential for re-processing physics data and affect the determination of jet and missing transverse energy related uncertainties. Compared to previous studies on the subject, for the first time, the track-counting luminosity was used as a reference to have a stable measurement over a large period of time. The study estimated the effect of damage and ageing of the scintillators and wavelength shifting fibres in TileCal cells to be between 10% to 30% depending on the location of the cell from the interaction point.

The latter measurement affects counting of the measured number of events of a certain theoretical process, is used by every ATLAS measurement using the dataset and is a limiting factor in precision analyses measuring physics cross-sections. The work done on this subject emphasizes the role of TileCal in the ATLAS luminosity measurement in the 2022 and 2023 data-taking periods in Run 3. The overall uncertainty in the luminosity determination in 2022 was estimated to be 2.19% (1.91% from TileCal) and in 2023 was estimated to be 2.04% (1.2% from TileCal).

Appendix A

Discriminating variables used in the g2HDM search

The discriminating variables used as input to the signal-versus-signal and signal-versus-background categorisation neural networks (NN) in the g2HDM search presented in Chapter 9 are shown in Figures A.1-A.7. In each figure, the total SM background is shown in grey and signal processes from the benchmark set of couplings, i.e. $\rho_{tt} = 0.4$ and $\rho_{tq} = 0.20$ with $m_H = 400$ GeV, are shown in different colours. In each category, only most relevant signals are shown, normalised to a cross-section of 12 fb^{-1} . The definitions of the discriminating variables is summarised in Table 9.1. The following variables, used for training the signal-versus-signal NNs, are shown:

- Sum of p_T of the jets ($H_{T,\text{jets}}$)
- Sum of p_T of the leptons ($H_{T,\text{lep}}$)
- Number of jets (N_{jets})
- Sum of pseudo-continuous b-tagging scores of jets (sumPCB)
- Pseudo-continuous b-tagging score of 1st, 2nd, 3rd leading jet in p_T ($N_{\text{b-jets}}$)
- Angular distance of leptons, $dR(l, l)$
- Missing transverse energy (E_T^{miss})

The following variables, used for training the signal-versus-background NNs in addition to the ones mentioned above, are shown:

- Leading p_T of jet
- Invariant mass of leading lepton and missing transverse energy ($MT(\text{lep}, E_T^{\text{miss}})$)

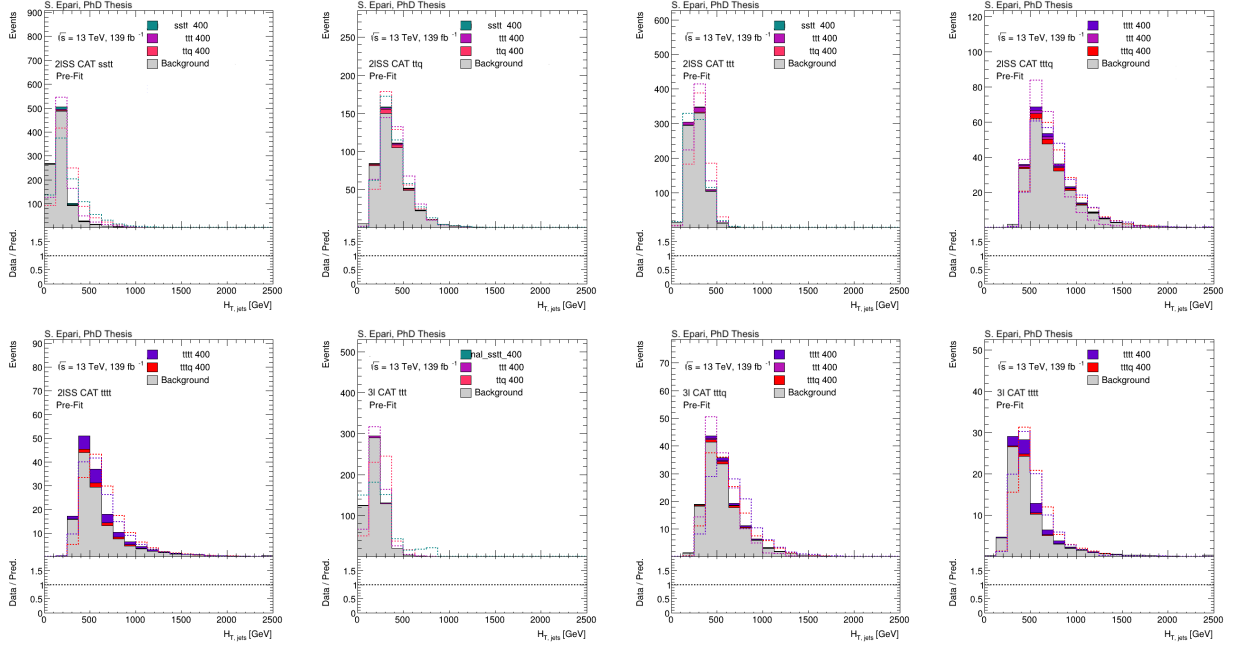


Figure A.1: Sum of p_T of jets for 2 ℓ SS categories sstt, ttq, ttt, ttq and tttt (top) and for 3 ℓ categories ttt, ttq and tttt (bottom).

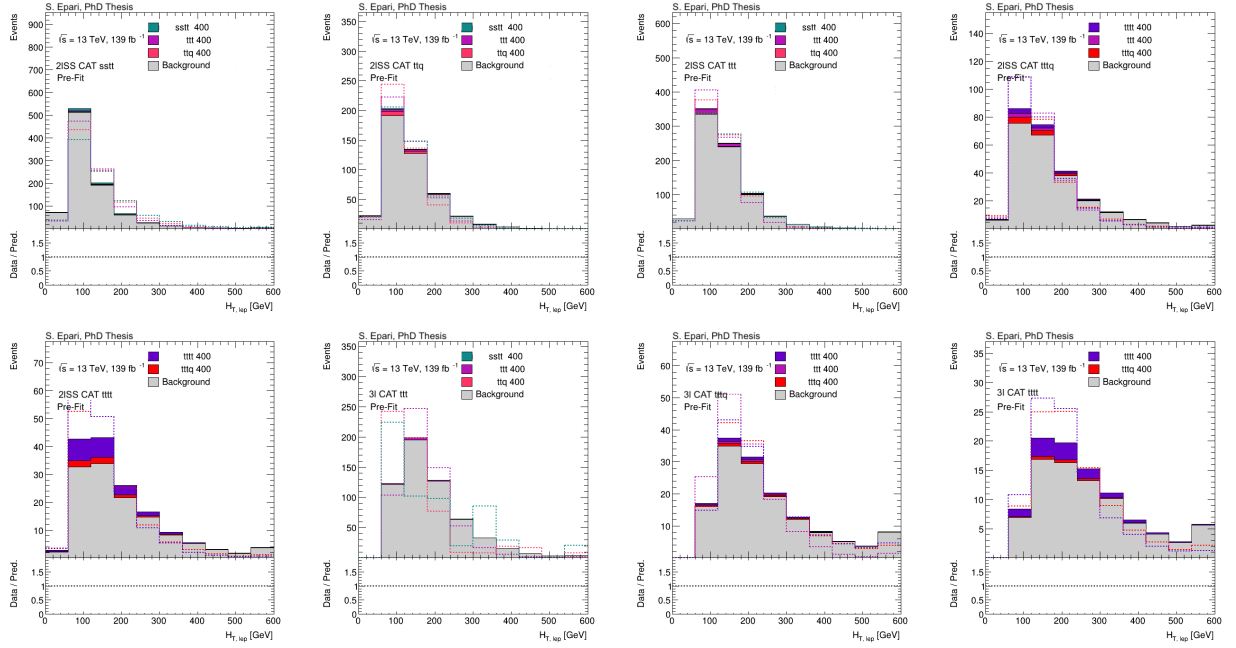


Figure A.2: Sum of p_T of leptons for 2ℓSS categories sstt, ttq, ttt, tttq and tttt (top) and for 3ℓ categories ttt, tttq and tttt (bottom).

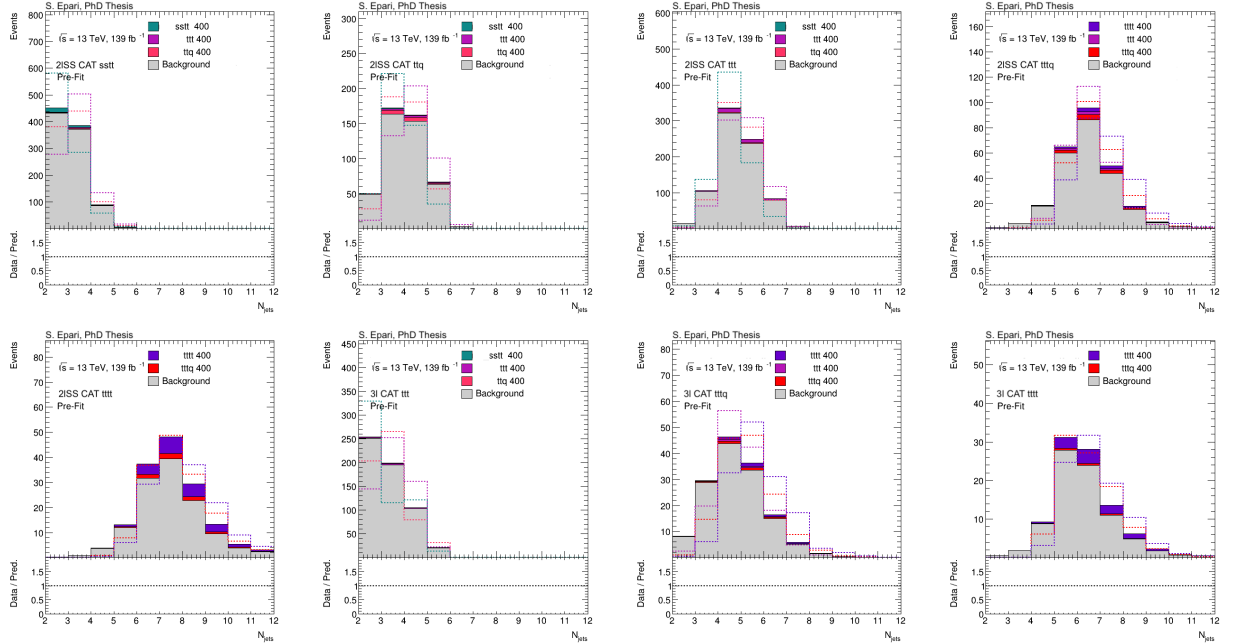


Figure A.3: Number of jets for 2ℓSS categories sstt, ttq, ttt, tttq and tttt (top), for 3ℓ categories ttt, tttq and tttt (bottom).

