

Reconstruction and Identification of Boosted Di- τ Decays in a Search for Higgs Boson Pairs with the ATLAS Detector

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Kurzfassung

Die Entdeckung des Higgs-Bosons ebnete den Weg für neue experimentelle Suchen am Large Hadron Collider am CERN. Die resonante Produktion von zwei Higgs-Bosonen ist eine vielversprechende Signatur zur Suche nach neuer Physik, die von Erweiterungen des Standardmodells wie dem Minimalen Supersymmetrischen Standardmodell vorhergesagt wird. Eine Suche nach schweren Resonanzen mit Massen oberhalb von 1 TeV ist eine experimentelle Herausforderung. In diesem Bereich werden die Higgs-Bosonen mit großen Impulsen erzeugt. Die dabei entstehenden Zerfallsprodukte sind stark kollimiert, so dass sie nicht mehr von den gängigen Methoden der Teilchenrekonstruktion im ATLAS-Detektor erkannt werden. In dieser Arbeit wird eine neue Methode zur Rekonstruktion von Paaren hadronisch zerfallender τ -Leptonen mit hohem Lorentz-Boost vorgestellt. Diese Di- τ -Rekonstruktion erlaubt eine Rekonstruktion von geboosteten τ -Paaren mit Effizienzen von über 80%. Die multivariate Di- τ -Identifikation erkennt τ -Paare mit einer Effizienz von mehr als 60%. Die Wahrscheinlichkeit Quark- oder Gluon-Untergrund als Signal fehlzuinterpretieren ist geringer als 0,01%. Die Di- τ -Algorithmen werden anhand von Daten aus 139 fb^{-1} Proton-Proton-Kollisionen mit einer Schwerpunktsenergie von 13 TeV validiert und kalibriert. Bei der Anwendung dieser neuen Methoden in einer Suche nach resonanter Produktion von zwei Higgs-Bosonen im $b\bar{b}\tau^+\tau^-$ Endzustand wurden keine signifikanten Abweichungen vom erwarteten Untergrund beobachtet. Es wurden obere Ausschlussgrenzen bestimmt auf den Wirkungsquerschnitt zur Produktion einer schmalen skalaren Resonanz multipliziert mit dem Verzweigungsverhältnis für ihren Zerfall in zwei Higgs-Bosonen. Im Massenbereich von 1 TeV bis 3 TeV wurden Ausschlussgrenzen von 858 fb bis 27 fb beobachtet bei einem Konfidenzniveau von 95%.

Abstract

The discovery of the Higgs boson opened the way for new experimental searches at the Large Hadron Collider at CERN. The resonant production of two Higgs bosons is a promising signature for searches for new physics phenomena that are predicted by extensions of the Standard Model such as the Minimal Supersymmetric Standard Model. Searches for heavy resonances with masses above 1 TeV are experimentally challenging. In this regime, the Higgs bosons are produced with high momenta. Their decay products are highly collimated to the extent that the standard techniques for particle reconstruction become inefficient. A novel method, referred to as di- τ reconstruction, is developed for the reconstruction of pairs of hadronically decaying τ leptons with a large Lorentz boost in the ATLAS detector. Highly boosted pairs of τ leptons are reconstructed with an efficiency of more than 80%. The multi-variate di- τ identification recognizes pairs of τ leptons with an efficiency of more than 60%, whereas the probability to misidentify the background of a quark- or gluon-initiated jet is less than 0.01%. The di- τ algorithms are calibrated and validated using data of 139 fb^{-1} of proton-proton collisions at a center-of-mass energy of 13 TeV. These novel techniques are employed in a search for resonant production of Higgs boson pairs in the $b\bar{b}\tau^+\tau^-$ final state. No significant deviations from the background expectation are observed. Upper limits are derived on the production cross section of a narrow scalar resonance times its branching ratio to decay into a Higgs boson pair. Exclusion limits between 858 fb and 27 fb are observed at 95% confidence level for resonance masses from 1 TeV to 3 TeV.

Contents

1	Introduction	1
2	The Standard Model of Particle Physics and Beyond	3
2.1	The Standard Model of Particle Physics	4
2.1.1	Strong and Electroweak Interactions	4
2.1.2	Electroweak Symmetry Breaking	6
2.1.3	Production of Higgs Boson Pairs in the Standard Model	8
2.1.4	Challenges of the Standard Model	9
2.2	New Physics Beyond the Standard Model	10
2.2.1	The Minimal Supersymmetric Standard Model	11
2.2.2	The Next-to-Minimal Supersymmetric Standard Model	19
2.2.3	Extra Dimensions	19
2.3	Monte Carlo Event Simulations	21
2.3.1	Monte Carlo Event Generation	21
2.3.2	Signal Monte Carlo Samples	22
3	The Large Hadron Collider and the ATLAS Experiment	25
3.1	The Large Hadron Collider	25
3.2	The ATLAS Experiment	27
3.2.1	Inner Detector	28
3.2.2	Calorimeter Systems	30
3.2.3	Muon Spectrometer	32
3.2.4	Trigger Systems	33
3.3	Data Taking in LHC Run 2	34
4	Physics Object Reconstruction	37
4.1	Low-Level Objects	37
4.2	Calorimeter Jets	39
4.3	Track Jets	41
4.4	b -Tagging	41
4.5	Electrons	42
4.6	Muons	42
4.7	Missing Transverse Momentum	43

5	Boosted Di-τ Reconstruction and Identification	45
5.1	Resolved τ Reconstruction	46
5.2	Boosted Di- τ Reconstruction	47
5.2.1	Seeding Jet and Subjet Reconstruction	48
5.2.2	Track and Vertex Association	49
5.2.3	Reconstruction Performance	49
5.3	Di- τ Energy Response	52
5.4	Di- τ Identification	53
5.4.1	Training Event Selection	54
5.4.2	Identification Variables	54
5.4.3	Identification Training	61
5.4.4	Identification Performance	62
5.5	Track-Multiplicity Selection	64
5.6	Systematic Uncertainties from Simulation Variations	64
5.6.1	Efficiency Uncertainties	66
5.6.2	Energy Response Uncertainties	67
6	Event Selection and Categorization	69
6.1	Event Cleaning and Overlap Removal	69
6.2	Event Preselection	70
6.2.1	Trigger Selection	71
6.2.2	Di- τ Selection	71
6.2.3	Large- R Jet Selection	72
6.3	Event Categorization	72
7	Background Estimation	75
7.1	Background Monte Carlo Samples	75
7.2	Systematic uncertainties	77
7.3	Multi-Jet Background	78
7.3.1	Fake Factor Measurement	79
7.3.2	Multi-Jet Background Validation	81
7.4	Z + Heavy Flavor Background	82
7.5	Top Background	85
8	Data-Driven Di-τ Calibration	87
8.1	‘ Z 0- b -tag’ Control Region	87
8.2	Di- τ Event Normalization Calibration	88
8.3	Di- τ Energy Calibration	92
9	Search for Resonant Higgs Boson Pair Production	93
9.1	Signal Region	93
9.2	Signal Acceptance Uncertainties	98
9.3	Statistical Analysis	99
9.3.1	Statistical Analysis Method	100

9.3.2	The Likelihood Function	100
9.3.3	The Test Statistic	103
9.3.4	Exclusion Limit Calculation	104
9.4	Results	106
9.4.1	Nuisance Parameter Impact	106
9.4.2	Exclusion Limit Results	108
10	Summary	113
A	Implementation Details	117
B	Statistical Analysis	127
B.1	Test Statistic Distributions	128
B.2	Nuisance Parameter Ranking	130
B.3	Exclusion Limit Table	133
	List of Figures	135
	List of Tables	137
	List of Abbreviations	139
	Bibliography	141
	Acknowledgments	161

Chapter 1

Introduction

The discovery of the Higgs boson [1, 2] by the ATLAS and CMS experiments at the Large Hadron Collider marked the beginning of a new era in experimental particle physics. On the one hand, this is the era of precision measurements in the Higgs sector. With the discovery of the Higgs boson, the last particle predicted by the Standard Model of particle physics was found. So far, many of its properties were measured precisely and were found to be consistent with the predictions of the Standard Model. Nevertheless, there are still many important signatures to be discovered, such as the trilinear Higgs boson self-coupling, where one Higgs boson decays into a pair of Higgs bosons. A measurement of this process would give important insights into electroweak symmetry breaking, the mechanism that provides elementary particles with their masses. On the other hand, the discovery of the Higgs boson opened the way for searches for physics beyond the Standard Model, in which the Higgs boson is the decay product of a new heavier particle. There is definite evidence that the descriptions of the Standard Model are not complete. This led to the formulation of extensions to the Standard Model to solve currently unanswered questions in particle physics and cosmology.

Various searches for the production of Higgs boson pairs, both within the Standard Model and beyond, were performed by the ATLAS [3–14] and CMS [15–23] collaborations. With the large amount of proton–proton collisions provided by the Large Hadron Collider at unprecedented energies, experimental searches became increasingly sensitive to very high masses. Nevertheless, there are many scenarios beyond the Standard Model that are still mostly unconstrained in the high-mass regime.

Searches for a high-mass resonance X , decaying into two Higgs bosons, $X \rightarrow hh$, are experimentally very challenging. The Higgs bosons are neutral, weakly interacting and too short-lived to be detected directly, but can only be identified by their decay products. In this thesis, this is the decay into a pair of b quarks, $h \rightarrow b\bar{b}$, and the decay into a pair of τ leptons, $h \rightarrow \tau^+\tau^-$. The decay channel $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ is very promising, as it combines the high branching ratio of the decay into a b pair, the moderately high branching ratio of the decay into a τ pair, and a high background separation that can be achieved with τ leptons. When the mass of the heavy resonance is very high compared to the mass of the Higgs bosons, they are produced with large momenta. In this case, their decay products have typically large momenta and small distances. In the mass regime above 1 TeV, each the

b pair and the τ pair become so collimated that the individual particles can not be resolved by the standard reconstruction techniques of the ATLAS experiment. Dedicated algorithms for the reconstruction of b pairs with a large Lorentz boost were previously developed by the ATLAS collaboration [24]. In this thesis, a novel technique for the reconstruction of a boosted pair of hadronically decaying τ leptons, referred to as di- τ reconstruction, is proposed. Furthermore, a dedicated di- τ identification is developed. It uses multi-variate techniques to reduce the background of quark- or gluon-initiated jets that are produced at high rates at the Large Hadron Collider. A calibration and validation of the di- τ algorithms is performed using a data set enriched with the process $Z/\gamma^* \rightarrow \tau^+\tau^- + \text{jets}$. Here, the pair of τ leptons recoils against a jet, providing the τ pair with a substantial Lorentz boost. Finally, the di- τ techniques are applied in a search for $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$.

This thesis is organized as follows. In Chapter 2, the theoretical foundations of this thesis are covered. These are the Standard Model of particle physics and beyond the Standard Model scenarios, such as the Minimal Supersymmetric Standard Model, that predict the existence of heavy resonances that decay into a pair of Higgs bosons. Chapter 3 introduces the experimental setup. This is the Large Hadron Collider with proton–proton collisions at a center-of-mass energy of 13 TeV and the ATLAS experiment that recorded 139 fb^{-1} of those collisions for physics analyses. In Chapter 4, it is outlined how the different final state particles of a proton–proton collision are reconstructed in the ATLAS detector. This is followed by a description of the di- τ reconstruction and identification techniques in Chapter 5. The performance of the di- τ reconstruction is compared with the standard reconstruction of single τ leptons in the ATLAS experiment. The event selection that is common in the subsequent parts of this thesis is described in Chapter 6. The events are categorized into distinct selection regions that serve different purposes. This is, for example, the estimation of background processes, the calibration of the di- τ reconstruction techniques, and the search for new physics. The background estimation is outlined in Chapter 7. It is based, depending on the background process, on Monte Carlo simulations or on data-based approaches. In Chapter 8, a data-based calibration and validation of the di- τ reconstruction techniques is presented. For this purpose, a selection region is used that is enriched with $Z/\gamma^* \rightarrow \tau^+\tau^- + \text{jets}$. Finally, Chapter 9 shows the application of the di- τ reconstruction in a search for a heavy scalar resonance X decaying via $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$. A statistical analysis is performed to set exclusion limits on the production of such a resonance with masses from 1 TeV to 3 TeV.

Chapter 2

The Standard Model of Particle Physics and Beyond

The Standard Model (SM) of particle physics is a very successful theory for describing the elementary particles that are known today and their interactions via strong, weak, and electromagnetic forces. Since its first formulation, all particles predicted by the SM have been observed and many of their properties have been tested with high precision. The SM and its phenomenology is introduced at the beginning of this chapter. Despite the success of this model, it still faces challenges, both from a theoretical and experimental perspective.

There is definite evidence that the current understandings of the laws of particle physics are incomplete. This led to the formulation of theories that go beyond the SM (BSM), which are the subject of the second part of this chapter. These models extend the particle content of the SM, for example, by postulating a new symmetry, the Supersymmetry, or by including a description of the gravitational force. In this chapter, a particular emphasis is given to the Higgs sector of such models and to processes that can lead to the production of two Higgs bosons in a hadron collider experiment. In particular, the production of a Higgs boson pair is an important signature to test the predictions of the SM and to eventually discover new BSM resonances decaying into two Higgs bosons.

The last part of this chapter is devoted to the description of Monte Carlo event simulations. These are used to simulate the interactions of particles at a collider experiment. This is crucial for the planning of a particle physics analysis and to estimate signal and background processes.

Large parts of this chapter are built upon the descriptions of the *Review of Particle Physics* [25], *The Higgs Hunter's Guide* [26], and the following two reviews of Supersymmetry [27, 28]. These references, as well as those given throughout this chapter, are highly recommended for their comprehensive coverage of the rich phenomenology of the Standard Model and beyond.

In this thesis natural units are used, i.e., the vacuum speed of light, the reduced Planck constant, and the Boltzmann constant are defined to be one, $c = \hbar = k_B = 1$, so that energies and momenta are measured in eV, and time and distances are measured in eV^{-1} .

2.1 The Standard Model of Particle Physics

The Standard Model of particle physics is a relativistic quantum field theory that describes the interactions among the known elementary particles via strong, weak, and electromagnetic forces. The elementary particles that are described by the SM are summarized in Figure 2.1. There are spin-one-half fermions, which are further divided into quarks and leptons; there are spin-one bosons that mediate the electromagnetic, weak, and strong forces; and there is a Higgs boson, which is the outcome of the Brout–Englert–Higgs mechanism [29–31] that describes electroweak symmetry breaking. The fermions are grouped in three generations, where the particles of the second and third generation differ from their first-generation counterparts only by higher masses. Fermions have a corresponding anti-particle with opposite charges.¹ The following descriptions apply to both particles and their corresponding anti-particles.