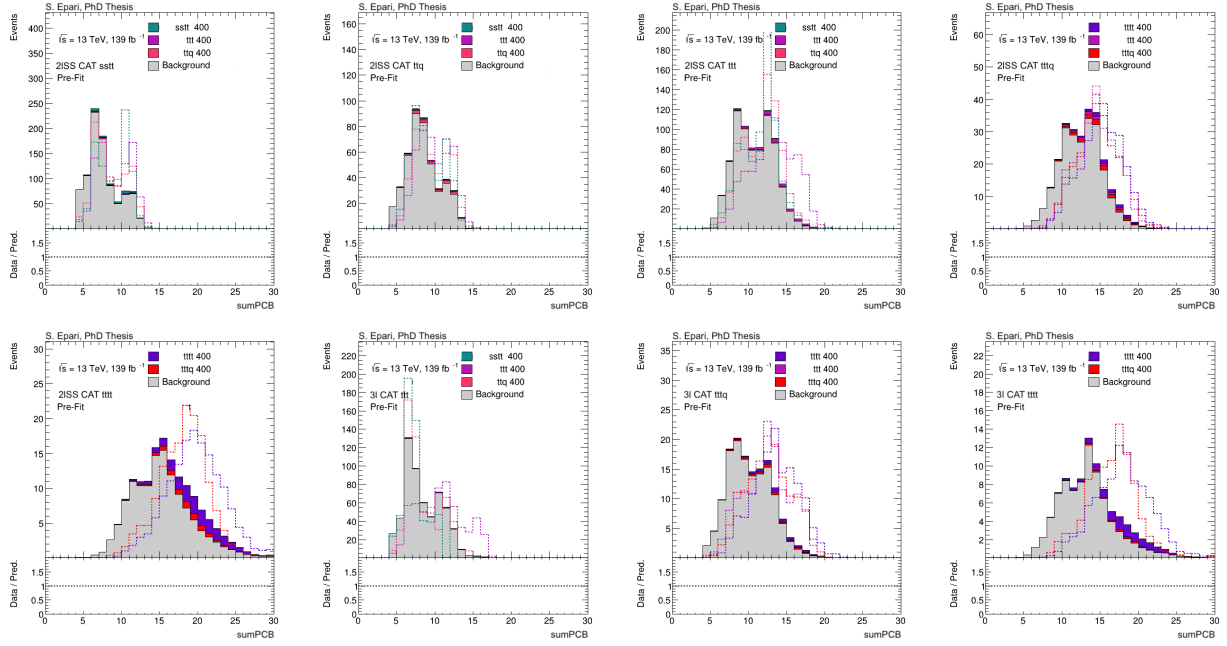


Figure A.4: Pseudo-continuous b-tagging scores for 2ℓSS categories sstt, ttq, ttt, ttq and tttt (top), for 3ℓ categories ttt, ttq and tttt (bottom).

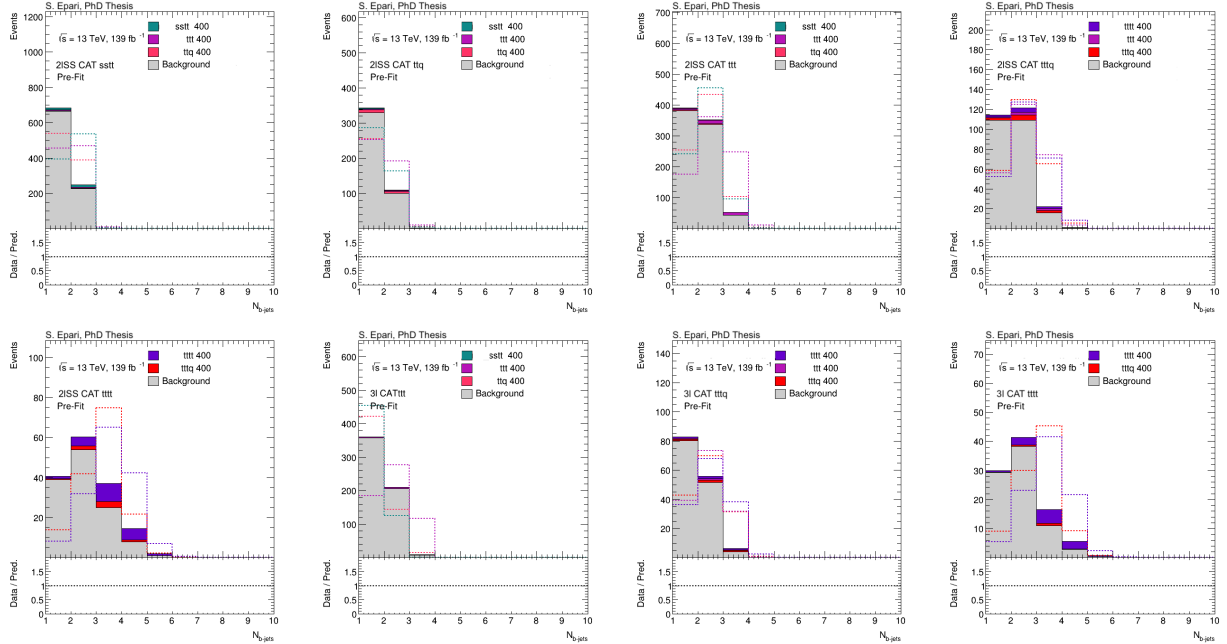


Figure A.5: Number of central b -jets (77% WP) for 2ℓSS categories sstt, ttq, ttt, ttq and tttt (top), for 3ℓ categories ttt, ttq and tttt (bottom).

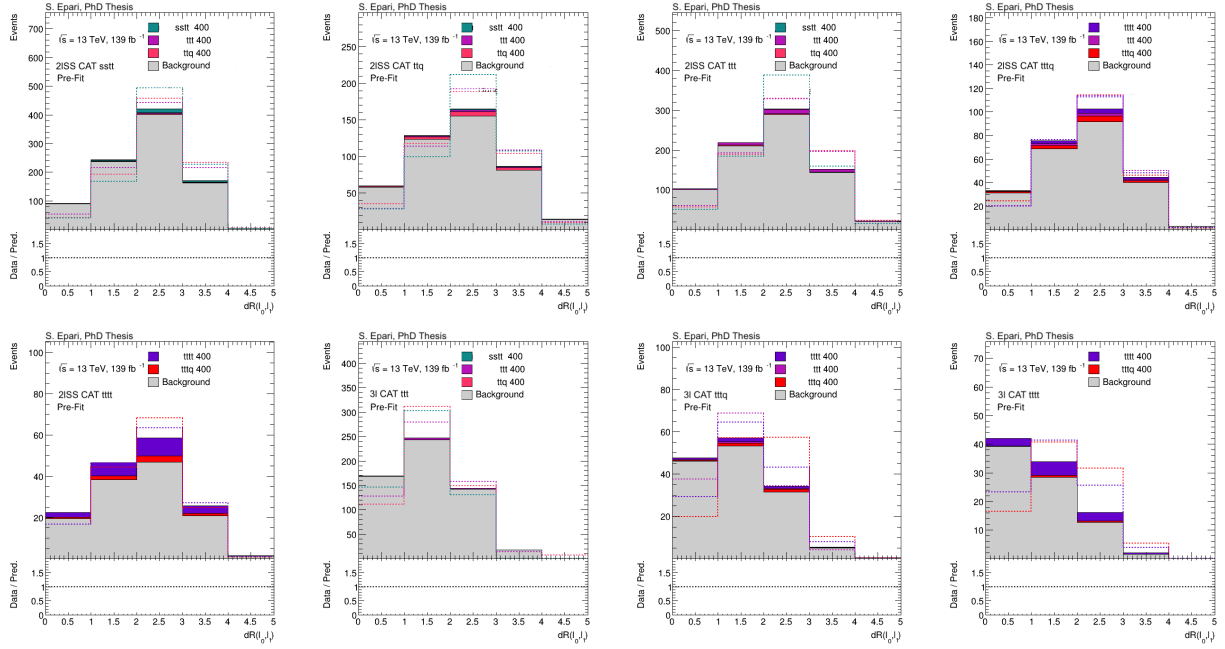


Figure A.6: Angular distance between first and second lepton for 2ℓ SS categories sstt, ttq, ttt, ttq and tttt (top), for 3ℓ categories ttt, ttq and tttt (bottom).

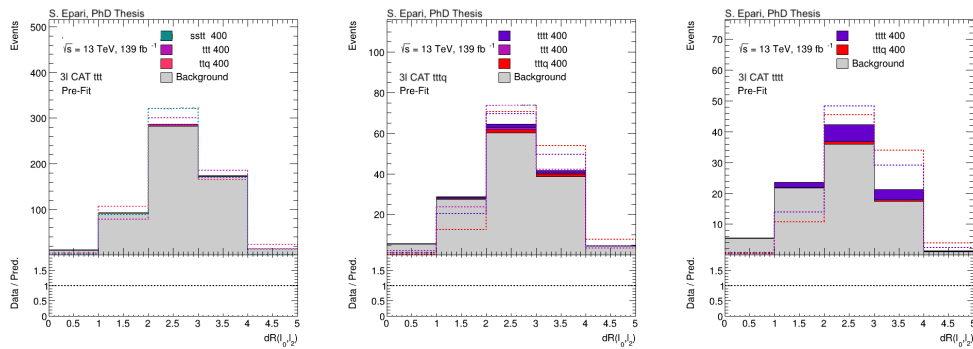


Figure A.7: Angular distance between leading and the third lepton for 3ℓ categories ttt, ttq and tttt.

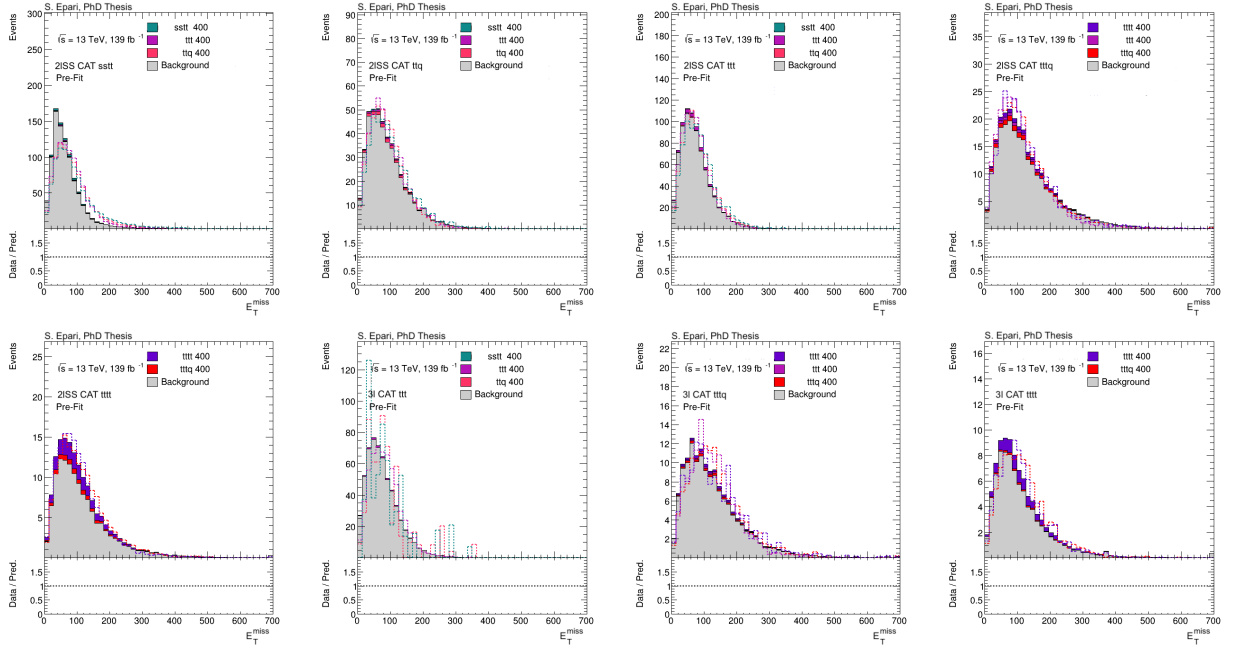


Figure A.8: Missing transverse energy for 2ℓSS categories sstt, ttq, ttt, ttq and tttt (top), for 3ℓ categories ttt, ttq and tttt (bottom).

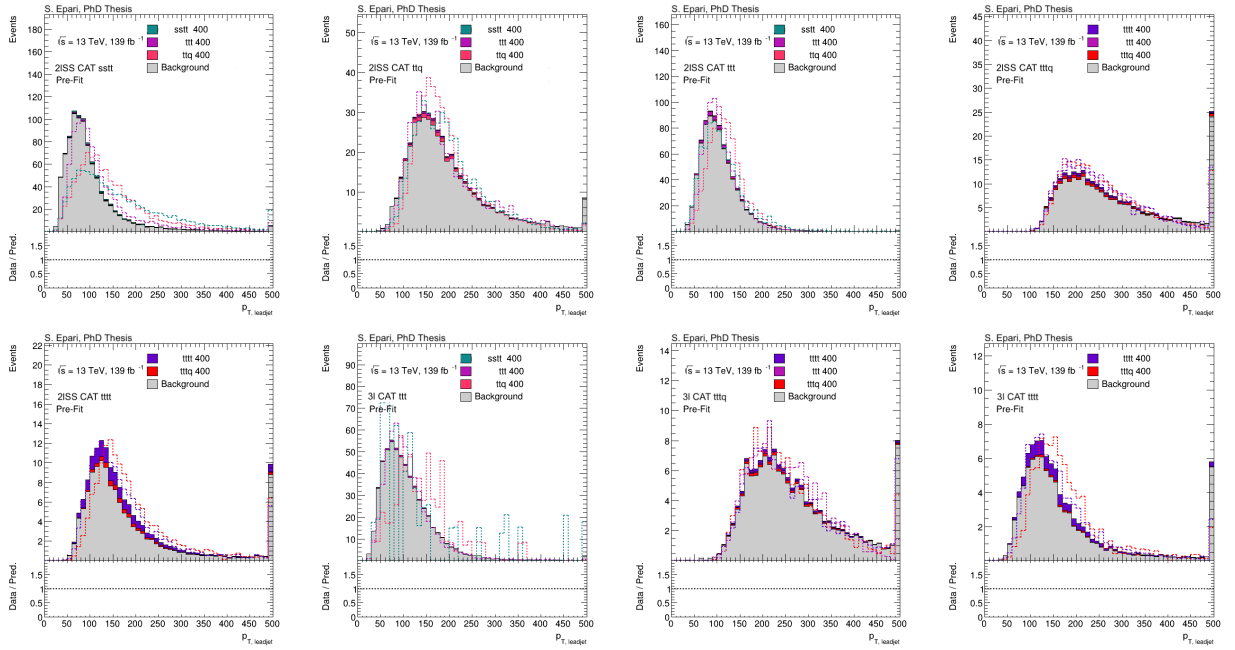


Figure A.9: p_T of the leading jet for 2ℓSS categories sstt, ttq, ttt, ttq and tttt (top), for 3ℓ categories ttt, ttq and tttt (bottom).

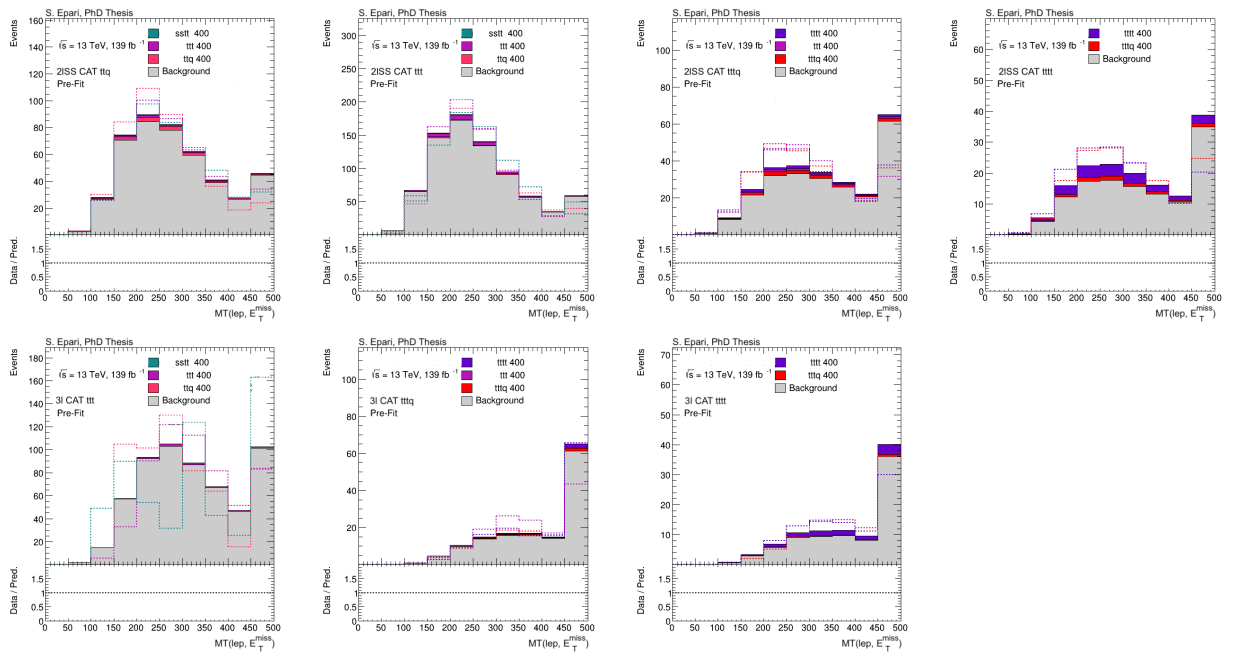


Figure A.10: Invariant mass of leading lepton and missing transverse energy for $2\ell\text{SS}$ categories ttq , tt̄t , tt̄t̄ and tt̄t̄t̄ (top), for 3ℓ categories tt̄t , tt̄t̄q and tt̄t̄t̄t̄ (bottom).

Appendix B

Discriminating variables used in the multilepton channels of the VLL4321 search

The discriminating variables used as input to the signal-versus-background categorisation neural networks (NN) in the VLL4321 search presented in Chapter 11 are shown in this Appendix. Figure B.1 shows the variables used to train the NN for the combined $2\ell SS/3\ell/4\ell+ \geq 0\tau_{\text{had}}$ channel, against signal from a VLL of mass 500 GeV. Similarly, Figure B.2 shows the variables used to train the NN for the $2\ell OS+\geq 1\tau_{\text{had}}$ channel, against signal from a VLL of mass 500 GeV. The definitions of the discriminating variables is summarised in Table 11.2. The following variables, used for training the $2\ell SS/3\ell/4\ell$ NN, are shown:

- Number of jets (N_{jets})
- Number of hadronic tau candidates (N_{τ})
- Type of di-leptonic event (ee , $e\mu$ or $\mu\mu$)
- Type of tri-leptonic event (eee , $ee\mu$, $e\mu\mu$ or $\mu\mu\mu$)
- Total number of light leptons
- Total charge of all leptons (including hadronic taus) (sumQ)
- p_T sum of all light leptons ($H_{T,\text{lep}}$)
- p_T sum of all jets ($H_{T,\text{jets}}$)
- p_T sum of all hadronically decaying taus ($H_{T,\text{tau}}$)

- Missing transverse energy (E_T^{miss})
- Sum of pseudo-continuous b-tagging scores of jets (sumPCB)
- Sum of pseudo-continuous tau tagging WPs (sumPCT)
- Sum of pseudo-continuous PLIV WPs (sumPLIV)

For training the $2\ell\text{OS}+\geq 1\tau_{\text{had}}$ DNN, N_τ , the variable identifying the type of tri-leptonic event, the variable counting the total number of light leptons and sumPLIV are dropped and the following variables are introduced in addition:

- Invariant mass of two closest b -jets in ΔR (m_{bb})
- Average ΔR between two b -jets ($\Delta R_{bb}^{\text{avg}}$)
- Minimum of invariant mass of light-lepton and τ_{had} pairs ($m_{\ell\tau}^{\text{min}}$)