	Fermions			Bosons	
Quarks	u up 2.16 MeV +2/3 1/2	c charm 1.27 GeV +2/3 1/2	t top 172.8 GeV +2/3 1/2	g gluon 0 0 1	h Higgs boson 125.1 GeV 0 0
	d down 4.67 MeV -1/3 1/2	s strange 93 MeV -1/3 1/2	b bottom 4.18 GeV -1/3 1/2	γ photon 0 0 1	
	e electron 511.0 keV -1 1/2	μ muon 105.7 MeV -1 1/2	τ τ lepton 1.777 GeV -1 1/2	Z Z boson 91.19 GeV 0 1	
Leptons	ν_e electron neutrino <1.1 eV 0 1/2	ν_μ muon neutrino <190 keV 0 1/2	ν_τ τ neutrino <18.2 MeV 0 1/2	W W boson 80.38 GeV ± 1 1	

Figure 2.1: The elementary particles in the Standard Model of particle physics. The mass, electric charge, and spin are given in the upper right corner for each particle [25].

2.1.1 Strong and Electroweak Interactions

In the Standard Model, every particle is represented by a field in the SM Lagrangian. The interactions between fermions are mediated by the exchange of gauge bosons. The latter are represented by gauge fields. Gauge fields ensure the invariance of the SM Lagrangian under local gauge transformations. According to Noether’s theorem [33], a symmetry in the sense of an invariance under a certain group of gauge transformations always implies the existence of a conservation law. The fundamental symmetry of the SM is given by the $SU(3)_C \times SU(2)_L \times U(1)_Y$ gauge group.

¹ Only for neutrinos it is yet unknown if they are so-called Majorana particles [32], which means they are their own anti-particles.

The interactions of quarks via the strong force is described by quantum chromodynamics (QCD) [34–38] and the $SU(3)_C$ gauge group. The charge in strong interactions is the so-called color charge. Each quark of flavor q and mass m_q is represented in the SM Lagrangian by a quark-field spinor $\psi_{q,a}$, where a can take three different color charges, often referred to as red, green, and blue. In interactions between a quark-field spinor and a gluon field $\mathcal{A}_\mu^C$, the color of the quark is rotated in the $SU(3)_C$ space. The index C of the gluon field can take values between one and eight, giving rise to eight kinds of gluons. The strength of strong interactions is given by the strong coupling constant g_s . Quarks and gluons, also called partons, have never been observed as free particles. They rather form colorless bound states, called hadrons, of multiple quarks, anti-quarks, and gluons. Hadrons are classified as either mesons, which have an integer spin, such as the pions π^+ , π^- , and π^0 , or baryons with a half-integer spin, like the proton p or the neutron n . Apart from the dynamic production of gluons, quarks, and anti-quarks within a hadron, a meson can be viewed as a bound state of a quark and an anti-quark, and a baryon can be viewed as a bound state of an odd number of quarks. High-energy quarks and gluons produced in hadron collisions like at the LHC undergo soft and collinear radiation of additional quarks and gluons, before they finally hadronize. These particle showers are typically reconstructed as jets in a particle detector.

The electromagnetic and weak forces are described in the unified model of electroweak interactions based on the $SU(2)_L \times U(1)_Y$ gauge group [39–42]. This is the unification of quantum flavordynamics (QFD) and quantum electrodynamics (QED). The index L denotes that only left-handed quarks and leptons take part in weak interactions, as only they carry a weak isospin $\vec{I}$, the charge of weak interactions. The weak hypercharge Y is another conserved quantity in the unified model of electroweak interactions and can be computed via $Y = 2(Q - I_3)$ from the electromagnetic charge Q and the third component I_3 of the weak isospin. Left-handed fermions are represented by doublets in the Lagrangian for electroweak interactions:

$$\psi_i = \begin{pmatrix} \nu_i \\ l_i^- \end{pmatrix} \quad \text{and} \quad \psi_i = \begin{pmatrix} u_i \\ d_i' \end{pmatrix}$$

for leptons and quarks, respectively. Here, l_i^- is the charged lepton of the i^{th} generation and ν_i is its corresponding neutrino. The up- and down-type quarks of the i^{th} generation are represented by u_i and d_i . The flavors of quarks mix in weak interactions with the Cabibbo-Kobayashi-Maskawa mixing matrix V_{ij} [43, 44]. Hence, the second component of the quark doublet is given with $d_i' = \sum_j V_{ij} d_j$. This concept incorporates flavor-changing processes in the quark sector into the theory of weak interactions. It explains CP violation, the violation of the combined symmetry of charge and parity conjugation, which is observed in weak interactions. Right-handed fermions are represented by singlets: (l_i^-) , (u_i) , and (d_i') , whereas right-handed neutrinos have not been observed to take part in weak interactions, so they are not represented by a singlet term in the Lagrangian. Similar to the mixing of quarks, a flavor mixing in the lepton sector is introduced by the Pontecorvo-Maki-Nakagawa-Sakata matrix [45, 46]. This allows a description of the mass-induced flavor oscillations of neutrinos

that are observed experimentally. The gauge fields of electroweak interactions are W_μ^i , with i running from one to three, for the $SU(2)_L$ group and B_μ for the $U(1)_Y$ group. The coupling constants of W_μ^i and B_μ are given with g and g' , respectively.

2.1.2 Electroweak Symmetry Breaking

The gauge fields that are discussed above are introduced into the SM Lagrangian without any mass terms, as those would violate local gauge invariance. However, this is in contradiction to the experimental observations that in particular the W and Z bosons have distinct masses, as shown in Figure 2.1. The inclusion of mass terms for these gauge bosons, as well as for the left- and right-handed fermions, is explained by the spontaneous symmetry breaking of electroweak interactions in the Brout–Englert–Higgs (BEH) mechanism [29–31]. For that purpose, an additional scalar field Φ and a potential $V(\Phi)$ are introduced, which leads to a non-zero vacuum expectation value v . In the state of lowest energy, at the vacuum expectation value, the $SU(3)_C \times SU(2)_L \times U(1)_Y$ symmetry is broken into $SU(3)_C \times U(1)_Q$. After electroweak symmetry breaking, the gauge groups of strong and electromagnetic interactions remain unbroken. Their mediators, the gluons and photons, remain massless, whereas the W and Z bosons, as mediators of the weak force, acquire masses.

Even after the discovery of a Higgs boson, which finally confirmed the BEH mechanism, the exact shape of the potential $V(\Phi)$ is still partly unknown.² In its minimal form it is given by

$$V(\Phi) = \mu^2 \Phi^\dagger \Phi + \lambda (\Phi^\dagger \Phi)^2 \quad (2.1)$$

with a complex scalar Higgs doublet

$$\Phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}.$$

Alternative representations of the Higgs field and its potential are discussed later in this chapter. Here, the potential develops a minimum at $v = \sqrt{-\mu^2/\lambda}$ if μ^2 is negative and λ positive.

The Higgs field, with foremost four degrees of freedom due to its two complex components, is redefined around the vacuum expectation value:

$$\Phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h \end{pmatrix},$$

where h can be identified with a spin-zero particle, the Higgs boson, and the remaining three degrees of freedom become the longitudinal components of the Z and $W^\pm$ bosons after electroweak symmetry breaking. The photon field A_μ and the fields of the charged

² As discussed further below and in References [47, 48], it is possible that the Higgs potential includes operators of higher orders than $(\Phi^\dagger \Phi)^2$. The values of μ and λ can be deduced to some extent from their relations to the measured mass of the Higgs boson and the vacuum expectation value v . However, their relations change if higher-order operators are included in the potential. In particular the trilinear and quartic Higgs self-interactions, whose strengths are parameterized by λ , have not been observed yet, hence, only indirect constraints exist so far.

and neutral weak bosons, $W_\mu^\pm$ and Z_μ , arise from a mixture of the electroweak gauge fields B_μ and W_μ^i :

$$\begin{aligned} A_\mu &= B_\mu \cos \theta_W + W_\mu^3 \sin \theta_W, \\ W_\mu^\pm &= \frac{1}{\sqrt{2}}(W_\mu^1 \mp iW_\mu^2), \\ Z_\mu &= -B_\mu \sin \theta_W + W_\mu^3 \cos \theta_W, \end{aligned}$$

where $\theta_W = \tan^{-1}(g'/g)$ is the weak mixing angle. The vacuum expectation value is related to the Fermi constant G_F via $v^2 = (\sqrt{2}G_F)^{-1}$. The Fermi constant is known with high precision from measurements of the muon lifetime. From this relation, the vacuum expectation value is determined to be $v = 246.22$ GeV [25]. The masses of the bosons are given by:

$$\begin{aligned} m_h &= \sqrt{2\lambda}v = \sqrt{-2\mu^2}, \\ m_W &= \frac{1}{2}gv, \\ m_Z &= \frac{1}{2}\sqrt{(g')^2 + g^2}v, \\ m_\gamma &= 0. \end{aligned}$$

The masses of the fermions are generated, after electroweak symmetry breaking, by a coupling between a right-handed fermion singlet, a left-handed fermion doublet, and the Higgs field. The mass of each fermion f is parameterized by its Yukawa coupling y_f to the Higgs field:

$$m_f = \frac{1}{\sqrt{2}}y_f v.$$

The couplings $g_{hf\bar{f}}$ of the Higgs boson to fermions and the couplings g_{hVV} to the vector bosons Z and $W^\pm$ are, respectively, proportional to the fermion mass m_f and to the square of the vector boson mass m_V :

$$g_{hf\bar{f}} = \frac{m_f}{v}, \quad g_{hVV} = \frac{2m_V^2}{v}.$$

The most important process to produce a Higgs boson in a high-energy hadron collider is via gluon–gluon fusion. As the Higgs boson does not couple directly to the massless gluons, this process is mediated by the exchange of virtual heavy quarks, which are mainly top quarks and a small contribution from bottom quarks. Contributions from other quarks are strongly suppressed due to their lower masses. The SM also predicts trilinear and quartic Higgs boson self-interactions, with strengths g_{hhh} and g_{hhhh} , as well as couplings between two Higgs bosons and two vector bosons with the strength g_{hhVV} :

$$g_{hhh} = \frac{3m_h^2}{v}, \quad g_{hhhh} = \frac{3m_h^2}{v^2}, \quad g_{hhVV} = \frac{2m_V^2}{v^2}. \quad (2.2)$$

2.1.3 Production of Higgs Boson Pairs in the Standard Model

The production of Higgs boson pairs is an important signature to test the predictions of the Standard Model. In particular the observation of the trilinear Higgs boson self-coupling would be a direct probe of the shape of the Higgs potential near the vacuum expectation value.³ In proton–proton collisions, the dominant process for the production of a Higgs boson pair is gluon–gluon fusion. It consists of two different amplitudes that are depicted in Figure 2.2: the production via a heavy quark loop and via trilinear Higgs boson self-interaction. These amplitudes interfere negatively, leading to a very low cross section for Higgs boson pair production in the SM.

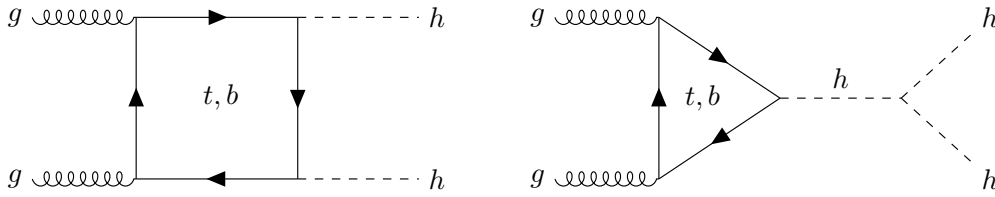


Figure 2.2: Feynman diagrams for the production of two Higgs bosons via gluon–gluon fusion. The production via a heavy quark loop is shown in the left diagram. The production via Higgs boson self-interaction is shown in the right diagram.

Searches for Higgs boson pairs are performed in a variety of final states. The branching ratios of the decays of two Higgs bosons are shown in Table 2.1 for the most important decay channels. Combinations of searches in different final states that used the data takings of the years 2015 and 2016 were published by the ATLAS collaboration and by the CMS collaboration [9, 20]. From those two combinations, the ATLAS collaboration provided the most stringent constraints on the SM production of Higgs boson pairs. An upper limit on the cross section for Higgs boson pair production of 6.9 times the SM prediction was observed at 95% confidence level, whereas in particular the search in the $b\bar{b}\tau^+\tau^-$ final state showed the highest sensitivity [5]. The search in the $b\bar{b}b\bar{b}$ final state was recently updated by the CMS collaboration by using the full LHC Run 2 data, which observed an upper limit on the Higgs boson pair production of 3.9 times the SM prediction [23].

Although the SM prediction for the trilinear Higgs boson self-coupling is very small, the coupling strength changes when operators of higher orders are introduced to the Higgs potential in Equation 2.1 [47, 48]. This effect is parameterized by κ_λ , the ratio of the Higgs boson self-coupling to the SM prediction. The SM predictions are reproduced in the case of $\kappa_\lambda = 1$. Due to the negative interference between the production via quark loop and the production via trilinear self-interaction, a modification of the strength of Higgs self-interaction would have large effects on the cross section and kinematics of the Higgs boson pair production. To this date, the most stringent constraints on κ_λ were set by the ATLAS collaboration with $-1.5 < \kappa_\lambda < 6.7$ at 95% confidence level in a search in the $b\bar{b}\gamma\gamma$ final state using the full LHC Run 2 data [12].

³ The trilinear Higgs boson self-coupling g_{hhh} in Equation 2.2 can also be written as $g_{hhh} = 6\lambda v$ to illustrate its relation to the parameter λ of the Higgs potential.

Table 2.1: Branching ratios of the most important decay channels of Higgs boson pairs. Only final states that were considered in the ATLAS or CMS searches [9, 20] are listed. The branching ratios are derived from the values given in Reference [49] for the decay of a single Higgs boson with a mass of 125 GeV.

Decay channel	Branching ratio
$hh \rightarrow b\bar{b}b\bar{b}$	33.9 %
$hh \rightarrow b\bar{b}W^+W^-$	24.9 %
$hh \rightarrow b\bar{b}\tau^+\tau^-$	7.3%
$hh \rightarrow W^+W^-W^+W^-$	4.6%
$hh \rightarrow b\bar{b}ZZ$	3.0%
$hh \rightarrow b\bar{b}\gamma\gamma$	0.3%
$hh \rightarrow W^+W^-\gamma\gamma$	0.1%

2.1.4 Challenges of the Standard Model

The Standard Model of particle physics is a very successful theory for describing the interactions between the elementary particles that are known today. All particles predicted by the SM have been observed and many of their properties have been scrutinized with high precision in a large number of experiments. However, the SM faces challenges, both from a theoretical and experimental standpoint, which show that the current understandings of the laws of particle physics are incomplete. Some of those problems are briefly introduced in this section.

As is the case for most models, the validity of the SM is limited to a certain energy range. For the SM, a definitive upper bound for its validity is the Planck scale with energies of about 10^{19} GeV. At those energies, quantum effects of gravity become important in particle interactions. This energy scale is far beyond the accessibility of particle accelerators that would ever be built, but it points to one of the most striking shortcomings of the SM, that it does not include a description of the fourth fundamental force, gravity. It is also rather unsatisfactory that the SM does not offer explanations for fundamental questions, such as whether there is an underlying principle that generates the very different fermion masses. This is related to the question of what determines the strengths of the Yukawa couplings of fermions to the Higgs field. It also cannot explain whether the three forces described by the SM have a common origin.

The observation of neutrino oscillations make it necessary to add a description of massive neutrinos to the SM. This is accomplished in multiple models by extending the particle content of the SM [50]. To determine which model best describes the nature of neutrinos, further experimental insight is needed into the exact neutrino masses, whether there are CP-violating processes in the leptonic sector, and whether neutrinos are their own antiparticles.

The SM does not explain the presence of dark matter, which accounts for 84.4% of the total matter density in the universe [25]. Dark matter is a non-baryonic kind of matter that is electromagnetically neutral or close-to-neutral. The only particles of the SM with such properties, the neutrinos, make up only between 0.5% and 1.6% of the non-baryonic

matter content of the universe. Also, the SM can not explain the large difference between the amounts of baryonic matter and anti-matter in the observed universe [51].

As discussed in the previous section, the SM prediction for the shape of the Higgs potential is not confirmed experimentally. Neither is it clear how the phase transition from a state of unbroken electroweak symmetry to a state of broken symmetry happened in the early universe. However, this has important cosmological implications. For example, the theory of electroweak baryogenesis [52] connects the generation of baryons to the electroweak phase transition in order to explain the asymmetry between matter and anti-matter. This explanation requires a first-order phase transition and CP violating processes that are large enough for the observed asymmetry. This would require the existence of new particles with masses not too far above the electroweak energy scale that couple to SM particles and in particular to the Higgs boson. Concerning the stability of the electroweak vacuum, it is remarkable that the measured mass of the Higgs boson is near-critical, meaning it is very close to the boundary between a stable and a metastable region [53]. This suggests that there might be an energy scale well below the Planck scale at which the electroweak vacuum is unstable. Although this observation is not in direct contradiction to the SM, the intermediate energy scale can be interpreted as a threshold at which new physics phenomena may take place.

The so-called *hierarchy problem* [54–57] arises from the large difference between the energy scale of the electroweak symmetry breaking and the Planck scale. In particular the mass of the Higgs boson is susceptible to large quantum corrections from virtual particles that couple to the Higgs boson. If the SM is valid up until the Planck scale it will require a significant fine-tuning of the free SM parameters, which is often perceived as unnatural. This fine-tuning is avoided if the SM is not valid up until the Planck scale or if there are contributions from new particles that cancel most of the terms that correct the mass of the Higgs boson.

Precision measurements of the magnetic moment of the muon found significant discrepancies between SM predictions and experimental results. In particular the anomalous magnetic moment of the muon, a_μ , is of interest as it arises from virtual effects, with contributions from electromagnetic, weak, and strong interactions. The most precise measurement of a_μ was presented by the Muon $g - 2$ collaboration [58]. It combines former results of the E821 experiment at the Brookhaven National Laboratory [59] with the latest measurement of the E989 experiment [60] at the Fermi National Laboratory. There, a discrepancy between the SM prediction [61] and the experimentally observed value was found with a significance of 4.2 standard deviations. This tension could be caused by particles that are yet unknown but interact with muons.

2.2 New Physics Beyond the Standard Model

As discussed in the previous section, there are good reasons to search for new physics phenomena and particles beyond the Standard Model. An appealing approach to extend the SM with new particles is by assuming a new symmetry, the Supersymmetry (SUSY) [27], which allows transformations from a boson into a fermion and vice versa. In this theory, a

superpartner exists for every particle degree of freedom with exactly the same properties, except for the spin. The Minimal Supersymmetric Standard Model (MSSM) extends the SM with the minimal amount of superpartners to achieve this symmetry. Since no such superpartners have been observed experimentally the new symmetry must be broken, similar to the electroweak symmetry that is also broken in the observable universe. This model can provide solutions to several shortcomings of the SM, as explained below.

If the SUSY breaking occurs at an energy scale M_{SUSY} that is not too far above⁴ the scale of electroweak symmetry breaking, it can provide a natural solution to the hierarchy problem. This mechanism is referred to as soft SUSY breaking. Due to the additional SUSY particles, large quantum corrections to the mass of the Higgs boson are avoided, because the contributions of the virtual fermions and their bosonic superpartners cancel each other, as they enter the calculation with opposite signs [27]. This also changes the evolution of the gauge couplings towards higher energies. Coincidentally, the gauge couplings evolve to a common scale in the MSSM, which could suggest a grand unification of the electromagnetic, weak, and strong forces [27]. In fact, SUSY is often incorporated into theories of grand unification [62]. Another remarkable feature of certain supersymmetric theories is that they can induce electroweak symmetry breaking without explicitly setting the Higgs mass parameter μ^2 to a negative value. A non-zero vacuum expectation value can arise even for positive μ^2 values from radiative quantum corrections to the Higgs potential in particular due to large top Yukawa couplings [27]. The MSSM also predicts stable electrically neutral particles, which are convincing dark matter candidates [63].

In Section 2.2.1, the phenomenology of the MSSM is introduced with an emphasis on its implications for the Higgs sector. There is the important requirement, that there must be two Higgs doublets, instead of only one as in the SM. This requirement can also be formulated in the more general Two-Higgs-Doublet Model (2HDM) [64]. The 2HDM can be considered without assuming Supersymmetry. It offers an alternative explanation of the electroweak symmetry breaking and answers certain open questions of the SM, e.g., it can provide additional sources of CP-violation that are needed for electroweak baryogenesis [65].

There are certain motivations to extend the Higgs sector even further, as done in the Next-to-Minimal Supersymmetric Standard Model (NMSSM) [66, 67]. This is discussed in Section 2.2.2. An alternative approach to solving the hierarchy problem and explaining the weakness of gravity is realized by introducing extra dimensions, as shown in Section 2.2.3.

2.2.1 The Minimal Supersymmetric Standard Model

The particles of the MSSM are organized in *supermultiplets* [27]. Each supermultiplet contains the fermionic and bosonic superpartners. Each fermion that is known in the SM is accompanied by a new scalar, i.e., a particle with a spin of zero.⁵ The superpartners of the quarks are called squarks and the superpartners of the leptons are called sleptons. The

⁴ An energy scale not above a few TeV is often mentioned in the literature, although this depends on the measure of fine-tuning and what level of fine-tuning is considered acceptable, as pointed out in the review on Supersymmetry theory in Reference [25].

⁵ Since the SM already distinguishes between right- and left-handed fermions, this must also be taken into account in any supersymmetric extension by distinguishing between superpartners of left- and right-handed fermions.

gauge bosons of the SM are accompanied by new spin-one-half fermions, called gauginos. In the MSSM, there are two Higgs supermultiplets, resulting in five Higgs bosons, as explained later. This is necessary to formulate a consistent quantum theory. With only one Higgs multiplet, the new fermionic partners of the Higgs boson would lead to gauge anomalies. Additionally, within the MSSM it is necessary that the two Higgs multiplets couple independently to either up-type quarks or to down-type quarks and charged leptons. The spin-one-half superpartners of Higgs bosons are called higgsinos. The higgsinos mix with gauginos to form the mass eigenstates of four electrically neutral neutralinos and two charged charginos.

In the MSSM, there are two Higgs doublets H_1 and H_2

$$H_1 = \begin{pmatrix} H_1^0 \\ H_1^- \end{pmatrix}, \quad H_2 = \begin{pmatrix} H_2^+ \\ H_2^0 \end{pmatrix}$$

with opposite weak hypercharges of -1 and $+1$, respectively. The Higgs potential is derived from the superpotential that describes the fundamental interaction between supermultiplets in the MSSM and from additional terms related to soft SUSY breaking. It is given by [28]

$$\begin{aligned} V_H = & (|\mu|^2 + m_{H_1}^2)(|H_1^0|^2 + |H_1^-|^2) + (|\mu|^2 + m_{H_2}^2)(|H_2^0|^2 + |H_2^+|^2) \\ & - B\mu(H_1^- H_2^+ - H_1^0 H_2^0 + \text{h.c.}) + \frac{g^2 + g'^2}{8}(|H_1^0|^2 + |H_1^-|^2 - |H_2^0|^2 - |H_2^+|^2)^2 \\ & + \frac{g^2}{2}|H_1^- H_1^0 + H_2^{0*} H_2^+|^2. \end{aligned}$$

The mass terms of this potential, i.e., the terms with the squared Higgs fields, depend on the supersymmetric higgsino mass parameter μ , the mass parameters of the Higgs doublets m_{H_1} and m_{H_2} and the term with $B\mu$ that arises from soft SUSY breaking. The quartic couplings of the Higgs bosons are fixed by the electroweak coupling constants g and g' .

Electroweak symmetry breaking can occur if the potential is bounded from below and has a non-zero vacuum expectation value. This is fulfilled under the following conditions:

$$\begin{aligned} 2|B\mu| & < 2|\mu|^2 + m_{H_1}^2 + m_{H_2}^2, \\ (B\mu)^2 & > (|\mu|^2 + m_{H_1}^2)(|\mu|^2 + m_{H_2}^2). \end{aligned}$$

Then the Higgs fields can be developed around their vacuum expectations values v_1 and v_2 :

$$H_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} v_1 + H_1^0 + iP_1^0 \\ H_1^- \end{pmatrix}, \quad H_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} H_2^+ \\ v_2 + H_2^0 + iP_2^0 \end{pmatrix}.$$

The real fields H_1^0 and H_2^0 will mix to the physical fields of two scalar CP-even Higgs bosons h and H . The imaginary parts P_1^0 and P_2^0 mix to a pseudoscalar CP-odd Higgs boson A and a massless Goldstone boson G^0 . The Higgs boson A is also referred to as pseudoscalar whereas h and H are referred to as scalar Higgs bosons. The fields H_1^- and H_2^+ and their complex conjugates mix to charged Higgs bosons $H^\pm$ and Goldstone bosons $G^\pm$. The Goldstone bosons G^0 and $G^\pm$ become the longitudinal components of the Z and

$W^\pm$ bosons after electroweak symmetry breaking. The mixing of the CP-even Higgs bosons is described by the mixing angle α , whereas the mixings of the other charged and CP-odd Higgs bosons are given by the angle β . Conveniently, the mixing angle β can be expressed via the vacuum expectation values:

$$\tan \beta = \frac{v_2}{v_1}.$$

The vacuum expectation values are, as in the SM, connected to the Fermi constant, leading to the following constraint:

$$v^2 = v_1^2 + v_2^2 = (246 \text{ GeV})^2.$$

After electroweak symmetry breaking there are only two free parameters of the Higgs sector of the MSSM: α and β , or the more commonly used m_A and $\tan \beta$. Those parameters fix the masses of all five Higgs bosons at tree level:

$$\frac{\tan(2\alpha)}{\tan(2\beta)} = \frac{m_A^2 + m_Z^2}{m_A^2 - m_Z^2}, \quad (2.3)$$

$$m_{h,H}^2 = \frac{1}{2} \left(m_A^2 + m_Z^2 \mp \sqrt{(m_A^2 + m_Z^2)^2 - 4m_A^2 m_Z^2 \cos^2(2\beta)} \right), \quad (2.4)$$

$$m_{H^\pm}^2 = m_A^2 + m_W^2. \quad (2.5)$$

By convention, α is defined to be in the range of $-\pi/2 \leq \alpha \leq 0$, and h is lighter than H . In the MSSM, the Higgs boson h is typically identified with the observed Higgs boson with a mass of about 125 GeV. There are certain MSSM benchmark scenarios that take H to be compatible with the observed Higgs boson, but this is only possible in a highly constrained region of the MSSM parameter space, as can be seen, for example, in References [68, 69]. For the sake of clarity, h is taken to be the already observed Higgs boson in the following descriptions. It must be noted that the above equations for the Higgs boson masses are derived at tree level. For example, Equation 2.4 suggests that the mass of h would be smaller than the mass of the Z boson. However, radiative corrections, in particular the contributions from top quarks, bottom quarks, and their superpartners, can push m_h above the mass of the Z boson.

A few examples of important couplings are given in the following, whereby a focus is given on the interactions of particles known in SM with the Higgs bosons h and H , which are of central interest in this thesis. Comprehensive overviews that also discuss quartic couplings, couplings with charged Higgs bosons and potential couplings to new supersymmetric particles are given in References [26, 28]. The generic 2HDM that is not constrained by an underlying supersymmetric theory has typically a higher number of free parameters than the 2HDM implemented in the MSSM. An overview of the Higgs couplings in a more generic 2HDM can be found in References [64, 70].

In the MSSM, the fermion masses are generated by a coupling of the Higgs doublet H_1

to down-type fermions and a coupling of the Higgs doublet H_2 to up-type fermions.⁶ This results in different Yukawa couplings y_u and y_d for up- and down-type fermions,

$$y_u = \frac{\sqrt{2}m_u}{v_2} = \frac{\sqrt{2}m_u}{v \sin \beta}, \quad y_d = \frac{\sqrt{2}m_d}{v_1} = \frac{\sqrt{2}m_d}{v \cos \beta}.$$

As in the SM, the couplings to fermions with high masses, i.e., in particular to top quarks, bottom quarks, and τ leptons, are enhanced. This results in the following dependencies for the couplings of the CP-even Higgs bosons to a pair of fermions

$$\begin{aligned} g_{h uu} &\propto \frac{\cos \alpha}{\sin \beta} = \sin(\beta - \alpha) + \frac{\cos(\beta - \alpha)}{\tan \beta}, \\ g_{h dd} &\propto -\frac{\sin \alpha}{\cos \beta} = \sin(\beta - \alpha) - \tan \beta \cos(\beta - \alpha), \\ g_{H uu} &\propto \frac{\sin \alpha}{\sin \beta} = \cos(\beta - \alpha) - \frac{\sin(\beta - \alpha)}{\tan \beta}, \\ g_{H dd} &\propto \frac{\cos \alpha}{\cos \beta} = \cos(\beta - \alpha) + \tan \beta \sin(\beta - \alpha). \end{aligned}$$

From those relations, one can see that the couplings to down-type fermions are enhanced with $\tan \beta$, whereas the couplings to up-type fermions are suppressed with $\tan \beta$. Therefore, to search for H in the MSSM parameter space with large $\tan \beta$, the decay modes $H \rightarrow \bar{b}b$ and $H \rightarrow \tau^+\tau^-$ are important. This is also the case for the pseudoscalar A whose couplings to down-type and up-type fermions are directly proportional to $\tan \beta$ and $1/\tan \beta$, respectively. So far, the couplings of the observed Higgs boson agree well with the SM prediction, leading to constraints on the parameter space of the MSSM. In the so-called ‘alignment limit’, $\sin(\beta - \alpha) = 1$, the couplings of h are the same as in the SM. In the MSSM, this is fulfilled at tree level when $m_{H,A,H^\pm} \gg m_h$. Such a large mass hierarchy is also referred to as ‘decoupling limit’ because the interactions of h decouple from the Higgs bosons H , A , and $H^\pm$ with much higher masses. Alignment without decoupling can be achieved in the MSSM by a specific choice of SUSY parameters that enable certain radiative corrections [69]. In a generic 2HDM, alignment can be achieved without decoupling at tree level because the mixing angle α can be chosen independently from m_A [70]. The measurements of the coupling strengths of the observed Higgs boson give important constraints on the available parameter space of the MSSM. However, small deviations from perfect alignment can still be compatible with the most precise Higgs boson measurements, and the available MSSM parameter space is still large, as will be shown later in this section.