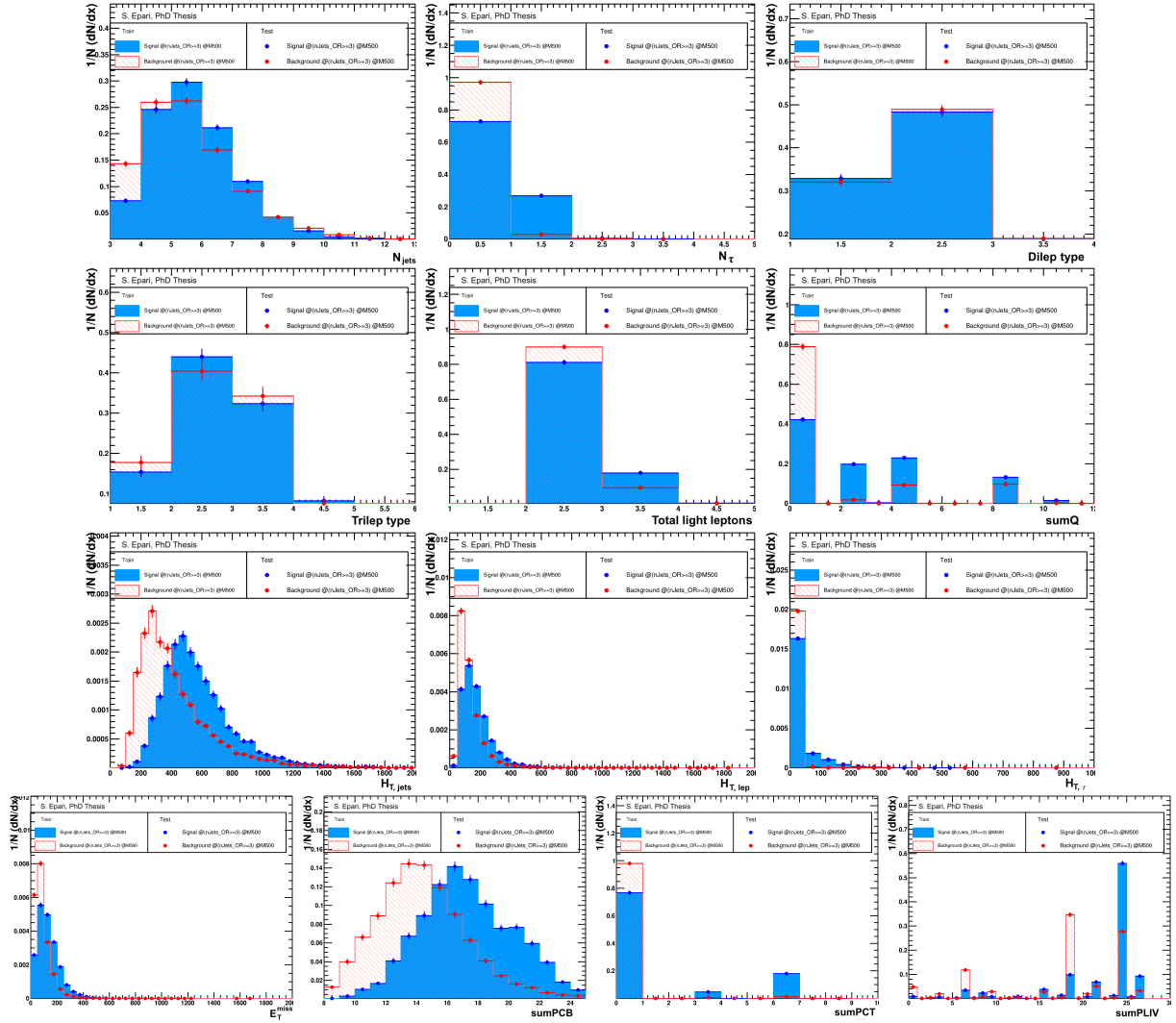


Figure B.1: Signal and background distributions of training variables for the $2\ell SS/3\ell/4\ell + \geq 0\tau_{\text{had}}$ channels against signal from a VLL of mass 500 GeV.

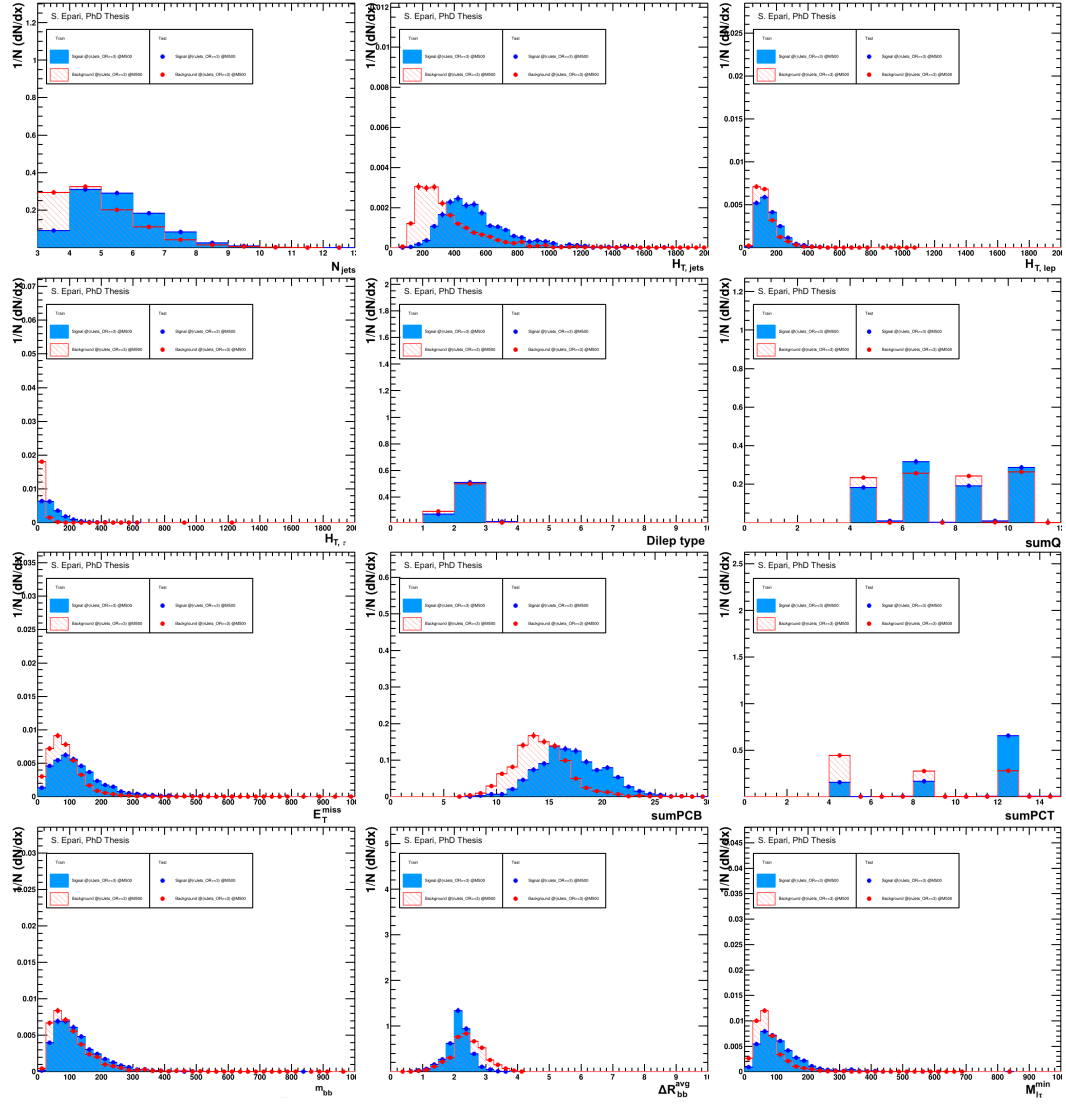


Figure B.2: Signal and background distributions of training variables in $2\ell\text{OS} + \geq 1\tau_{\text{had}}$ channel against signal from a VLL of mass 500 GeV.

Bibliography

- [1] J. J. Thomson, *Cathode Rays*, [Philosophical Magazine Series 44](#) (1897) 293–316.
- [2] P. Dirac, *The Principles of Quantum Mechanics*. Clarendon Press, Oxford, 1930.
- [3] M. Gell-Mann, *Isotopic Spin and New Unstable Particles*, [Phys. Rev. Lett. 12](#) (1964) 627–629.
- [4] G. Zweig, *An SU_3 model for strong interaction symmetry and its breaking*, 1964.
<http://cds.cern.ch/record/570209>.
- [5] F. Englert and R. Brout, *Broken Symmetry and the Mass of Gauge Vector Mesons*, [Phys. Rev. Lett. 13](#) (1964) 321–323.
- [6] P. W. Higgs, *Broken Symmetries and the Masses of Gauge Bosons*, [Phys. Rev. Lett. 13](#) (1964) 508–509.
- [7] G. S. Guralnik, C. R. Hagen, and T. W. B. Kibble, *Global Conservation Laws and Massless Particles*, [Phys. Rev. Lett. 13](#) (1964) 585–587.
- [8] ATLAS Collaboration, *Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC*, [Phys. Lett. B 716](#) (2012) 1–29.
- [9] CMS Collaboration, *Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC*, [Phys. Lett. B 716](#) (2012) 30–61.
- [10] Muon $g - 2$ Collaboration, *Measurement of the Positive Muon Anomalous Magnetic Moment to 0.46 ppm*, [Phys. Rev. Lett. 126](#) (2021) 141801.
- [11] LHCb Collaboration, *Measurement of the Ratios of Branching Fractions $\mathcal{R}(D^*)$ and $\mathcal{R}(D^0)$* , [Phys. Rev. Lett. 131](#) (2023) 111802.

- [12] S. L. Glashow, *Partial-symmetries of weak interactions*, *Nucl. Phys.* **22** (1961) 579–588.
- [13] A. Pais and S. B. Treiman, *How Many Charm Quantum Numbers are There?*, *Phys. Rev. Lett.* **35** (1975) 1556–1559.
- [14] A. Salam, *Gauge unification of fundamental forces*, *Rev. Mod. Phys.* **52** (1980) 525–538.
- [15] E. Noether, *Invariant Variation Problems*, *Transport Theory and Statistical Physics* **1** (1971) 186–207.
- [16] A. Purcell, *Go on a particle quest at the first CERN webfest*, 2012.
<https://cds.cern.ch/record/1473657>.
- [17] W. Pauli, *Über den Zusammenhang des Abschlusses der Elektronengruppen im Atom mit der Komplexstruktur der Spektren*, *Zeitschrift für Physik* **31** (1925) 765–783.
- [18] Y.-R. Liu, H.-X. Chen, W. Chen, X. Liu, and S.-L. Zhu, *Pentaquark and Tetraquark States*, *Progress in Particle and Nuclear Physics* **107** (2019) 237–320.
- [19] M. D. Schwartz, *Quantum Field Theory and the Standard Model*. Cambridge University Press, 2014.
- [20] Particle Data Group, *Review of Particle Physics*, *PTEP* **2020** (2020) 083C01.
- [21] “The Nobel Prize in Physics 2004.”
<https://www.nobelprize.org/prizes/physics/2004/summary/>.
- [22] M. Gell-Mann and K. Nishijima, *The Eightfold Way: A Theory of Strong Interaction Symmetry*, *Phys. Rev.* **106** (1957) 1339.
- [23] Particle Data Group, *Review of Particle Physics*, *PTEP* **2022** (2022) 083C01.
- [24] UA1 Collaboration, *Discovery of the W and Z Particles*, *Phys. Lett. B* **129** (1983) 449–457.
- [25] Y. Nambu, *Quasi-Particles and Gauge Invariance in the Theory of Superconductivity*, *Phys. Rev.* **117** (1960) 648–663.

- [26] *Planck2018 results: VI. Cosmological parameters*, *Astronomy & Astrophysics* **641** (2020) A6.
- [27] D. Clowe, M. Bradac, A. H. Gonzalez, M. Markevitch, S. W. Randall, C. Jones, and D. Zaritsky, *A direct empirical proof of the existence of dark matter*, *The Astrophysical Journal Letters* **648** (2006) L109–L113.
- [28] A. Crivellin and M. Hoferichter, *Beta decays as Sensitive Probes of Lepton Flavor Universality*, *Phys. Rev. Lett.* **125** (2020).
- [29] T. P. Gorringer and D. W. Hertzog, *Precision Muon Physics*, *Prog. Part. Nucl. Phys.* **84** (2015) 73–123.
- [30] A. Crivellin, M. Hoferichter, and C. A. Manzari, *Fermi Constant from Muon Decay Versus Electroweak Fits and Cabibbo-Kobayashi-Maskawa Unitarity*, *Phys. Rev. Lett.* **127** (2021).
- [31] Particle Data Group, *Review of Particle Physics*, *PTEP* **2020** (2020) 083C01.
- [32] T. Aoyama et al., *The anomalous magnetic moment of the muon in the Standard Model*, *Phys. Rept.* **887** (2020) 1–166.
- [33] “Standard Model Summary Plots October 2023.” https://atlas.web.cern.ch/Atlas/GROUPS/PHYSICS/PUBNOTES/ATL-PHYS-PUB-2023-039/fig_02.png. Accessed on 2024-09-11.
- [34] CERN, *The Large Hadron Collider*, *JINST* **3** (2008) S08001.
- [35] D. Boussard and T. P. R. Linnecar, *The LHC superconducting RF system*, 1999.
- [36] ATLAS Collaboration, *The ATLAS Experiment at the CERN Large Hadron Collider*, *JINST* **3** (2008) S08003.
- [37] CMS Collaboration, *The CMS Experiment at the CERN Large Hadron Collider*, *JINST* **3** (2008) S08004.
- [38] LHCb Collaboration, *The LHCb Detector at the CERN Large Hadron Collider*, *JINST* **3** (2008) S08005.
- [39] ALICE Collaboration, *The ALICE Experiment at the CERN Large Hadron Collider*, *JINST* **3** (2008) S08002.

- [40] D. Boussard and T. P. R. Linnecar, *The LHC Superconducting RF System*, 1999.
- [41] P. Pugnat and A. Siemko, *Review of Quench Performance of LHC Main Superconducting Magnets*, *IEEE Transactions on Applied Superconductivity* **17** (2007) 1091–1096.
- [42] P. Lebrun, *Cryogenics for the Large Hadron Collider*, *Applied Superconductivity, IEEE Transactions on* **10** (2000) 1500 – 1506.
- [43] ATLAS Collaboration, *Luminosity determination in pp collisions at $\sqrt{s} = 13$ TeV using the ATLAS detector at the LHC*, *Eur. Phys. J. C* **83** (2023).
- [44] J. Wenninger, *Operation and Configuration of the LHC in Run 2*, 2019. <https://cds.cern.ch/record/2668326>.
- [45] S. Fartoukh, S. Kostoglou, M. Solfaroli Camillocci, G. Arduini, H. Bartosik, C. Bracco, K. Brodzinski, R. Bruce, X. Buffat, M. Calviani, F. Cerutti, I. Efthymiopoulos, B. Goddard, G. Iadarola, N. Karastathis, A. Lechner, E. Metral, N. Mounet, F.-X. Nuiy, P. S. Papadopoulou, Y. Papaphilippou, B. Petersen, T. H. B. Persson, S. Redaelli, G. Rumolo, B. Salvant, G. Sterbini, H. Timko, R. Tomas Garcia, and J. Wenninger, *LHC Configuration and Operational Scenario for Run 3*, 2021. <https://cds.cern.ch/record/2790409>.
- [46] G. Strong, *On the impact of selected modern deep-learning techniques to the performance and celerity of classification models in an experimental high-energy physics use case*, *Machine Learning: Science and Technology* **1** (2020).
- [47] ATLAS Collaboration, *ATLAS Magnet System: Magnet Project Technical Design Report*, 1997. <https://cds.cern.ch/record/338080>.
- [48] T. Saleem, *Development of pixel detector for ATLAS Inner Tracker (ITK) upgrade at HL-LHC and Searching for the Standard Model Higgs boson decay into b-quark pair with ATLAS experiment*. PhD thesis, Université Paris Saclay (COMUE), 2019. <https://theses.hal.science/tel-02275808>.
- [49] A. L. Rosa and on behalf of ATLAS collaboration, *The ATLAS Insertable B-Layer: from construction to operation*, *JINST* **11** (2016) C12036.
- [50] ATLAS Collaboration, *Jet energy scale and resolution measured in proton–proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, *Eur. Phys. J. C* **81** (2021) 689.

- [51] P. Strizenec, *Performance of the ATLAS Liquid Argon Calorimeter after three years of LHC operation and plans for a future upgrade*, *JINST* **9** (2014) C09007.
- [52] ATLAS Collaboration, *Jet reconstruction and performance using particle flow with the ATLAS Detector*, *Eur. Phys. J. C* **77** (2017).
- [53] ATLAS Collaboration, *Standalone vertex finding in the ATLAS muon spectrometer*, *JINST* **9** (2014) P02001–P02001.
- [54] ATLAS Collaboration, *Performance of the ATLAS Trigger System in 2015*, *Eur. Phys. J. C* **77** (2017).
- [55] W. Buttinger, *The ATLAS Level-1 Trigger System*, in *Journal of Physics: Conference Series*, vol. 396. 2012.
- [56] E. Starchenko, G. Blanchot, M. Bosman, M. Cavalli-Sforza, A. Karyukhin, S. Kopikov, A. Miagkov, M. Nessi, A. Shalimov, N. Shalanda, M. Soldatov, A. Solodkov, A. Soloviev, V. Tsoupko-Sitnikov, and A. Zaitsev, *Cesium monitoring system for ATLAS Tile Hadron Calorimeter*, *Nucl. Instrum. Methods A* **494** (2002) 381 – 384.
- [57] S. Viret, *LASER monitoring system for the ATLAS tile calorimeter*, *Nucl. Instrum. Methods A* **617** (2010) 120–122.
- [58] K. Andersona, A. Gupta, F. Merritt, M. Oreglia, J. Pilcher, H. Sanders, M. Shochet, F. Tang, R. Teuscher, H. Wu, G. Blanchot, M. Cavalli-Sforza, and I. Korolkov, *Design of the front-end analog electronics for the ATLAS tile calorimeter*, *Nucl. Instrum. Methods A* **551** (2005) 469 – 476.
- [59] P. Anand, A. Gonzalez, and A. Radl, *Cesium and Laser Calibration of ATLAS Tile Calorimeter*, 08, 2018. <https://cds.cern.ch/record/2633181>.
- [60] ATLAS Collaboration, S. Fracchia, V. Gangiobbe, I. Korolkov, J. Abdallah, and A. Cortes Gonzalez, *Study of TileCal scintillators irradiation using the Minimum Bias integrators*,. <https://cds.cern.ch/record/1621932>.
- [61] M. Agaras, A. Ahmad, A. Blanco, D. Boumediene, R. Bonnefoy, D. Calvet, M. Calvetti, R. Chadelas, P. Conde Muino, A. Cortes Gonzalez, M. Crouau, C. Crozatier, F. Daudon, T. Davidek, G. Di Gregorio, L. Fiorini, B. Galhardo, P. Gris, P. Klimek, P. Lafarguette, D. Lambert, S. Leone, A. Maio, M. Marjanovic,

- F. Martins, M. Mlynarikova, B. Pereira, R. Pedro, K. Petukhova, S. Polacek, R. Rosten, C. Santoni, F. Scuri, D. Simon, Y. Smirnov, A. Solodkov, O. Solovyanov, M. Van Woerden, F. Veloso, and H. Wilkens, *Laser calibration of the ATLAS Tile Calorimeter during LHC Run 2*, *JINST* **18** (2023) P06023.
- [62] *Tucs GitLab Repository*, 2024.
<https://gitlab.cern.ch/atlas-tile-offline/Tucs/-/tree/master>. Accessed on 2024-06-12.
- [63] ATLAS Collaboration, “Approved Plots for Tile Calibration.” <https://twiki.cern.ch/twiki/bin/view/AtlasPublic/ApprovedPlotsTileCalibrationCombined>. Accessed on 2024-08-28.
- [64] ATLAS Collaboration, *Operation and performance of the ATLAS tile calorimeter in LHC Run 2*, 2024. <https://arxiv.org/abs/2401.16034>.
- [65] P. Grafström and W. Kozanecki, *Luminosity determination at proton colliders*, *Progress in Particle and Nuclear Physics* **81** (2015) 97–148.
- [66] S. van der Meer, *Calibration of the effective beam height in the ISR*, 1968.
<https://cds.cern.ch/record/296752>.
- [67] ATLAS Collaboration, *Preliminary analysis of the luminosity calibration for the ATLAS 13.6 TeV data recorded in 2023*, 2024.
<https://cds.cern.ch/record/2897259>.
- [68] ATLAS Collaboration, *Luminosity determination in pp collisions at $\sqrt{s} = 13$ TeV using the ATLAS detector at the LHC*, *Eur. Phys. J. C* **83** (2023).
- [69] ATLAS Collaboration, *Preliminary analysis of the luminosity calibration of the ATLAS 13.6 TeV data recorded in 2022*, 2023.
<https://cds.cern.ch/record/2852380>.
- [70] S. Agostinelli, J. Allison, K. Amako, J. Apostolakis, H. Araujo, P. Arce, M. Asai, D. Axen, S. Banerjee, G. Barrand, et al., *GEANT4: a simulation toolkit*, *Nucl. Instrum. Methods A* **506** (2003) 250–303.
- [71] J. C. Collins, D. E. Soper, and G. F. Sterman, *Factorization of Hard Processes in QCD*, *Adv. Ser. Direct. High Energy Phys.* **5** (1988) 1–91.