The trilinear couplings between two vector bosons Z or $W^\pm$ and a scalar Higgs boson are

$$\begin{aligned} g_{hVV} &\propto \sin(\beta - \alpha), \\ g_{HVV} &\propto \cos(\beta - \alpha). \end{aligned}$$

In the alignment limit, the MSSM and SM predictions for hVV coincide, whereas HVV

⁶ Up- and down-type refers to the third component I_3 of the weak isospin. Up-type fermions have $I_3 = +1/2$ and down-type fermions have $I_3 = -1/2$.

vanishes. The allowed couplings between a neutral Higgs boson and vector bosons are strongly restricted by CP-invariance. There is no coupling between one pseudoscalar A and two vector bosons. Also, if one vector bosons interacts with two neutral Higgs bosons, they must have opposite parity, which is only the case for AZh and AZH . The trilinear couplings hhh and Hhh are given by

$$\begin{aligned} g_{hhh} &\propto 3 \cos(2\alpha) \sin(\beta + \alpha), \\ g_{Hhh} &\propto 2 \sin(2\alpha) \sin(\beta + \alpha) - \cos(2\alpha) \cos(\beta + \alpha). \end{aligned}$$

The trilinear self-coupling hhh vanishes at $\alpha = 0$. Trilinear Higgs boson couplings with pseudoscalars must have exactly two pseudoscalars involved, like AAh and AAH . Accordingly, a decay of A into two lighter Higgs bosons is not allowed.

The couplings typically receive large radiative corrections, just like the tree-level mass predictions mentioned before. The tree-level predictions of the MSSM Higgs sector depend only on two free parameters, but due to the radiative corrections they become sensitive to additional SUSY parameters, like the soft-SUSY-breaking scale, the masses of new supersymmetric particles, and their mixing terms. To reduce this complexity, *benchmark scenarios* are defined that fix the additional parameters to specific values that, e.g., feature unique phenomenological signatures or have a high potential to be discovered with current or future experiments.

Several popular benchmark scenarios can be found in Reference [69], which all have in common that the SUSY mass parameters are chosen to be in the TeV scale. At this scale, the new SUSY particles may still be within experimental reach. However, it has the consequence that the parameter space $\tan\beta \lesssim 8$ is largely ruled out from those scenarios. At lower $\tan\beta$ values, the SUSY mass parameters would need to be much higher than assumed in the scenarios in order to bring the mass and couplings of h into agreement with the values of the observed Higgs boson.

The hMSSM [71–74] reduces the complexity of multiple free parameters with a certain approximation. All new SUSY particles are assumed to be heavy enough that their effect on the Higgs boson couplings can be neglected. This results in only one additional free parameter that describes the radiative corrections, which can be fixed by setting m_h to the measured mass of the observed Higgs boson. In this case, the masses and couplings with corrections are again fully determined by the tree-level parameters. However, the above assumptions are not fulfilled in the entire parameter space of $\tan\beta$ and m_A , as detailed in References [74, 75]. For example, for every $\tan\beta$ exists a minimum m_A that is needed to reproduce the observed value for m_h . The contributions from bottom quarks and their superpartners must be sufficiently small to be negligible, which is naturally fulfilled at low values of $\tan\beta$. Also, it is known that further corrections are required for the decay $H \rightarrow hh$ to achieve a good agreement between the hMSSM approximation and a full MSSM calculation [76].

The $M_{h,\text{EFT}}^{125}$ [77] benchmark scenario is explicitly designed for the low $\tan\beta$ region.⁷

⁷ The range of $1 \leq \tan\beta \leq 10$ is considered in the $M_{h,\text{EFT}}^{125}$ benchmark scenario.

Agreement of m_h with the observed value of about 125 GeV is realized by a flexible SUSY mass scale that is adjusted for every point of m_A and $\tan\beta$ in the parameter space. The MSSM Higgs sector is modeled by an effective field theory (EFT) in the framework of a low-energy 2HDM. The predictions of the $M_{h,\text{EFT}}^{125}$ benchmark scenario for the most important decay channels of H are illustrated in Figure 2.3. The values for the branching ratios are provided by the LHC Higgs Cross Section Working Group [49]. The Higgs boson masses and their mixing is computed in the FeynHiggs program [78–85]. The branching ratios are obtained from the most precise results of the FeynHiggs, HDECAY [86–89], and PROPHECY4f [90–92] programs.

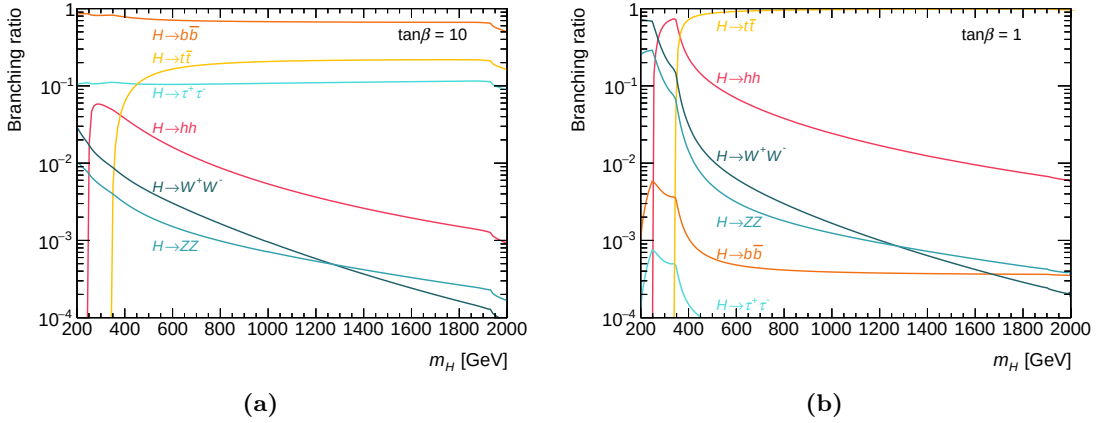


Figure 2.3: Branching ratios of the most important decay modes of the heavy scalar H in the $M_{h,\text{EFT}}^{125}$ [77] benchmark scenario for $\tan\beta = 10$ (a) and $\tan\beta = 1$ (b) as a function of the mass m_H of the heavy scalar Higgs boson. The branching ratio values are provided by the LHC Higgs Cross Section Working Group [49].

In Figure 2.3(a) it can be seen that for $\tan\beta = 10$ the decay channel $H \rightarrow b\bar{b}$ is dominant over the entire m_H range due to the $\tan\beta$ enhancement of couplings to down-type fermions. The decay channel $H \rightarrow \tau^+\tau^-$ gets the same $\tan\beta$ enhancement, but is suppressed due to the lower masses of the τ leptons. The branching ratio of $H \rightarrow t\bar{t}$ increases rapidly when it becomes kinematically available at $m_H > 2m_t$. At even higher masses of about 2 TeV, decays into new SUSY particles may contribute, as can be seen from the decrease in branching ratios at the upper end of the mass range.

The branching ratios of H under the assumption of $\tan\beta = 1$ are shown in Figure 2.3(b). At $m_H \approx 200$ GeV, the decays into two vector bosons are dominant. The decay channel $H \rightarrow hh$ is dominant in the region of $2m_h < m_H < 2m_t$. This is followed by an exceptionally high branching ratio of $H \rightarrow t\bar{t}$ at $m_H > 2m_t$. This leads to a difficult situation for experimental searches for H with a high mass in the low $\tan\beta$ regime. Searches in the $H \rightarrow t\bar{t}$ decay channel have been performed by the ATLAS [93] and CMS [94] collaborations with data from LHC Run 1 and early Run 2, respectively. Such analyses face a large background of $t\bar{t}$ events that are produced with a high cross section at the LHC. Additionally, interference effects between signal and non-resonant $t\bar{t}$ production must be accounted as they distort a signal peak to non-trivial line shapes [95, 96]. A different approach is chosen in this thesis, by searching in the $H \rightarrow hh$ decay channel, which has still the second highest

branching ratio, although it is only about 1% at $m_H = 1.5$ TeV, for example. Nevertheless, a much cleaner signal signature and a smaller background can be expected, depending on the decay channel of the lighter Higgs bosons h .

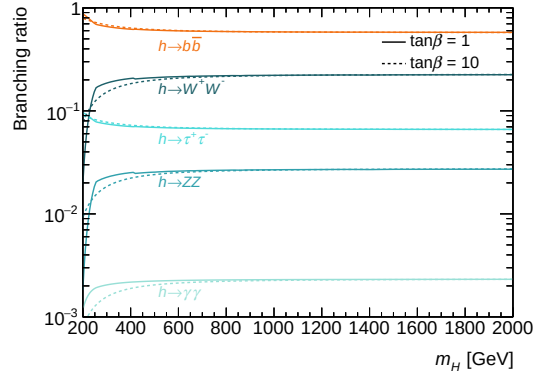


Figure 2.4: Branching ratios of the most important decay modes of the light scalar h in the $M_{h,\text{EFT}}^{125}$ [77] benchmark scenario for $\tan\beta = 1$ (solid lines) and $\tan\beta = 10$ (dashed lines) as a function of the mass m_H of the heavy scalar H . The branching ratio values are provided by the LHC Higgs Cross Section Working Group [49].

The branching ratios of the decays of the Higgs boson h with a mass of 125 GeV are shown in Figure 2.4. At the lowest shown masses, the branching ratios deviate from the SM prediction, but become very close to the SM predictions when approaching the decoupling limit at higher m_H . In the mass regime above a few hundred GeV, the dependence on $\tan\beta$ is small. For the final states of the $H \rightarrow hh$ decay, this gives very similar branching ratios as for the SM non-resonant hh production previously discussed in Section 2.1.3 and Table 2.2. Searches for BSM resonant hh production have been performed in a variety of final states by the ATLAS [3–9, 11–14] and CMS [15–22] collaborations. The $b\bar{b}b\bar{b}$ final state benefits from a high branching ratio, but has a large background from other quarks and gluons. The decay into $b\bar{b}\tau^+\tau^-$ has still a relatively high branching ratio and benefits from a good background separation that can be achieved with the τ leptons. Decays involving vector bosons also have a relatively high branching ratio, but typically only those decay channels with at least one leptonic decay of the vector boson are considered to achieve a decent background separation, which further reduces the number of available signal events. The $b\bar{b}\gamma\gamma$ final state has a small branching ratio but benefits from the clean signature of two photons.

The parameter spaces of the hMSSM approximation and the $M_{h,\text{EFT}}^{125}$ benchmark scenario are shown in Figures 2.5 and 2.6, respectively. Figure 2.5 shows the regions of the hMSSM parameter space that are excluded by various ATLAS analyses. This figure is regularly updated by the ATLAS collaboration. References to the contributing analyses can be found in the figure legend and in Reference [97]. Figure 2.6 shows the excluded parameter space of the $M_{h,\text{EFT}}^{125}$ benchmark scenario. This is calculated from the results of the most sensitive ATLAS and CMS analyses that were available when Reference [77] was published. The contributing analyses can be found in that reference. For both scenarios, significant constraints arise from precision measurements of the 125 GeV Higgs boson couplings, disfavoring low masses m_A for the entire $\tan\beta$ range. At high $\tan\beta$ values and high masses

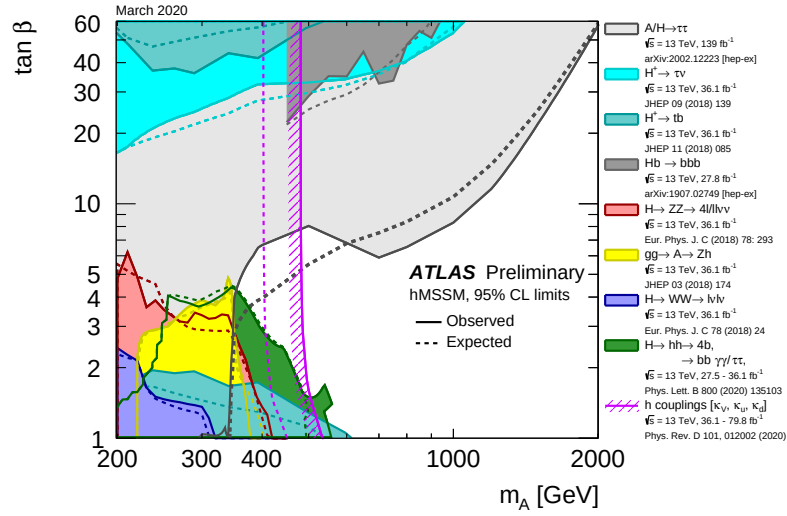


Figure 2.5: Regions of the $(m_A, \tan \beta)$ parameter space of the hMSSM approximation that are excluded at 95% confidence level by various analyses of the ATLAS collaboration. Observed and expected exclusion limits are represented by solid and dashed lines, respectively. The colored areas are excluded by direct searches for additional Higgs bosons. The purple line represents the exclusion from measurements of the 125 GeV Higgs boson couplings. This figure is regularly updated by the ATLAS collaboration. All analyses used the 2015 and 2016 data takings, except for the h couplings measurement that also included 2017 data and the $A/H \rightarrow \tau^+ \tau^-$ search that used the full LHC Run 2 data set. [97]

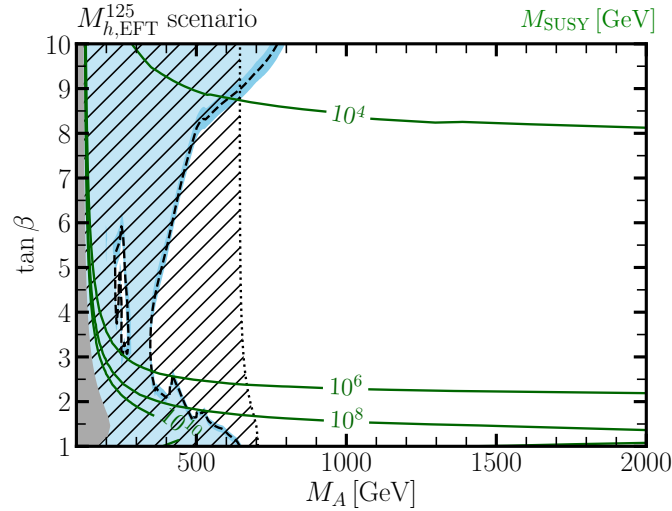


Figure 2.6: The $(m_A, \tan \beta)$ parameter space of the $M_{h, \text{EFT}}^{125}$ benchmark scenario. The blue region is excluded at 95% confidence level by direct LHC searches for additional Higgs bosons. The hatched area is disfavored at the 2σ level by measurements of the signal rates of the 125 GeV Higgs boson at the LHC. The green contour lines represent the energy scale M_{SUSY} that is required to get $m_h = 125$ GeV. The gray area represents the parameter space at which the predicted m_h is not compatible with 125 GeV. [77]

m_A , the most sensitive search channel is $H/A \rightarrow \tau^+\tau^-$. At low $\tan\beta$ values, the searches for $H \rightarrow hh$ and $H^\pm \rightarrow tb$ provide the strongest constraints. It can also be seen that large parts of the parameter space of high masses and low $\tan\beta$ values are yet unexplored, which is the main motivation for the search presented in this thesis.

2.2.2 The Next-to-Minimal Supersymmetric Standard Model

The NMSSM [66, 67] further extends the Higgs sector of the MSSM with an additional singlet field S , which only couples to the MSSM Higgs doublets. There are certain theoretical motivations for this extension. In the MSSM, there is no natural explanation for the mass parameter μ to lie in the electroweak energy scale, which is known as the μ problem [98]. This is solved in the NMSSM, as the parameter μ is generated dynamically when the Higgs singlet acquires a vacuum expectation value via spontaneous symmetry breaking. Also, the NMSSM requires less radiative corrections to render a Higgs boson with a mass of 125 GeV and provides an explanation for the current lack of experimental evidence for supersymmetric partners [49].

If CP is conserved in the NMSSM, it predicts two more neutral Higgs bosons, CP-even and CP-odd, which can mix with the other neutral Higgs bosons that are already described in the MSSM. This leads to a rich phenomenology of the NMSSM Higgs sector that is yet largely unconstrained [99]. A Higgs boson h_S , which has a large contribution from the singlet field S , would have only a small coupling to SM particles.⁸ This results in small cross sections of the usual production channels like gluon–gluon fusion or Higgs-strahlung off a Z boson. Therefore, it is possible that there is a Higgs boson considerably lighter than 125 GeV that has not yet been observed. The main production mode for such a Higgs boson would come from the decay of a heavier Higgs boson, e.g., via $H \rightarrow hh_S$ or $H \rightarrow h_S h_S$. Such signal topologies would not only allow for a search for NMSSM physics, but in case of discovery would also allow for a distinction from MSSM physics. However, the additional degree of freedom of the mass of h_S further complicates such analyses. With increasing masses of H or decreasing masses of h_S , a reliable reconstruction of boosted decay signatures becomes increasingly important. The LHC Higgs Cross Section Working Group provides several NMSSM benchmark points for which the $b\bar{b}\tau^+\tau^-$ final state is an important signature [49]. An interpretation of the results of this thesis in the NMSSM is not done, however. It would be worth to be considered in the future.

2.2.3 Extra Dimensions

The extension of the four-dimensional spacetime with an additional spacial dimension was initially proposed by Kaluza and Klein (KK) [100–102] in order to unify gravity and electromagnetism. In this theory the fifth dimension is closed like a circle in the direction of the extra dimension, meaning that it is periodic and has a compactification radius r_c . The periodicity and compactness was initially introduced to explain the quantization of the electric charge and to motivate the fact that the presence of the fifth dimension is not

⁸ This section focuses on the phenomenology of CP-even Higgs bosons, but analogous statements can be derived for CP-odd Higgs bosons.

noticeable in ordinary experiments. In later approaches, the periodicity rather leads to the interpretation of a field having an infinite number of excitation modes, like a massless graviton with an infinite number of excitations with increasing masses. This formalism is used, for example, in the proposals of Arkani-Hamed, Dimopoulos, and Dvali (ADD) [103] and in the model of Randall and Sundrum (RS) [104].

In the ADD scenario, there are at least two extra spacial dimensions, which are compactified, but can still be almost as big as a millimeter. The SM fields are located in the four-dimensional subspace, the so-called brane, whereas only the gravitational force can propagate the extra dimensions, which gives an explanation for its apparent weakness. Experimental constraints for this scenario are derived from investigations of gravity at small distances and from astrophysical and collider experiments. An overview of the most constraining experiments can be found in the review of extra dimensions in Reference [25].

The RS scenario is particularly interesting as it not only explains the weakness of the gravitational force but also provides a solution to the hierarchy problem and can explain the very different masses of the fermions by introducing only one extra dimension. The hierarchy between the weak scale and the Planck scale is generated by the warp factor e^{-2kr_c} that is introduced to the background metric

$$ds^2 = e^{-2kr_c\phi} \eta_{\mu\nu} dx^\mu dx^\nu + r_c^2 d\phi^2.$$

The curvature factor k must be of order of the Planck scale. The x^μ are the four-dimensional spacetime coordinates and ϕ is the coordinate of the extra dimension. The extra dimension is restricted by its size r_c and by the condition $0 \leq \phi \leq \pi$. There are two branes at the boundaries $\phi = 0$ and $\phi = \pi$, whose metric differs greatly due to the exponential warp factor. The $\phi = 0$ brane corresponds to the Planck scale and the $\phi = \pi$ brane corresponds to the electroweak scale if $ke^{-2kr_c\pi} \sim \text{TeV}$. In this case, no unnaturally high or low parameters are needed, as the hierarchy emerges from the exponential warp factor.

In the initial RS proposal, the SM fields are assumed to be located in the TeV brane. However, later proposals [105–108] extended this approach, with the possibility for SM fields to propagate between the branes, the so-called bulk. Only the Higgs field is required to be located close to the TeV brane in order to maintain the solution to the hierarchy problem. This generalization has the advantage that depending on the location of a fermion field in ϕ , an exponentially suppressed Yukawa coupling to the Higgs field can be constructed, which explains the very different fermion masses [108]. The two RS scenarios, often referred to as RS1 model and RS bulk model, have a very different phenomenology, but in general they manifest in the existence of KK excitations of SM particles, a spin-0 radion R [109–111], and a spin-2 KK excitation of a graviton G [112, 113] with masses in the TeV scale. The free dimensionless parameter $k/\bar{M}_{\text{Pl}}$, where $\bar{M}_{\text{Pl}}$ is the reduced four-dimensional Planck mass, is typically taken as a basic parameter of the model in combination with either kr_c or the mass of the lightest excitation of the graviton [114].

A comprehensive overview of the experimental constraints on the RS models can be found in Reference [25]. Here only a few important examples shall be mentioned. The dominant production mode of a KK excitation of a graviton in both the RS1 model and

the RS bulk model is gluon–gluon fusion [114]. The branching ratios of the decay of such a graviton depends strongly on the model and on the location of the SM fields in the bulk. For a search for KK gravitons in the RS1 model, the most appropriate search channels are the di-jet [115], di-lepton [116, 117], and di-photon [118–120] final states. From these analyses the searches in the di-photon final state are most sensitive. The ATLAS collaboration excluded an RS1 graviton with a mass below 4.5 TeV if $k/\bar{M}_{\text{Pl}} = 0.1$ [119], and the CMS collaboration excluded masses below 2.3–4.6 TeV in the parameter range $0.01 < k/\bar{M}_{\text{Pl}} < 0.2$ [120] at 95% confidence level. In the RS bulk model, the light fermions, photons, and gluons are assumed to be localized near the Planck brane, which strongly suppresses their couplings to G . If the field of a top quark is localized near the TeV brane, the decay into $t\bar{t}$ has the highest branching ratio. Otherwise the decays into two vector bosons [121–124] and into two Higgs bosons [9, 14, 20–22] become dominant. From those analyses the graviton excitations in the RS bulk model are excluded at 95% confidence level with masses below 2.3 TeV [121] if $k/\bar{M}_{\text{Pl}} = 1.0$ and with masses smaller than 850 GeV [124] and between 1 TeV and 1.2 TeV [21] if $k/\bar{M}_{\text{Pl}} = 0.5$.

In this thesis, an interpretation of the results in models of extra dimensions is not performed, although this is worth considering for future investigations. In particular the radion and the KK excitations of a graviton in the RS bulk model are potential signals that can decay into a pair of Higgs bosons and into the $b\bar{b}\tau^+\tau^-$ final state. However, in this thesis, graviton simulations are used to develop the di- τ reconstruction techniques, as discussed in more detail in the next section.

2.3 Monte Carlo Event Simulations

High-energy particle physics analyses, like the one presented in this thesis, use general-purpose Monte Carlo event generators [125] to simulate the proton–proton collisions at the LHC. A prediction as accurate as possible is crucial, in order to plan an analysis, evaluate techniques for particle reconstruction in the detector, and to estimate distributions of observables of signal and background processes, as well as their yields. The generation of a proton–proton collision event at the LHC is outlined in the following. The specific Monte Carlo generators that are used to simulate the BSM signal processes of this thesis are described afterwards.

2.3.1 Monte Carlo Event Generation

The simulation of a proton–proton collision event typically involves hundreds of final state particles, with momenta ranging over several orders of magnitude. To predict the cross section of a certain process of interest, phase space integrals over a large number of dimensions must be solved, which is an ideal application for Monte Carlo sampling techniques. The event generation is divided into multiple stages based on the scale of momentum transfer, from the simulation of the hard scattering process at the highest scale down to the order of 1 GeV where the hadronization of partons takes place.

The hard scattering process at the highest scales is calculated perturbatively. The

incoming partons of the proton beams interact and produce typically a small number of high-momentum outgoing particles. The cross section to produce the final state n from the initial partons a and b is determined by the factorization formula [125, 126]

$$\sigma = \sum_{a,b} \int_0^1 dx_a dx_b \int f_a^{h_1}(x_a, \mu_F) f_b^{h_2}(x_b, \mu_F) d\hat{\sigma}_{ab \rightarrow n}(\mu_F, \mu_R).$$

The parton distribution function (PDF) f_a^h models the probability of finding a parton a with a momentum fraction x relative to its parent hadron h when probed at the factorization scale μ_F . The parton-level cross section $\hat{\sigma}_{ab \rightarrow n}$ is determined from the matrix element squared $|\mathcal{M}_{ab \rightarrow n}|^2$ at any point of phase space. It also depends on the factorization scale μ_F and the renormalization scale μ_R . The choice of these scales is in principle arbitrary. Only in the limit of an infinite number of terms in the perturbation series, their dependencies cancel out. In practice, these scales are set to a hard scale that is characteristic for the process, e.g., to $\mu_F = \mu_R = M^2$ for the s -channel production of a resonance with mass M . An uncertainty is usually evaluated by varying these scales.

The incoming and outgoing partons of the hard scattering process can radiate gluons, which can produce pairs of quarks and anti-quarks or radiate more gluons. This is simulated by parton shower algorithms, which are based on step-wise Markov chains that add one or more partons probabilistically. It is also likely that in a given proton–proton scattering more than one parton pair interact. These multi-parton interactions produce a so-called underlying event with additional partons in the final state that must be modeled in addition to the primary hard scattering process. The simulation of electromagnetic radiation is either performed by using parton shower algorithms or by incorporating the Yennie-Frautschi-Suura [127] approach. The former approach is commonly preferred when both QCD and QED radiations are possible, while the latter is used by some generators for colorless particles where only electromagnetic radiations can occur.

At the scale of about 1 GeV, the hadronization of colored partons into colorless hadrons is modeled. At this scale, perturbation theory breaks down, and the hadronization is rather described by non-perturbative models. Afterwards, unstable hadrons as well as τ leptons must decay further into a set of particles that can be considered stable with respect to the typical time scale of a particle in a detector. These simulations utilize branching ratios known from experimental measurements, but also theoretical considerations are taken into account.

2.3.2 Signal Monte Carlo Samples

The following two BSM processes of resonant production of two Higgs bosons are used as signal samples in this thesis: a spin-2 resonance G in the decay channel $G \rightarrow hh \rightarrow \tau^+ \tau^- \tau^+ \tau^-$ and a spin-0 resonance X decaying via $X \rightarrow hh \rightarrow b\bar{b} \tau^+ \tau^-$. These processes are depicted in Figure 2.7. In both cases, the Higgs bosons h behave SM-like and have a mass of 125 GeV, and their branching ratios are set to the values predicted by the SM. The process $G \rightarrow hh \rightarrow \tau^+ \tau^- \tau^+ \tau^-$ describes a decay of the lightest KK excitation of a graviton in the RS bulk model. This process is used in Chapter 5 for the development of the boosted di- τ

reconstruction and identification techniques. A final state with four τ leptons is chosen in order to increase the number of boosted τ pairs per simulated event. The second process, $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$, is inspired by a 2HDM heavy Higgs boson decaying into two lighter Higgs bosons. If such a heavy spin-0 resonance exists it could be the manifestation of multiple theories, such as a heavy CP-even Higgs boson in the MSSM or NMSSM, or possibly a radion in the RS model. Hence, the general notation X is used in the following. This process is also used to validate the di- τ reconstruction techniques in Chapter 5, but primarily serves as a signal sample for the search for resonant Higgs boson pair production in Chapter 9. The MC samples of the SM backgrounds are described when the estimation of SM backgrounds is discussed in Chapter 7.

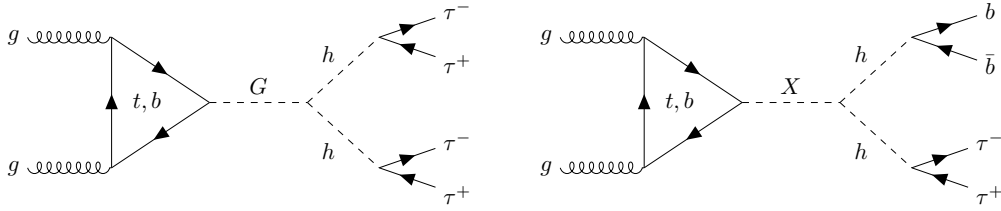


Figure 2.7: Feynman diagrams for the two BSM signal processes used in this thesis: a spin-2 resonance G in the decay channel $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ and a spin-0 resonance X decaying via $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$.

The gluon–gluon fusion production of a heavy spin-2 resonance G and its decay via $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ is simulated with MADGRAPH5_aMC@NLO 2.3.3 [128] at leading order accuracy in QCD. This process is simulated with $k/\bar{M}_{\text{Pl}} = 1$ and for nine different resonance masses m_G : 1.00 TeV, 1.50 TeV, 1.75 TeV, 2.00 TeV, 2.25 TeV, 2.50 TeV, 3.00 TeV, 4.00 TeV, and 5.00 TeV. The parton distribution functions are given by the NNPDF2.3LO set [129]. The parton shower, underlying event, and the hadronization are simulated with PYTHIA 8.211 [130]. Their phenomenological parameters are adjusted to the A14 tune [131]. Decays of unstable hadrons and τ leptons are simulated with PYTHIA, except for the decays of b and c hadrons, which are modeled by the EVTGEN 1.2.0 program [132].