- [72] G. Altarelli and G. Parisi, *Asymptotic freedom in parton language*, *Nucl. Phys. B* **126** (1977) 298.
- [73] NNPDF Collaboration, *Parton distributions for the LHC Run II*, *JHEP* **04** (2015) 040.
- [74] S. Catani, F. Krauss, R. Kuhn, and B. R. Webber, *QCD matrix elements + parton showers*, *JHEP* **11** (2001) 063.
- [75] M. L. Mangano, *Multijet matrix elements and shower evolution in hadronic collisions: $Wb\bar{b} + n$ jets as a case study*, *JHEP* **07** (2006) 028.
- [76] B. Andersson, G. Gustafson, G. Ingelman, and T. Sjostrand, *Parton Fragmentation and String Dynamics*, *Phys. Rept.* **97** (1983) 31–145.
- [77] B. R. Webber, *A QCD Model for Jet Fragmentation Including Soft Gluon Interference*, *Nucl. Phys. B* **238** (1984) 492–528.
- [78] B. R. Webber, *Fragmentation and hadronization*, *Int. J. Mod. Phys. A* **15** (2000) 577.
- [79] ATLAS Collaboration, *Measurement of the underlying event in jet events from 7 TeV proton-proton collisions with the ATLAS detector*, *Eur. Phys. J. C* **74** (2014) 2965.
- [80] T. Sjöstrand, S. Mrenna, and P. Skands, *PYTHIA 8.1: A general-purpose event generator*, *Comput. Phys. Commun.* **178** (2008) 852–867.
- [81] M. Bähr, S. Gieseke, M. A. Gigg, D. Grellscheid, J. Papavassiliou, S. Plätzer, M. H. Seymour, A. Sherstnev, and S. Hoeche, *Herwig++ Physics and Manual*, *Eur. Phys. J. C* **58** (2008) 639–707.
- [82] T. Gleisberg, S. Höche, F. Krauss, S. Schumann, F. Siegert, and J. Winter, *Event generation with SHERPA 1.1*, *JHEP* **02** (2009) 007.
- [83] S. Catani and M. H. Seymour, *A General algorithm for calculating jet cross sections in NLO QCD*, *Nucl. Phys. B* **485** (1997) 291–419.
- [84] P. Nason, *A new method for combining NLO QCD with shower Monte Carlo algorithms*, *JHEP* **11** (2004) 040.

- [85] J. Alwall, R. Frederix, S. Frixione, V. Hirschi, F. Maltoni, O. Mattelaer, H.-S. Shao, T. Stelzer, P. Torrielli, and M. Zaro, *The automated computation of tree-level and next-to-leading order differential cross sections, and their matching to parton shower simulations*, *JHEP* **07** (2014) 079.
- [86] D. J. Lange, *The EvtGen particle decay simulation package*, *Nucl. Instrum. Methods A* **462** (2001) 152.
- [87] P. Artoisenet, R. Frederix, O. Mattelaer, and R. Rietkerk, *Automatic spin-entangled decays of heavy resonances in Monte Carlo simulations*, *JHEP* **03** (2013) 15.
- [88] M. Dobbs and P. K. Hansen, *The HepMC C++ Monte Carlo event record for High Energy Physics*, *Comput. Phys. Commun.* **134** (2001) 41–46.
- [89] ATLAS Collaboration, *The ATLAS Simulation Infrastructure*, *Eur. Phys. J. C* **70** (2010) 823–874.
- [90] ATLAS Collaboration, *The simulation principle and performance of the ATLAS fast calorimeter simulation FastCaloSim*, 2010. <https://cds.cern.ch/record/1300517>.
- [91] K. Edmonds, *The Fast ATLAS Track Simulation (FATRAS)*, Mar, 2008. <https://cds.cern.ch/record/1091969>.
- [92] “ATLAS Inner Detector Overview.” <https://atlassoftwaredocs.web.cern.ch/trackingTutorial/idooverview/>. Accessed on 2024-01-29.
- [93] ATLAS Collaboration, *Performance of the reconstruction of large impact parameter tracks in the inner detector of ATLAS*, 2017. <https://cds.cern.ch/record/2275635>.
- [94] “ATLAS Software Documentation - Tracking Tutorial.” <https://atlassoftwaredocs.web.cern.ch/trackingTutorial/lrtvertexmisc/>.
- [95] ATLAS Collaboration, *Early Inner Detector Tracking Performance in the 2015 Data at $\sqrt{s} = 13$ TeV*, 2015. <https://cds.cern.ch/record/2110140>.
- [96] ATLAS Collaboration, *Reconstruction of primary vertices at the ATLAS experiment in Run 1 proton–proton collisions at the LHC*, *Eur. Phys. J. C* **77** (2017).

- [97] ATLAS Collaboration, *Topological cell clustering in the ATLAS calorimeters and its performance in LHC Run 1*, *Eur. Phys. J. C* **77** (2016).
- [98] M. Valente, *Supersymmetric Beasts and Where to Find Them: From Novel Hadronic Reconstruction Methods to Search Results in Large Jet Multiplicity Final States at the ATLAS Experiment*, 2024. <https://cds.cern.ch/record/2721059>.
- [99] ATLAS Collaboration, *Electron and photon performance measurements with the ATLAS detector using the 2015–2017 LHC proton-proton collision data*, *JINST* **14** (2019) P12006–P12006.
- [100] ATLAS Collaboration, *Measurement of the Higgs boson production cross section in association with a vector boson and decaying into WW^* with the ATLAS detector at $\sqrt{s} = 13$ TeV*, 2021. <https://cds.cern.ch/record/2765898>.
- [101] ATLAS Collaboration, *Electron and photon energy calibration with the ATLAS detector using data collected in 2015 at $\sqrt{s} = 13$ TeV*, 2016. <https://cds.cern.ch/record/2203514>.
- [102] ATLAS Collaboration, *Muon reconstruction performance of the ATLAS detector in proton–proton collision data at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **76** (2016) 292.
- [103] ATLAS Collaboration, *Muon reconstruction and identification efficiency in ATLAS using the full Run 2 pp collision data set at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **81** (2021) 578.
- [104] ATLAS Collaboration, *Jet reconstruction and performance using particle flow with the ATLAS Detector*, *Eur. Phys. J. C* **77** (2017).
- [105] M. Cacciari, G. P. Salam, and G. Soyez, *The anti- k_t jet clustering algorithm*, *JHEP* **04** (2008) 063.
- [106] ATLAS Collaboration, *Tagging and suppression of pileup jets*, 2014. <https://cds.cern.ch/record/1700870>. ATLAS-CONF-2014-018.
- [107] ATLAS Collaboration, *Identification and rejection of pile-up jets at high pseudorapidity with the ATLAS detector*, *Eur. Phys. J. C* **77** (2017) 580.

- [108] ATLAS Collaboration, *Optimisation and performance studies of the ATLAS b-tagging algorithms for the 2017-18 LHC run*, 2017.
<https://cds.cern.ch/record/2273281>.
- [109] ATLAS Collaboration, *Identification of Jets Containing b-Hadrons with Recurrent Neural Networks at the ATLAS Experiment*, 2017.
<https://cds.cern.ch/record/2255226>.
- [110] ATLAS Collaboration, *Secondary vertex finding for jet flavour identification with the ATLAS detector*, 2017. <https://cds.cern.ch/record/2270366>.
- [111] ATLAS Collaboration, *Topological b-hadron decay reconstruction and identification of b-jets with the JetFitter package in the ATLAS experiment at the LHC*, 2018.
<https://cds.cern.ch/record/2645405>.
- [112] ATLAS Collaboration, *Monte Carlo to Monte Carlo scale factors for flavour tagging efficiency calibration*, 2020.
<https://cds.cern.ch/record/2718610/files/ATL-PHYS-PUB-2020-009.pdf>.
- [113] ATLAS Collaboration, *ATLAS flavour-tagging algorithms for the LHC Run 2 pp collision dataset*, *Eur. Phys. J. C* **83** (2023) 681.
- [114] ATLAS Collaboration, *Measurement of b-tagging Efficiency of c-jets in $t\bar{t}$ Events Using a Likelihood Approach with the ATLAS Detector*, 2018.
<http://cds.cern.ch/record/2306649>.
- [115] ATLAS Collaboration, *Calibration of light-flavour b-jet mistagging rates using ATLAS proton-proton collision data at $\sqrt{s} = 13$ TeV*, 2018.
<https://cds.cern.ch/record/2314418>.
- [116] ATLAS Collaboration, “Measurement of the tau lepton reconstruction and identification performance in the ATLAS experiment using pp collisions at $\sqrt{s} = 13$ TeV.” ATLAS-CONF-2017-029, 2017.
<https://cds.cern.ch/record/2261772>.
- [117] ATLAS Collaboration, *Reconstruction, Energy Calibration, and Identification of Hadronically Decaying Tau Leptons in the ATLAS Experiment for Run-2 of the LHC*, 2015. <http://cds.cern.ch/record/2064383>.

- [118] ATLAS Collaboration, “Identification of hadronic tau lepton decays using neural networks in the ATLAS experiment.” ATL-PHYS-PUB-2019-033, 2019.
<https://cds.cern.ch/record/2688062>.
- [119] ATLAS Collaboration, *Performance of missing transverse momentum reconstruction with the ATLAS detector using proton-proton collisions at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **78** (2018) 903.
- [120] ATLAS Collaboration, *Luminosity determination in pp collisions at $\sqrt{s} = 13$ TeV using the ATLAS detector at the LHC*, 2019.
<https://cds.cern.ch/record/2677054/files/ATLAS-CONF-2019-021.pdf>.
- [121] ATLAS Collaboration, *Luminosity determination in pp collisions at $\sqrt{s} = 13$ TeV using the ATLAS detector at the LHC*,. <https://arxiv.org/pdf/2212.09379>.
- [122] ATLAS Collaboration, *Development of ATLAS Primary Vertex Reconstruction for LHC Run 3*, 2019. <https://cds.cern.ch/record/2670380>.
- [123] P. Golonka and Z. Was, *PHOTOS Monte Carlo: A Precision tool for QED corrections in Z and W decays*, *Eur. Phys. J. C* **45** (2006) 97–107.
- [124] ATLAS Collaboration, “ttH multi-analysis working group repository.”
<https://gitlab.cern.ch/atlasHTop/ttHMultiAna>. Accessed on 2024-06-15.
- [125] ATLAS Collaboration, “ATHENA: ATLAS Software Framework.”
<https://gitlab.cern.ch/atlas/athena>. Accessed on 2024-06-15.
- [126] ATLAS Collaboration, “ttH multi-GF working group repository.” https://gitlab.cern.ch/atlasHTop/ttHMultiGFW2/-/tree/master_ttH?ref_type=heads. Accessed on 2024-06-15.
- [127] “TRexFitter framework documentation.”
<https://trexfitter-docs.web.cern.ch/trexfitter-docs/>.
- [128] “TRexFitter framework gitlab project.”
<https://gitlab.cern.ch/TRExStats/TRExFitter/>.
- [129] ATLAS Collaboration, *Evidence for the associated production of the Higgs boson and a top quark pair with the ATLAS detector*, *Phys. Rev. D* **97** (2018) 072003.