The gluon–gluon fusion production of a heavy spin-0 resonance X and its decay via $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ is simulated with MADGRAPH5_aMC@NLO 2.6.1 [128] at leading order accuracy in QCD with the NNPDF2.3LO set [129]. This process is simulated separately for nine resonance masses m_X : 1.0 TeV, 1.1 TeV, 1.2 TeV, 1.4 TeV, 1.6 TeV, 1.8 TeV, 2.0 TeV, 2.5 TeV, and 3.0 TeV. The samples are generated with a narrow-width approximation, i.e., the natural width of the resonance X is fixed to a value of 10 MeV, which is considerably smaller than the experimental mass resolution. Parton shower and non-perturbative effects are simulated with HERWIG 7.1.3 [133, 134] using the HERWIG default set of tuned parameters [134] and the MMHT2014LO [135] PDF set. Decays of unstable hadrons and τ leptons are simulated with HERWIG, except for the decays of b and c hadrons, which are modeled by the EVTGEN 1.6.0 program [132].

Pileup effects, i.e., multiple interactions in the same or neighboring bunch crossings, are simulated with PYTHIA 8.186 [136] for both signal processes. The original hard-scattering event is overlaid with simulated inelastic proton–proton collision events by using the

NNPDF2.3LO set [129] and the A3 tune [137]. The generated events are weighted in such a way that they resemble the pileup profile of the ATLAS data. The interaction of particles with matter and the detector response are simulated with a model [138] of the ATLAS detector in the GEANT4 program [139].

Chapter 3

The Large Hadron Collider and the ATLAS Experiment

The Large Hadron Collider (LHC) [140] is a circular superconducting hadron accelerator at the European Organization for Nuclear Research (CERN). It provides particle physics experiments with particle collisions at high rates with unprecedented high energies. One of the detectors located at the LHC is the ATLAS experiment [141]. ATLAS is a general-purpose detector that enables the investigation of a wide range of particle physics phenomena, such as precision measurements of SM predictions and searches for BSM particles. ATLAS is an international collaboration with more than 5500 members spread across 181 institutions and 41 countries around the world [142]. The operation of the ATLAS experiment is only possible due to an extensive collaborative effort, with members working in a wide range of fields. This includes, for example, the maintenance, monitoring, and further development of the detector components, the data acquisition and validation, the software to reconstruct particles emerging from collision events, and finally the physics analyses that aim to extend current knowledge to a higher level of accuracy or to discover new phenomena. In the following, the LHC and the ATLAS experiment are introduced, as well as the data taking during the LHC Run 2, which provided the data used in this thesis.

3.1 The Large Hadron Collider

The LHC is designed to accelerate proton beams to energies of up to 7 TeV and beams of heavy ions, primarily lead nuclei, to energies of up to 2.8 TeV per nucleon. It is installed in a tunnel with a circumference of 26.7 km formally used by the large electron–positron storage ring LEP [143]. The LHC started operation with Run 1 using proton-beam energies of 3.5 TeV in the years 2009–2011 and energies of 4 TeV in 2012 [144]. This was followed by Run 2, which lasted from 2015 to 2018, with proton-beam energies of 6.5 TeV [145]. The design energy of 7 TeV, i.e., a center-of-mass energy of $\sqrt{s} = 14$ TeV, is expected to be reached in the next run of the LHC and in the phase of the High-Luminosity LHC [146].

In a collider experiment, the mean number of events N that can be expected after a

certain time T of operation is given by

$$N = \sigma \int_T \mathcal{L}(t) dt,$$

where σ is the cross section of the scattering process. The luminosity $\mathcal{L}$ is an accelerator parameter, which may be integrated over time to yield $\mathcal{L}_{\text{int}} = \int \mathcal{L} dt$. For a Gaussian beam profile the luminosity is given by the following beam parameters:

$$\mathcal{L} = \frac{N_b^2 n_b f_{\text{rev}} \gamma_r}{4\pi \epsilon_n \beta^*} \mathcal{F}.$$

The LHC employs bunched beams with N_b protons per bunch and n_b bunches per beam. The protons, with a relativistic gamma factor γ_r , are accelerated to a revolution frequency f_{rev} . It also depends on beam parameters like the spread of the particles within the beam, the beam focus, and the crossing angle of the beams at the interaction point, which are quantified by the normalized transverse beam emittance ϵ_n , the beta function at the interaction point β^* , and the geometric luminosity reduction factor $\mathcal{F}$. In 2017 and 2018, the LHC achieved peak luminosities above $2 \cdot 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$ [145]. These luminosities are more than twice as high as in the original design, primarily due to much lower emittance and β^* values than originally anticipated.

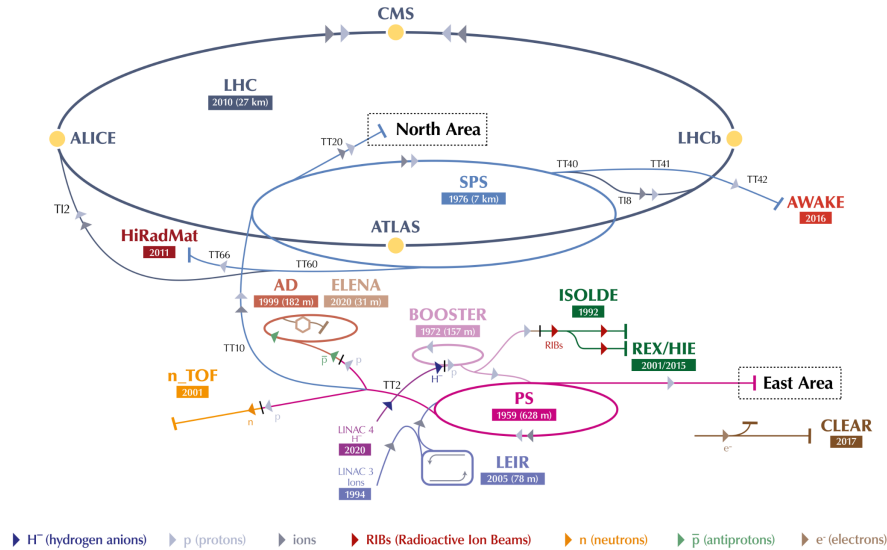


Figure 3.1: Schematic illustration of the CERN accelerator complex [147].

The LHC is the largest ring in CERN's accelerator complex, as depicted in Figure 3.1. The smaller accelerators are used to pre-accelerate the protons for the LHC. The protons are extracted from hydrogen gas and are injected into LINAC2 where they are accelerated to 50 MeV. This is followed by the Proton Synchrotron Booster (PSB) with energies of up to 1.4 GeV, the Proton Synchrotron (PS) with 25 GeV, and the Super Proton Synchrotron (SPS) with 450 GeV. Finally, the protons are injected into two separate rings of the LHC, where they are accelerated in opposite directions to their final energies. To bend the proton beams, the LHC accommodates 1232 superconducting dipole magnets. They are cooled

with superfluid helium to a temperature of 1.9 K and produce magnetic fields of up to 8.3 T. Quadrupole magnets and various configurations of other multipole magnets ensure a focused beam and apply corrections to the beam profile and trajectory.

The LHC ring consists of eight straight sections and eight arcs. The beams are brought to collision on four of the straight sections. These interaction points are the locations of the experimental detectors ATLAS [141], CMS [148], ALICE [149], and LHCb [150]. ATLAS and CMS are general-purpose experiments and investigate a wide range of particle physics phenomena at high energies and luminosities. The ALICE experiment is specialized in the investigation of strongly interacting matter in heavy ion collisions. The LHCb experiment focuses on measurements of CP violations and rare decays of b hadrons.

3.2 The ATLAS Experiment

The ATLAS experiment is located at Point 1 of the LHC ring, which is the interaction point closest to the main campus of CERN. An overview of the detector is shown in Figure 3.2. With a length of more than 44 m, a diameter of 25 m and a weight of approximately 7000 t the ATLAS detector is the largest detector ever constructed at a particle collider. It is build forward-backward symmetrically and consists of a barrel region with multiple detector components placed in cylindrical layers around the beam and two end-caps with disk-shaped detector layers perpendicular to the beam axis. The inner detector measures the trajectories of charged particles with high granularity close to the beam pipe. This particularly requires a fast readout and radiation resistant detector elements. The ATLAS calorimeters induce electromagnetic and hadronic showers and measure their energies. The outermost layers of the ATLAS detector are part of the muon spectrometer, which enables the identification of muons. Two magnet systems bend the trajectories of charged particles. This allows the determination of the momentum of a particle from the curvature of its trajectory. The trigger system monitors multiple detector components during data-taking, to preselect events for recording that may contain processes of interest.

The ATLAS coordinate system used to describe particle trajectories in the detector is introduced in the following. The origin of the coordinate system is set to the center of the detector at the nominal proton–proton interaction point. The z -axis of a right-handed Cartesian coordinate system is defined to follow the beam direction. The positive x -axis points to the center of the LHC ring and the positive y -axis points upwards. Transverse variables, like the transverse momentum p_T , are projections into the x - y plane. The azimuthal angle ϕ is measured in this transverse plane. The polar angle θ is measured to the z -axis in the plane longitudinal to the beam direction. Based on θ , the pseudorapidity is defined as

$$\eta = -\ln \left(\tan \frac{\theta}{2} \right).$$

The pseudorapidity is commonly used as a coordinate because a difference in η is invariant under Lorentz boosts in z -direction for particles with negligible masses. In this case it

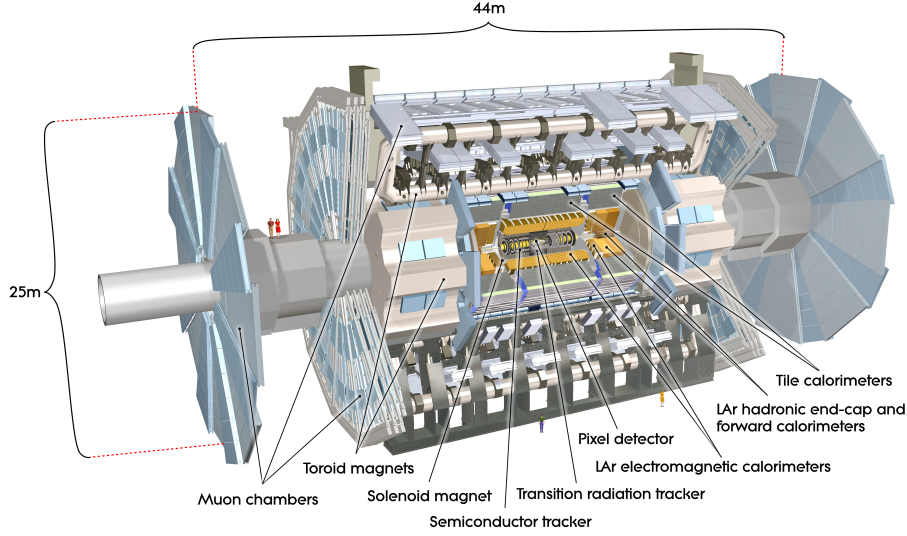


Figure 3.2: Schematic representation of the ATLAS Detector and its subsystems [151].

converges to the rapidity

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

The angular distance between two particles is measured with

$$\Delta R = \sqrt{(\eta_1 - \eta_2)^2 + (\phi_1 - \phi_2)^2}.$$

The main detector components of the ATLAS experiment, i.e., the inner detector, the calorimeter systems, the muon spectrometer, and the trigger systems, are presented in the following.

3.2.1 Inner Detector

The measurement of tracks and momenta of charged particles is performed in the inner detector. A large number of particles is typically produced in proton–proton collisions, e.g., due to multiple interactions in a bunch crossing, or due to the dense environments that emerge from the decays of boosted particles and within high-energy jets. Their detection requires detector components with fine granularity. A particle track is reconstructed from multiple position measurements, as detailed in Chapter 4. This is one of the foundations for distinguishing different particle types. For example, the number of tracks assigned to the decay of a τ lepton is an important characteristic to distinguish it from a hadronic jet. Also, the recognition of a displaced track vertex is important for the identification of τ leptons and b hadrons. They have a mean lifetime long enough to resolve a decay vertex with a certain distance to the primary collision vertex from their decay products. The inner detector is shown in Figure 3.3 and consists of three sub-systems: the pixel detector, the semiconductor tracker (SCT), and the transition radiation tracker (TRT). This is surrounded by a thin superconducting solenoid magnet that produces a 2 T magnetic

field inside the sub-detectors.

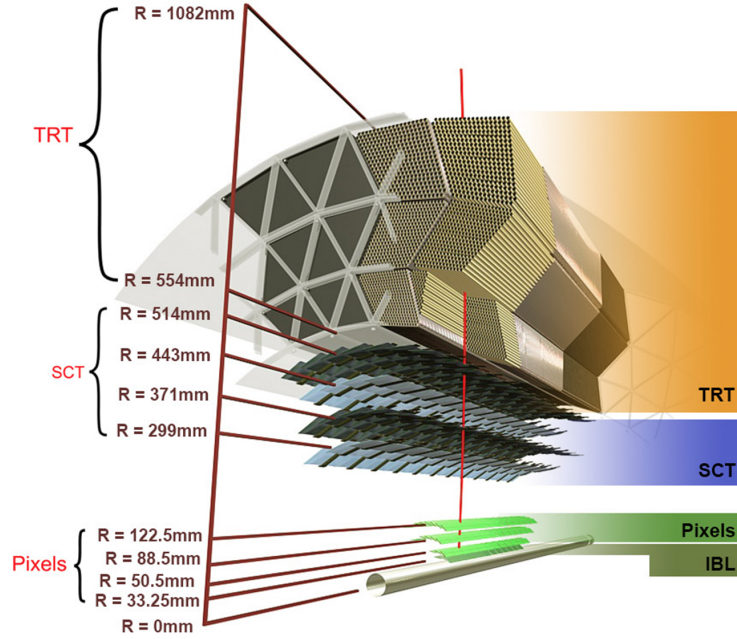


Figure 3.3: Schematic representation of the barrel region of the ATLAS inner detector [152].

Pixel Detector

The pixel detector is the sub-system closest to the beam pipe. As such, it must withstand the highest radiation doses, but must also have the finest granularity to achieve the required resolutions of the track and vertex reconstructions. It consists of four layers of silicon pixel sensors in the barrel region and three disks of sensors in each end-cap. This configuration allows four discrete spacial measurements per track in the pseudorapidity region $|\eta| < 2.5$. A portion of the energy of an ionizing particle is absorbed in the semiconductor sensors, leading to electron-hole pairs. Under an applied electric field, this results in a detectable signal current. The innermost cylindrical layer is the Insertable B-Layer (IBL) [153], which was installed as a major upgrade between LHC Run 1 and Run 2. It comes as close as 33 mm to the beam axis and provides a pixel size of about $50\text{ }\mu\text{m}$ in the transverse direction and $250\text{ }\mu\text{m}$ in the longitudinal direction. The sizes of the pixels in the remaining layers are mostly $50\text{ }\mu\text{m}$ by $400\text{ }\mu\text{m}$.