- [130] ATLAS Collaboration, *Electron reconstruction and identification in the ATLAS experiment using the 2015 and 2016 LHC proton–proton collision data at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **79** (2019) 639.
- [131] ATLAS Collaboration, *Selection of jets produced in 13 TeV proton-proton collisions with the ATLAS detector*,. <https://cds.cern.ch/record/2037702>. ATLAS-CONF-2015-029.
- [132] “Jet-based event cleaning.” <https://twiki.cern.ch/twiki/bin/view/AtlasProtected/HowToCleanJetsR21>.
- [133] ATLAS Collaboration, *ATLAS b-jet identification performance and efficiency measurement with $t\bar{t}$ events in pp collisions at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **79** (2019) 970.
- [134] ATLAS Collaboration, *Measurement of the c-jet mistagging efficiency in $t\bar{t}$ events using pp collision data at $\sqrt{s} = 13$ TeV collected with the ATLAS detector*, *Eur. Phys. J. C* **82** (2022) 95.
- [135] ATLAS Collaboration, *Calibration of the light-flavour jet mistagging efficiency of the b-tagging algorithms with Z +jets events using 139 fb^{-1} of ATLAS proton–proton collision data at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **83** (2023) 728.
- [136] D. P. Kingma and J. Ba, *Adam: A Method for Stochastic Optimization*, 2017. <https://arxiv.org/abs/1412.6980>.
- [137] F. Chollet et al., “Keras.” <https://keras.io>, 2015.
- [138] *TensorFlow: Large-Scale Machine Learning on Heterogeneous Systems*, 2015. <https://www.tensorflow.org/>.
- [139] R. Frederix, D. Pagani, and M. Zaro, *Large NLO corrections in $t\bar{t}W$ and $t\bar{t}t\bar{t}$ hadroproduction from supposedly subleading EW contributions*, *JHEP* **2018** (2018).
- [140] CERN, *CERN Yellow Reports: Monographs, Vol 2 (2017): Handbook of LHC Higgs cross sections: 4. Deciphering the nature of the Higgs sector*, 2017. <https://e-publishing.cern.ch/index.php/CYRM/issue/view/32>.
- [141] J. Butterworth, S. Carrazza, A. Cooper-Sarkar, A. D. Roeck, J. Feltesse, S. Forte, J. Gao, S. Glazov, J. Huston, Z. Kassabov, R. McNulty, A. Morsch, P. Nadolsky,

- V. Radescu, J. Rojo, and R. Thorne, *PDF4LHC recommendations for LHC Run II*, *Journal of Physics G: Nuclear and Particle Physics* **43** (2016) 023001.
- [142] “TTbarNNLOReweighter package.”
<https://gitlab.cern.ch/pinamont/TTbarNNLOReweighter>.
- [143] G. Cowan, K. Cranmer, E. Gross, and O. Vitells, *Asymptotic formulae for likelihood-based tests of new physics*, *Eur. Phys. J. C* **71** (2011) 1554.
- [144] T. Junk, *Confidence level computation for combining searches with small statistics*, *Nucl. Instrum. Methods A* **434** (1999) 435.
- [145] K. Cranmer, G. Lewis, L. Moneta, A. Shibata, and W. Verkerke, *HistFactory: A tool for creating statistical models for use with RooFit and RooStats*, 2012.
<https://cds.cern.ch/record/1456844>.
- [146] W. Verkerke and D. Kirkby, *The RooFit toolkit for data modeling*, 2003.
<https://arxiv.org/abs/physics/0306116>.
- [147] W. Verkerke and D. Kirkby, “Roofit users manual.”
<http://roofit.sourceforge.net>.
- [148] W.-S. Hou and M. Kikuchi, *Approximate Alignment in Two Higgs Doublet Model with Extra Yukawa Couplings*, *EPL* **123** (2018) 11001.
- [149] K. Fuyuto, W.-S. Hou, and E. Senaha, *Electroweak baryogenesis driven by extra top Yukawa couplings*, *Phys. Lett. B* **776** (2018) 402–406.
- [150] W. Altmannshofer, J. Eby, S. Gori, M. Lotito, M. Martone, and D. Tuckler, *Collider Signatures of Flavorful Higgs Bosons*, *Phys. Rev. D* **94** (2016) 115032.
- [151] M. Kohda, T. Modak, and W.-S. Hou, *Searching for new scalar bosons via triple-top signature in $cg \rightarrow tS^0 \rightarrow t\bar{t}\bar{t}$* , *Phys. Lett. B* **776** (2018) 379–384.
- [152] W.-S. Hou, M. Kohda, and T. Modak, *Implications of Four-Top and Top-Pair Studies on Triple-Top Production*, *Phys. Lett. B* **798** (2019) 134953.
- [153] G. W. S. Hou, *Top-Higgs Associated Production involving A^0 , H^0 with Mass at 300 GeV*, *PoS* (2020) 337.

- [154] ATLAS Collaboration, *Observation of four-top-quark production in the multilepton final state with the ATLAS detector*, *Eur. Phys. J. C* **83** (2023).
- [155] ATLAS Collaboration, *Search for top-philic heavy resonances in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, *Eur. Phys. J. C* **84** (2024) 157.
- [156] ATLAS Collaboration, “Search for $t\bar{t}H/A \rightarrow t\bar{t}t\bar{t}$ production in the multilepton final state in proton–proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector.” ATLAS-CONF-2022-008, 2022. <https://cds.cern.ch/record/2805212>.
- [157] ATLAS Collaboration, *Search for top-quark-associated production of heavy scalar or pseudoscalar in pp collisions at 13 TeV*, 2024. <https://cds.cern.ch/record/2891814>.
- [158] CMS Collaboration, *Observation of four top quark production in proton-proton collisions at $\sqrt{s} = 13$ TeV*, *Phys. Lett. B* **847** (2023) 138290.
- [159] CMS Collaboration, *Search for standard model production of four top quarks with same-sign and multilepton final states in proton–proton collisions at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **78** (2018) 140.
- [160] CMS Collaboration, *Search for the production of four top quarks in the single-lepton and opposite-sign dilepton final states in proton–proton collisions at $\sqrt{s} = 13$ TeV*, *JHEP* **11** (2019) 082.
- [161] CMS Collaboration, *Search for production of four top quarks in final states with same-sign or multiple leptons in proton–proton collisions at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **80** (2020) 75.
- [162] CMS Collaboration, *Search for physics beyond the standard model in events with two leptons of same sign, missing transverse momentum, and jets in proton–proton collisions at $\sqrt{s} = 13$ TeV*, *Eur. Phys. J. C* **77** (2017) 578.
- [163] ATLAS Collaboration, *Measurement of the total and differential cross-sections of $t\bar{t}W$ production in pp collisions at 13 TeV with the ATLAS detector*, 2023. <http://cds.cern.ch/record/2855337>.
- [164] ATLAS Collaboration, “Analysis of $t\bar{t}H$ and $t\bar{t}W$ production in multilepton final states with the ATLAS detector.” ATLAS-CONF-2019-045, 2019. <https://cds.cern.ch/record/2693930>.

- [165] ATLAS Collaboration, *Measurement of the $t\bar{t}Z$ and $t\bar{t}W$ cross sections in proton–proton collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, *Phys. Rev. D* **99** (2019) 072009, [arXiv:1901.03584](#).
- [166] ATLAS Collaboration, *Measurement of the $t\bar{t}t\bar{t}$ production cross section in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, *JHEP* **11** (2021) 118.
- [167] ATLAS Collaboration, *Search for R-parity-violating supersymmetry in a final state containing leptons and many jets with the ATLAS experiment using $\sqrt{s} = 13$ TeV proton–proton collision data*, *Eur. Phys. J. C* **81** (2021) 1023.
- [168] B. Altunkaynak, W.-S. Hou, C. Kao, M. Kohda, and B. McCoy, *Flavor Changing Heavy Higgs Interactions at the LHC*, *Phys. Lett. B* **751** (2015) 135–142.
- [169] A. Crivellin, A. Kokulu, and C. Greub, *Flavor-phenomenology of two-Higgs-doublet models with generic Yukawa structure*, *Phys. Rev. D* **87** (2013) 094031.
- [170] *Autonomio Talos*, 2020. <https://autonomio.github.io/talos>.
- [171] ATLAS Collaboration, *Search for heavy Higgs bosons with flavour-violating couplings in multi-lepton plus b-jets final states in pp collisions at 13 TeV with the ATLAS detector*, *JHEP* **12** (2023) 081.
- [172] G. J. Székely, M. L. Rizzo, and N. K. Bakirov, *Measuring and testing dependence by correlation of distances*, *Ann. Statist.* **35** (2007) 2769–2794.
- [173] G. Kasieczka and D. Shih, *Robust Jet Classifiers through Distance Correlation*, *Phys. Rev. Lett.* **125** (2020) 122001.
- [174] ATLAS Collaboration, *Internal note of “Search for the associated production of a Higgs Boson and a Top Quark Pair in multilepton final states in 80 fb^{-1} pp Collisions at $\sqrt{s} = 13$ TeV with the ATLAS Detector”*, <https://cds.cern.ch/record/2314122>.
- [175] ATLAS Collaboration, *Internal note of “Measurement of the total and differential cross sections of a top-quark-antiquark pair in association with a W boson in proton-proton collisions at a centre-of-mass energy of 13 TeV with ATLAS detector at the Large Hadron Collider”*, <https://cds.cern.ch/record/2712986>.

- [176] Belle Collaboration, *Measurement of $\mathcal{R}(D)$ and $\mathcal{R}(D^*)$ with a semileptonic tagging method*, *Phys. Rev. Lett.* **124** (2020) 161803.
- [177] Belle Collaboration, *Test of Lepton-Flavor Universality in $B \rightarrow K^* \ell^+ \ell^-$ Decays at Belle*, *Phys. Rev. Lett.* **126** (2021) 161801.
- [178] Belle Collaboration, *Test of lepton flavor universality and search for lepton flavor violation in $B \rightarrow K \ell \ell$ decays*, *JHEP* **03** (2021) 105.
- [179] LHCb Collaboration, *Angular Analysis of the $B^+ \rightarrow K^{*+} \mu^+ \mu^-$ Decay*, *Phys. Rev. Lett.* **126** (2021) 161802.
- [180] LHCb Collaboration, *Measurement of CP -Averaged Observables in the $B^0 \rightarrow K^{*0} \mu^+ \mu^-$ Decay*, *Phys. Rev. Lett.* **125** (2020) 011802.
- [181] LHCb Collaboration, *Measurement of the ratio of the $B^0 \rightarrow D^{*-} \tau^+ \nu_\tau$ and $B^0 \rightarrow D^{*-} \mu^+ \nu_\mu$ branching fractions using three-prong τ -lepton decays*, *Phys. Rev. Lett.* **120** (2018) 171802.
- [182] LHCb Collaboration, *Test of lepton universality with $B^0 \rightarrow K^{*0} \ell^+ \ell^-$ decays*, *JHEP* **08** (2017) 055.
- [183] LHCb Collaboration, *Test of lepton universality in beauty-quark decays*, *Nat. Phys.* **18** (2022) 277–282.
- [184] Muon $g - 2$ Collaboration, *Measurement of the Positive Muon Anomalous Magnetic Moment to 0.46 ppm*, *Phys. Rev. Lett.* **126** (2021) 141801.
- [185] A. Chakraborty and S. Chakraborty, *Probing $(g - 2)_\mu$ at the LHC in the paradigm of R -parity violating MSSM*, *Phys. Rev. D* **93** (2016) 075035.
- [186] M.-D. Zheng and H.-H. Zhang, *Studying the $b \rightarrow s \ell^+ \ell^-$ anomalies and $(g - 2)_\mu$ in R -parity violating MSSM framework with the inverse seesaw mechanism*, *Phys. Rev. D* **104** no. 11, (2021) 115023, [arXiv:2105.06954 \[hep-ph\]](#).
- [187] W. Altmannshofer, P. S. B. Dev, A. Soni, and Y. Sui, *Addressing $R_{D^{(*)}}$, $R_{K^{(*)}}$, muon $g - 2$ and ANITA anomalies in a minimal R -parity violating supersymmetric framework*, *Phys. Rev. D* **102** (2020) 015031.