Semiconductor Tracker

The SCT consists of silicon microstrip detectors, arranged as four double strip layers in the barrel region and nine disk layers in each end-cap. The silicon microstrip detectors are semiconductor sensors, but use readout strips instead of pixels to reduce the number of readout channels. Each layer consists of modules with strips on both sides that are rotated by 40 mrad to each other to allow for space point measurements. Rectangular strip modules are distributed in parallel to the beam direction in the barrel region and trapezoidal modules

are radially distributed in the end-caps. The mean strip pitch is approximately $80\,\mu\text{m}$. A track with a pseudorapidity $|\eta| < 2.5$ passes on average four SCT layers.

Transition Radiation Tracker

Transition radiation occurs when a highly relativistic charged particle crosses the boundary between two media with different dielectric constants. The total radiated energy is proportional to the Lorentz factor γ of the particle. This can be used to distinguish particles of different masses. Transition radiation is used in the TRT to differentiate in particular electrons from pions and other charged hadrons. It covers a pseudorapidity range of $|\eta| < 2.0$. There are 73 layers of so-called straw tubes in the barrel region and 160 planes of straw tubes in the end-caps. The straws are drift tubes with a diameter of 4 mm filled with a xenon-based gas mixture. Due to leakage problems, some modules were modified to use the less expensive argon instead of xenon [154]. The ionization induced by a charged particle in the gas is measured by an anode wire in the center of each straw tube. Spatial information is provided by the TRT only for the transversal direction. However, this can be matched to the measurements in the silicon detectors to further improve the tracking performance of the inner detector. To induce transition radiation, the straws are interleaved with polypropylene fibers in the barrel and foils in the end-caps. The radiation is absorbed by the gas and increases the measured current in the anode wire.

3.2.2 Calorimeter Systems

The ATLAS calorimeter systems surround the inner detector, as depicted in Figure 3.4. The calorimeters measure the energy and direction of electromagnetic and hadronic showers induced by particles. ATLAS uses various sampling calorimeters in which an active medium is interleaved with metallic absorbers. The interaction of a particle with the absorber material induces a shower of secondary particles of lower energy, which are then detected in the active material. The active material is either liquid argon (LAr) or consists of scintillators. When LAr is ionized, it allows direct measurement of an electric current. Ionizing particles in a scintillator induce scintillation light that is transported through a wavelength-shifting fiber to a photomultiplier tube for readout.

The innermost layers are occupied by the electromagnetic calorimeters, which measure the showers of electrons and photons. Hadronic showers already interact with the electromagnetic calorimeters, but are only fully absorbed by outer components, the hadronic calorimeters. The calorimeter systems must be sufficiently deep to achieve full absorption of electromagnetic and hadronic showers. A precise measurement of energy and direction of electrons and photons requires a high granularity in the electromagnetic calorimeter. The reconstruction of hadronic jets requires usually less granularity. However, a decent segmentation is still needed to resolve substructures within jets in order to identify the decay signatures of boosted particles, as done in this thesis. The calorimeter systems cover a pseudorapidity range of $|\eta| < 4.9$ to allow for a reliable measurement of the missing transverse momentum, which indicates the presence of neutrinos or of BSM particles that leave the detector without interaction. At the highest pseudorapidities, the forward

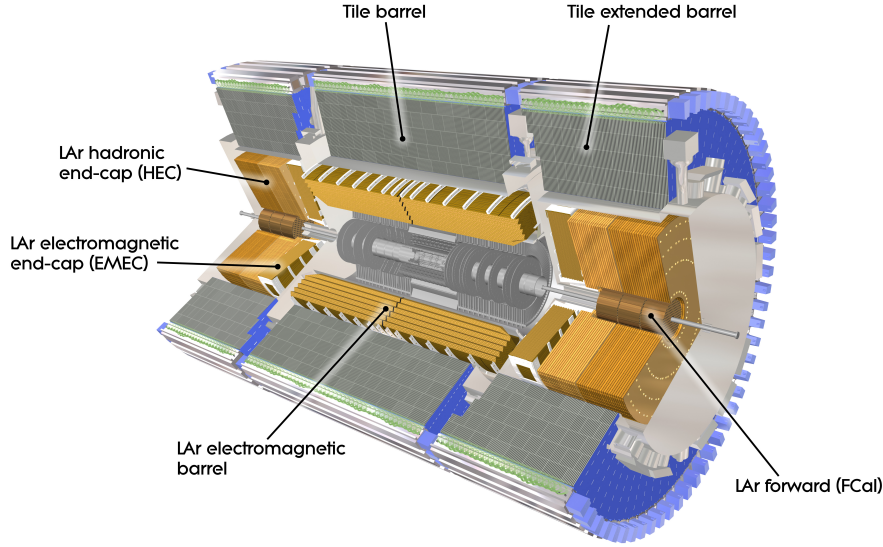


Figure 3.4: Schematic representation of the ATLAS calorimeter system [155].

calorimeter measures both, electromagnetic and hadronic showers.

Electromagnetic Calorimeters

The electromagnetic calorimeter is composed of a barrel region, covering $|\eta| < 1.475$, and two end-caps, covering $1.375 < |\eta| < 3.2$. It uses LAr as active medium and lead absorber plates. The absorber plates are interleaved with readout electrodes and are arranged in an accordion structure that provides full azimuthal coverage and symmetry. The barrel calorimeter is split at $z = 0$ into two identical rings with a small gap of 4 mm. Both end-cap calorimeters are made of two coaxial wheels. The finest granularity in $\Delta\eta$ and $\Delta\phi$ is provided in the region $|\eta| < 2.5$, which is also covered by the ATLAS inner detector, to enable precision measurements of electrons and photons. In this region, it is segmented into three layers in depth. At higher pseudorapidities there is a coarser granularity and only two layers in depth. A presampler detector is installed in front of the barrel and end-cap calorimeters to estimate the prior energy loss of electrons and photons. It consists of a thin layer of LAr that covers the pseudorapidity range of $|\eta| < 1.8$.

Hadronic Calorimeters

The hadronic calorimeter is composed of a tile calorimeter in the barrel region and two hadronic end-cap calorimeters. The tile calorimeter surrounds the electromagnetic calorimeter in the barrel region. It uses scintillator tiles as active medium and steel plates as absorbers. It consists of one component in the central barrel, covering $|\eta| < 1.0$, and two components in the so-called extended barrels, covering $0.8 < |\eta| < 1.7$. Each component of the tile calorimeter is segmented into three layers in depth.

The hadronic end-cap calorimeters cover a pseudorapidity range of $1.5 < |\eta| < 3.2$ and are installed behind the electromagnetic end-cap calorimeters. Copper plates are used as

absorbers interleaved with LAr gaps. Each hadronic end-cap calorimeter consists of two wheels. Every wheel is segmented into two layers in depth.

Forward Calorimeter

The forward calorimeter extends the reach of electromagnetic and hadronic calorimetry to high pseudorapidities of $3.1 < |\eta| < 4.9$. A high-density design is required for this calorimeter, as it is located about 1.2 m back in the end-cap compared to the electromagnetic calorimeter in order to reduce backscatterings into the inner detector. The forward calorimeter is composed of three modules per end-cap. In each module, longitudinal tubes of LAr are embedded in a metal matrix. The first module is optimized for electromagnetic calorimetry and uses copper as absorber material. The two outermost modules use tungsten as absorber and measure the energy of hadronic showers.

3.2.3 Muon Spectrometer

Muons are the only known charged particles that can traverse the calorimeters with only a few interactions. Hence, the muon spectrometer is the outermost component of the ATLAS detector. Three superconducting air-core toroids generate magnetic fields of up to 3.5 T to bend the trajectories of muons. There is one barrel toroid and two end-cap toroids, each consisting of eight coils that are installed radially around the beam pipe. As depicted in Figure 3.5, it consists of different chambers that are installed throughout the muon spectrometer, either with fine granularity for precise momentum measurements or for trigger decisions with a high rate. The monitored drift tubes (MDT) and the cathode strip chambers (CSC) are gaseous detectors that localize muon tracks in their bending direction with high precision. In addition, there are resistive-plate chambers (RPC) and thin-gap chambers (TGC) that provide fast trigger signals and measure the third coordinate of the muon track.

The MDT chambers are installed as three layers between the toroid coils in the barrel region and as three disks in front and behind the end-cap toroids. The MDT chambers have a pseudorapidity coverage of $|\eta| < 2.7$, except for the innermost layer, which covers only $|\eta| < 2.0$. In the center of the muon spectrometer, at $\eta \approx 0$, there is an area that is not equipped with muon chambers but with service structures of the ATLAS detector. The MDT chambers consist of up to eight layers of drift tubes. The drift tubes are filled with a pressurized argon-rich gas mixture. The ionization caused by a muon, generates free electrons, which are detected by an anode wire in the center of each drift tube.

In the innermost layer at $2.0 < |\eta| < 2.7$, CSCs are used instead of MDTs. Due to their better granularity and radiation hardness they are well suited for the high particle fluxes in the forward region. The CSCs are multiwire proportional chambers that can measure both the transversal and longitudinal coordinates of a muon track. Here, multiple parallel anode wires run in an argon-rich gas mixture between two layers of cathodes segmented into strips with orthogonal orientations. Each chamber consists of four of such planes. The muon position is determined from the charge collected on adjacent cathode strips.

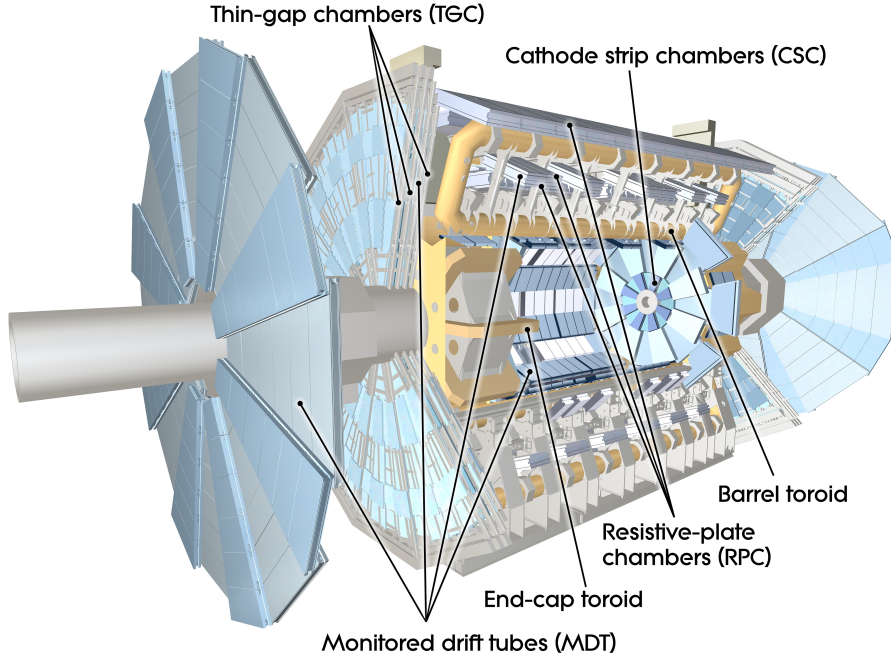


Figure 3.5: Schematic representation of the ATLAS muon spectrometer [156].

The muon trigger chambers provide fast information about the multiplicity of muons produced in a proton–proton collision event and their approximate energies on time scales smaller than the nominal bunch spacing of 25 ns. In addition, they complement the MDT chambers by locating muon tracks in the non-bending direction. Three layers of RPCs are used in the barrel region, $|\eta| < 1.05$. The RPCs consist of parallel resistive plates operated at high voltages and filled with gas. Ionizing particles cause an electron avalanche in the electric field between two plates. The signal is read out by two sets of metallic strips that are mounted orthogonally to each other on the outsides of the resistive plates.

The TGCs cover the end-caps, $1.05 < |\eta| < 2.7$, although only pseudorapidities up to $|\eta| < 2.4$ can be used for trigger decisions. The TGC units consist of doublets or triplets of multiwire proportional chambers. Each chamber comprises two cathodes and a plane of wires in between. Two of the cathodes per TGC doublet or triplet are segmented into strips. This allows the measurement of the azimuthal coordinate of a muon track while the longitudinal coordinate is determined from a signal in the anode wires.

3.2.4 Trigger Systems

The ATLAS trigger system processes the collision data during LHC operation in real time to find events that may contain physics processes of interest, and to reduce the event rate to a manageable level for recording. The trigger system received a significant upgrade between LHC Run 1 and Run 2 [157, 158] to meet the new experimental conditions. The higher center-of-mass energy of 13 TeV increases the cross sections of many processes of interest. Also, the reduction of the bunch spacing to 25 ns during Run 2 and the higher instantaneous luminosities increased the rate of simultaneous proton–proton collision events significantly. The trigger decisions are made in two stages: in the Level-1 (L1) trigger and

in the High-Level Trigger (HLT). Given a bunch-crossing rate of 40 MHz at the LHC, the L1 trigger reduces the number of events to be buffered to the ATLAS detector's maximum readout rate of 100 kHz. The data are passed to the HLT, which selects events for recording with an average rate of 1.2 kHz.

The hardware-based L1 trigger makes a decision based on reduced-granularity information from various detector sub-systems. Analog signals from the calorimeter systems are digitized and calibrated by a preprocessor. This is used to identify candidates for electrons, photons and hadronic decays of τ leptons, to reconstruct jets, and to compute a missing transverse energy in the calorimeter. The muon trigger chambers are examined for signals compatible with a muon coming from the interaction point. The L1 trigger accepts events based on, for example, the presence of a particle candidate with momentum above a certain threshold, the total energy in the calorimeter, or topological requirements such as multiplicities of certain particles, their invariant mass, or angular distribution. At this stage, Regions-of-Interest (RoIs) are defined, which are further investigated by the HLT. For events that are accepted by the L1 trigger, the full detector data is read out and temporarily stored.

The HLT system is software-based. After a fast preselection, particle reconstruction algorithms are used that are close to the offline event reconstruction. Here, offline refers to operations that are performed on the recorded data set, while online refers to operations running in real time during data taking. The triggers of the HLT have access to information not available at L1, like the full granularity of the calorimeters and tracking information from the inner detector and the high-precision muon chambers. To test whether the trigger conditions are fulfilled, it can request detector data from within an RoI, or if necessary, from the full detector. Events accepted by the HLT are exported to the Worldwide LHC Computing Grid [159, 160] for permanent storage and offline reconstruction. For both L1 and HLT, it is possible for a given trigger to exceed its available bandwidth. In this case, it is provided with a prescale value, that indicates that only a fraction of events that meet the trigger conditions are kept. A trigger can be given a prescale value already at the beginning of operation, or it can become prescaled due to changing experimental conditions during data taking.

3.3 Data Taking in LHC Run 2

Proton–proton collision data recorded by the ATLAS detector during LHC Run 2 are used in this thesis. Compared to Run 1, the high center-of-mass energy of 13 TeV increases the cross sections of many interesting physics processes, especially the production of heavy resonances. The proton bunches are accelerated with a bunch spacing of 25 ns. Only at the beginning of the data taking in 2015 a bunch spacing of 50 ns was employed, which is not used in this thesis, as it corresponds to a very small fraction of data that would require dedicated calibration. A so-called ATLAS run includes the data that are continuously recorded between LHC declared stable beams and beam dump. An ATLAS run is divided into time periods of typically 60 s, called luminosity blocks, with approximately constant experimental conditions and trigger configurations.