- [188] D. Das, C. Hati, G. Kumar, and N. Mahajan, *Scrutinizing R -parity violating interactions in light of $R_{K^{(*)}}$ data*, *Phys. Rev. D* **96** (2017) 095033.
- [189] K. Earl and T. Grégoire, *Contributions to $b \rightarrow s\ell\ell$ Anomalies from R -Parity Violating Interactions*, *JHEP* **08** (2018) 201.
- [190] N. G. Deshpande and X.-G. He, *Consequences of R -parity violating interactions for anomalies in $\bar{B} \rightarrow D^{(*)}\tau\bar{\nu}$ and $b \rightarrow s\mu^+\mu^-$* , *Eur. Phys. J. C* **77** (2017) 134.
- [191] Q.-Y. Hu, Y.-D. Yang, and M.-D. Zheng, *Revisiting the B -physics anomalies in R -parity violating MSSM*, *Eur. Phys. J. C* **80** (2020) 365.
- [192] Q.-Y. Hu and L.-L. Huang, *Explaining $b \rightarrow s\ell^+\ell^-$ data by sneutrinos in the R -parity violating MSSM*, *Phys. Rev. D* **101** (2020) 035030.
- [193] W. Altmannshofer, P. S. Bhupal Dev, and A. Soni, *$R_{D^{(*)}}$ anomaly: A possible hint for natural supersymmetry with R -parity violation*, *Phys. Rev. D* **96** (2017) 095010.
- [194] S. Trifinopoulos, *Revisiting R -parity violating interactions as an explanation of the B -physics anomalies*, *Eur. Phys. J. C* **78** (2018) 803.
- [195] F. del Aguila and M. J. Bowick, *The Possibility of New Fermions With $\Delta I = 0$ Mass*, *Nucl. Phys. B* **224** (1983) 107.
- [196] P. M. Fishbane, R. E. Norton, and M. J. Rivard, *Experimental Implications of Heavy Isosinglet Quarks and Leptons*, *Phys. Rev. D* **33** (1986) 2632.
- [197] P. M. Fishbane and P. Q. Hung, *Lepton Masses in a Dynamical Model of Family Symmetry*, *Z. Phys. C* **38** (1988) 649.
- [198] I. Montvay, *Three Mirror Pairs of Fermion Families*, *Phys. Lett. B* **205** (1988) 315–320.
- [199] K. Fujikawa, *A Vector-like extension of the standard model*, *Prog. Theor. Phys.* **92** (1994) 1149–1160.
- [200] D. B. Kaplan, H. Georgi, and S. Dimopoulos, *Composite Higgs Scalars*, *Phys. Lett. B* **136** (1984) 187–190.
- [201] K. Agashe, R. Contino, and A. Pomarol, *The minimal composite Higgs model*, *Nucl. Phys. B* **719** (2005) 165–187.

- [202] K. Kong, S. C. Park, and T. G. Rizzo, *A vector-like fourth generation with a discrete symmetry from Split-UED*, [JHEP **07** \(2010\) 059](#).
- [203] G.-Y. Huang, K. Kong, and S. C. Park, *Bounds on the Fermion-Bulk Masses in Models with Universal Extra Dimensions*, [JHEP **06** \(2012\) 099](#).
- [204] S. P. Martin, *Extra vector-like matter and the lightest Higgs scalar boson mass in low-energy supersymmetry*, [Phys. Rev. D **81** \(2010\) 035004](#).
- [205] S. Zheng, *Minimal vector-like model in supersymmetric unification*, [Eur. Phys. J. C **80** \(2020\) 273](#).
- [206] R. Nevzorov, *E_6 inspired supersymmetric models with exact custodial symmetry*, [Phys. Rev. D **87** \(2013\) 015029](#).
- [207] I. Dorsner, S. Fajfer, and I. Mustac, *Light vector-like fermions in a minimal $SU(5)$ setup*, [Phys. Rev. D **89** \(2014\) 115004](#).
- [208] A. Joglekar and J. L. Rosner, *Searching for signatures of E_6* , [Phys. Rev. D **96** \(2017\) 015026](#).
- [209] K. Agashe, T. Okui, and R. Sundrum, *A Common Origin for Neutrino Anarchy and Charged Hierarchies*, [Phys. Rev. Lett. **102** \(2009\) 101801](#).
- [210] M. Redi, *Leptons in Composite MFV*, [JHEP **09** \(2013\) 060](#).
- [211] P. Schwaller, T. M. P. Tait, and R. Vega-Morales, *Dark Matter and Vectorlike Leptons from Gauged Lepton Number*, [Phys. Rev. D **88** \(2013\) 035001](#).
- [212] J. Halverson, N. Orlofsky, and A. Pierce, *Vectorlike Leptons as the Tip of the Dark Matter Iceberg*, [Phys. Rev. D **90** \(2014\) 015002](#).
- [213] S. Bahrami, M. Frank, D. K. Ghosh, N. Ghosh, and I. Saha, *Dark matter and collider studies in the left-right symmetric model with vectorlike leptons*, [Phys. Rev. D **95** \(2017\) 095024](#).
- [214] S. Bhattacharya, P. Ghosh, N. Sahoo, and N. Sahu, *Mini Review on Vector-Like Leptonic Dark Matter, Neutrino Mass, and Collider Signatures*, [Front. in Phys. **7** \(2019\) 80](#).

-
- [215] ATLAS Collaboration, *Exploration at the high-energy frontier: ATLAS Run 2 searches investigating the exotic jungle beyond the Standard Model*, [arXiv:2403.09292](#).
- [216] Muon g-2 Collaboration, *Final Report of the Muon E821 Anomalous Magnetic Moment Measurement at BNL*, *Phys. Rev. D* **73** (2006) 072003.
- [217] Muon g-2 Collaboration, *Measurement of the Positive Muon Anomalous Magnetic Moment to 0.20 ppm*, *Phys. Rev. Lett.* **131** (2023) 161802.
- [218] R. H. Parker, C. Yu, W. Zhong, B. Estey, and H. Müller, *Measurement of the fine-structure constant as a test of the Standard Model*, *Science* **360** (2018) 191, [arXiv:1812.04130](#).
- [219] L. Morel, Z. Yao, P. Cladé, and S. Guellati-Khélifa, *Determination of the fine-structure constant with an accuracy of 81 parts per trillion*, *Nature* **588** (2020) 61–65.
- [220] X. Fan, T. G. Myers, B. A. D. Sukra, and G. Gabrielse, *Measurement of the Electron Magnetic Moment*, *Phys. Rev. Lett.* **130** (2023) 071801.
- [221] B. Belfatto, R. Beradze, and Z. Berezhiani, *The CKM unitarity problem: A trace of new physics at the TeV scale?*, *Eur. Phys. J. C* **80** (2020) 149.
- [222] Y. Grossman, E. Passemar, and S. Schacht, *On the Statistical Treatment of the Cabibbo Angle Anomaly*, *JHEP* **07** (2020) 068.
- [223] A. Crivellin, F. Kirk, C. A. Manzari, and M. Montull, *Global Electroweak Fit and Vector-Like Leptons in Light of the Cabibbo Angle Anomaly*, *JHEP* **12** (2020) 166.
- [224] N. Kumar and S. P. Martin, *Vectorlike Leptons at the Large Hadron Collider*, *Phys. Rev. D* **92** (2015) 115018.
- [225] P. N. Bhattiprolu and S. P. Martin, *Prospects for vectorlike leptons at future proton-proton colliders*, *Phys. Rev. D* **100** (2019) 015033.
- [226] M. S. Chanowitz and M. K. Gaillard, *The TeV Physics of Strongly Interacting W's and Z's*, *Nucl. Phys. B* **261** (1985) 379–431.

- [227] L3 Collaboration, P. Achard et al., *Search for heavy neutral and charged leptons in e^+e^- annihilation at LEP*, *Phys. Lett. B* **517** (2001) 75–85.
- [228] ATLAS Collaboration, *Search for heavy lepton resonances decaying to a Z boson and a lepton in pp collisions at $\sqrt{s} = 8$ TeV with the ATLAS detector*, *JHEP* **09** (2015) 108.
- [229] ATLAS Collaboration, *Search for third-generation vector-like leptons in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, *JHEP* **07** (2023) 118.
- [230] CMS Collaboration, *Inclusive nonresonant multilepton probes of new phenomena at $\sqrt{s} = 13$ TeV*, *Phys. Rev. D* **105** (2022) 112007.
- [231] L. Di Luzio, A. Greljo, and M. Nardecchia, *Gauge leptoquark as the origin of B -physics anomalies*, *Phys. Rev. D* **96** (2017) 115011.
- [232] C. Cornella, D. A. Faroughy, J. Fuentes-Martin, G. Isidori, and M. Neubert, *Reading the footprints of the B -meson flavor anomalies*, *JHEP* **08** (2021) 050.
- [233] L. Di Luzio, J. Fuentes-Martin, A. Greljo, M. Nardecchia, and S. Renner, *Maximal Flavour Violation: a Cabibbo mechanism for leptoquarks*, *JHEP* **11** (2018) 081.
- [234] M. J. Baker, J. Fuentes-Martin, G. Isidori, and M. Konig, *High pT signatures in vector-leptoquark models*, *Eur. Phys. J. C* **79** (2019) 334.
- [235] CMS Collaboration, *Search for pair-produced vector-like leptons in final states with third-generation leptons and at least three b quark jets in proton-proton collisions at $\sqrt{s} = 13$ TeV*, *Phys. Lett. B* **846** (2023) 137713.
- [236] ATLAS Collaboration, *Search for electroweak production of vector-like leptons in multiple tau and b -jets final states in pp collisions at $\sqrt{s}=13$ TeV with the ATLAS detector*, tech. rep., CERN, Geneva, 2024. <https://cds.cern.ch/record/2904563>.
- [237] ROOT Collaboration, *TMVA - Toolkit for Multivariate Data Analysis*. CERN, 2022. https://root.cern/doc/master/group__TMVA.html.
- [238] “Software tool for MVA.” https://gitlab.cern.ch/asonay/tmva_tool.