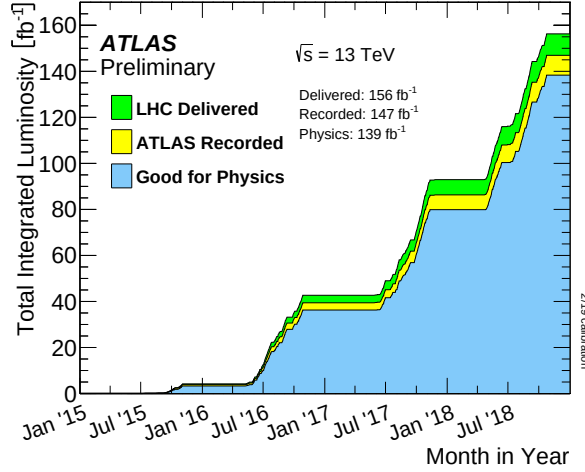


Figure 3.6: Integrated luminosity versus time of data taking. During Run 2, the LHC delivered 156 fb^{-1} of stable beams for proton–proton collision, as shown in green. The ATLAS experiment recorded 147 fb^{-1} of those collisions, as shown in yellow. Shown in blue are the 139 fb^{-1} of the proton–proton collisions that meet the requirements of the data quality assessment and can be used for physics analyses. [161]

The integrated luminosity versus time of data taking is shown in Figure 3.6. The LHC delivered 156 fb^{-1} of stable beams for proton–proton collisions during Run 2 [161]. The ATLAS collaboration was able to record more than 94% of that data. The small loss is mainly due to inefficiencies in the data acquisition and the time required to ramp up the high voltage in the tracking detectors and to activate the preamplifiers of the pixel system. The recorded data undergoes another data quality assessment [162]. It must be recorded under good detector conditions, i.e., all detector components were working stably, and the reconstructed collision events must be of good quality. Lists of luminosity blocks that were verified to fulfill those requirements are collected in so-called Good Run Lists. The ATLAS data that can be used for physics analyses amounts to a total integrated luminosity of 139 fb^{-1} . The primary luminosity measurement for ATLAS is performed with the LUCID-2 detector [163] by sampling the rate of inelastic interactions. This measurement is calibrated in dedicated LHC runs with low luminosities and is complemented by independent luminosity measurements in the ATLAS inner detector and calorimeters [164].

During Run 2, the beam performance was continuously improved at the LHC. While a peak luminosity of $0.55 \cdot 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$ was achieved in the year 2015, it was increased up to $2.1 \cdot 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$ in 2018 [145]. However, this also comes with an increase in pileup interactions, as shown in Figure 3.7. There, the mean number of interactions per bunch crossing is shown for each year of data taking and for the entire Run 2. Over the full Run 2, there are on average 33.7 interactions per bunch crossing, although occasionally there are events with more than 70 interactions. The pileup distribution of the 2017 data taking shows a double-peak structure, which is related to LHC operations with different beam types [145]. Those were needed to mitigate abnormal background radiation and beam losses that occurred after an accidental entry of air into the beam vacuum during accelerator maintenance. The issue was largely resolved by evacuating the beam pipe to an improved vacuum before the start of the 2018 data taking.

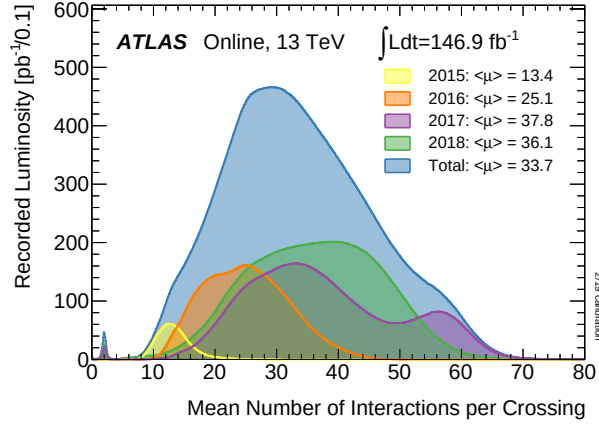


Figure 3.7: Distribution of the mean number of interactions per bunch crossing for each year of data taking and for the entire LHC Run 2. The small peak on the left corresponds to special data-taking periods with on average two interactions per bunch crossing. [161]

To reflect the different pileup conditions of the ATLAS data in simulations, the MC samples are produced in three campaigns: MC16a, MC16d, and MC16e. MC16 refers to a set of software releases used for processing Run 2 simulations. The MC16a campaign generates events of the combined 2015 and 2016 data takings with a pileup distribution similar to the observation in data. This is done accordingly in the MC16d campaign for the 2017 data taking. The generation of the MC16e samples is based on the pileup conditions that were expected for the 2018 data taking. A list of MC samples used in this thesis can be found in Appendix A. Their usage in the development of the of the boosted di- τ reconstruction techniques and for the estimate of SM background processes in the search for resonant Higgs boson pair production is described in the following chapters.

Chapter 4

Physics Object Reconstruction

The reconstruction and identification of the various final state particles is the foundation of any particle physics analysis. The responses of all ATLAS detector subsystems must be combined in order to distinguish particles among each other and from detector noise. There are specific reconstruction strategies and algorithms provided by the ATLAS collaboration for different particle types. The procedure starts with the detection of low-level objects, such as tracks, vertices and energy clusters. These form the basis for the reconstruction of higher-level objects, like jets or leptons, which finally permit the search for boosted $h \rightarrow b\bar{b}$ and $h \rightarrow \tau^+\tau^-$ decays.

Jets are particularly important for the detection of the particle showers of hadronic final states. There are multiple jet definitions employed in this thesis with varying size definitions and different jet constituents, such as energy clusters in the calorimeter or tracks in the inner detector. After jet reconstruction, dedicated algorithms are utilized to identify jets that originate from decays of b hadrons, τ leptons, or from other background processes.

Events with electrons and muons are mostly rejected in this thesis in order to suppress background events. However, they are employed in a dedicated control region that is used to better understand the background of Z boson production. Finally, in the calculation of the missing transverse energy all of the above information is combined to find momentum imbalances that indicate the presence of neutrinos, as they are expected in decays of τ leptons.

This chapter serves as an overview of all object reconstruction, identification and calibration methods that are employed in the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ analysis, except for the novel boosted di- τ tagging techniques, which are described separately in Chapter 5.

4.1 Low-Level Objects

The reconstruction of low-level objects, such as tracks, vertices and energy clusters, out of raw detector measurements are an essential first step towards finding higher-level physics signatures like jets, leptons, or Higgs boson decays. A precise and efficient reconstruction of such low-level objects becomes particularly important in the high-energy regime where the typical particle distances are close to the granularity of the detector sensors.

The trajectories of charged particles are reconstructed as so-called *tracks* in the inner

detector [165]. Sensor signals in the pixel or SCT detector systems that exceed a certain energy threshold and share a common edge or corner are grouped by a connected component analysis [166]. These groups are used to calculate the three-dimensional interaction points at which charged particles traversed the active material. This is the basis for a first iterative track finding, performed by a combinatorial Kalman filter [167]. Certain requirements are applied to the track candidate momentum and the track impact parameters. Impact parameters are the distances of a track to the estimated location of the proton–proton collision. At this stage a single charged particle can lead to multiple track candidates. The best-fitting track is to be determined by the following steps. The track candidates are rated based on the quality of the track fit, the track momentum, the number of assigned energy deposits and potential intersections with the detector in which no energy deposit is found. A neural network is trained to identify energy deposits that originate from multiple charged particles. An ambiguity-resolving algorithm reassigns energy deposits to track candidates, giving priority to tracks with a previously high rating. These tracks are extended to the outermost radii of the inner detector by searching for compatible sets of TRT measurements [168]. Finally, the tracks are rated again and those fulfilling further quality criteria are passed to a high-resolution track fit. Here, additional neural networks are applied [169] for a precise position and uncertainty estimation. The track reconstruction performance was measured in the core of jets with transverse momenta between 200 GeV and 1600 GeV [165]. The fraction of charged particles that fail to be reconstructed was found to range between 6.1% and 9.3% as the jet momentum increases.

The locations of proton–proton interactions are reconstructed as *primary vertices*. Primary vertices are typically distributed along the beam axis. Their reconstruction uses a collection of tracks as input and is divided into two stages: vertex finding and vertex fitting [170]. For the first vertex an initial seed position is set. This seed position is refined in an iterative fit. In each iteration the vertex position is recomputed and tracks that are less compatible with this vertex are down-weighted. After converging on a vertex position, incompatible tracks are used for the reconstruction of the next vertex. The primary vertex with the highest sum of track p_T^2 is considered as the main hard-scatter vertex of the event. The reconstruction performance was tested in a dedicated data taking period with low pileup in early Run 2 [171]. At least two reconstructed tracks are needed to reliably reconstruct a vertex. While for events with only two tracks the efficiency of the vertex reconstruction is about 83%, it becomes almost fully efficient for events with more than four tracks.

The energies measured by the calorimeter sensors are deposited in three-dimensional calorimeter cells. For better calibration and to control detector noise, those cells are grouped into massless topological *energy clusters* [172]. A nearest-neighbour algorithm [173] adds cells to a cluster by considering the ratio between the cell energy and the expected noise in that cell. Typically energy deposits from electrons or photons lead to different calorimeter responses than energy deposits from hadrons. This is reflected in two different cluster calibrations either of which can be applied: the ‘electromagnetic scale’ has a better resolution for energy deposits from electromagnetic showers, while the ‘hadronic scale’

provides a better measurement for hadrons by applying a local hadronic cell weighting scheme [172–174].

4.2 Calorimeter Jets

The *calorimeter jet* reconstruction uses energy clusters as input. A sequential recombination algorithm, the anti- k_t algorithm [175], is used to form a reconstructed jet. Hereby two distance measures are defined:

$$d_{ij} = \min(p_{Ti}^{-2}, p_{Tj}^{-2}) \frac{\Delta R_{ij}^2}{R^2},$$

$$d_{iB} = p_{Ti}^{-2},$$

where $\Delta R_{ij}^2 = (\eta_i - \eta_j)^2 + (\phi_i - \phi_j)^2$ measures the distance between two clusters, i and j , and p_{Ti} , η_i , and ϕ_i are the transverse momentum, pseudorapidity, and azimuth of a cluster i .¹ The radius parameter R influences the size of the reconstructed jet. For all possible pairs of clusters i and j , the above distances are calculated. If the smallest distance is a d_{ij} , the clusters i and j are merged. If the smallest distance is a d_{iB} , the cluster i is declared to be a jet and is not available for following recombinations. This procedure is repeated until no clusters are left. The anti- k_t algorithm is infrared and collinear safe, meaning that it is resilient with respect to radiations of soft particles and collinear splittings.

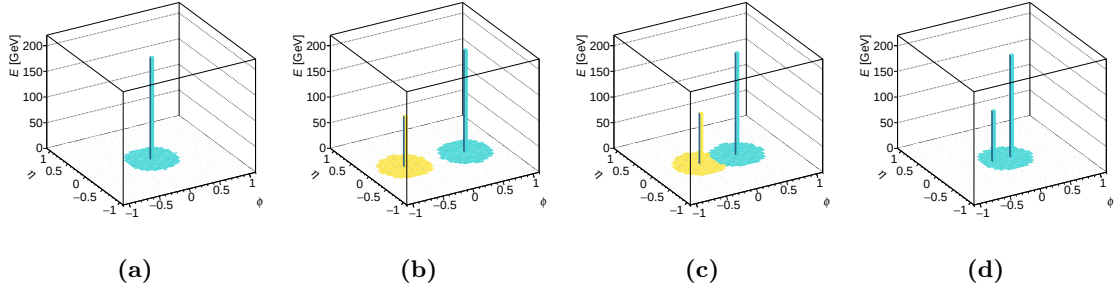


Figure 4.1: Illustration of the anti- k_t algorithm with radius parameter $R = 0.4$ on one high-energy cluster (a) and on two high-energy clusters with distance $\Delta R > 2R$ (b), $R < \Delta R < 2R$ (c) and $\Delta R < R$ (d). The high-energy clusters have energies of 100 GeV and 200 GeV respectively on top of a uniform background noise with energies between 1 MeV and 1 GeV. The clusters that are merged to an anti- k_t jet are colored.

Especially the distance parameter R has an important influence on whether the signatures of multiple particle decays can be resolved or not. To get a better understanding of how the anti- k_t algorithm behaves on different detector signatures, four idealized scenarios are explained below and illustrated in Figure 4.1. The trivial case of having exactly one high-energy deposit, with only low-energy deposits in its vicinity, results in one reconstructed jet with a conical shape. In this case the high-energy cluster is in the center and all low-energy

¹ In Reference [175] the distance is introduced by using the rapidity y_i instead of the pseudorapidity η_i . However, a slightly different definition is chosen here in order to be consistent with the definitions in Chapter 3. In this particular case the jet constituents, i.e., the energy clusters, are defined to be massless, so that the pseudorapidity converges to the rapidity and both distance measures become equivalent.

clusters within radius R are collected into the jet. If there are two high-energy deposits within a distance of $\Delta R > 2R$ the anti- k_t algorithm delivers two separate jets. Also the case of $R < \Delta R < 2R$ leads to two jets, but they share a border whose shape depends on the ratio of the energies of the clusters. Two high-energy clusters with a distance $\Delta R < R$ result in one reconstructed jet containing both clusters. The cluster with the higher energy tends to be in the center of the jet. In general, if closely spaced particle decays are to be resolved, a correspondingly small radius parameter R must be chosen. If a jet is supposed to contain multiple decay signatures, R must be accordingly large.

Calorimeter jets with $R = 0.4$ are used in the majority of the physics analyses of the ATLAS collaboration [172]. The reconstruction uses energy clusters that are calibrated to the electromagnetic scale. The resulting jets are calibrated using a sequence of simulation-based corrections, including pileup corrections and an energy scale calibration. These bring the reconstructed jet energy to the level of the simulated particles from which the jet originated. Finally, a data-based calibration corrects for differences between data and simulations. The performance of this jet definition was studied with up to 81 fb^{-1} of proton–proton collision data recorded by the ATLAS detector from 2015 to 2017 [172]. The relative resolution of the jet energy was found to range between 35% and 4% at transverse momenta from 20 GeV to 2 TeV. In this thesis, calorimeter jets with a radius parameter of $R = 0.4$ are mainly used for the calculation of the missing transverse energy (see Section 4.7) and are referred to as *small- R jets* in the following.

Analyses that search for massive particles with high momenta, such as decays of Higgs bosons, vector bosons, or top quarks, often see signatures where the decay products are collimated and can neither fit into one small- R jet nor be resolved by two such jets. This led to the definition of a second jet type in the ATLAS collaboration with a radius parameter of $R = 1.0$ [174], denoted as *large- R jet* in the following. Large- R jets are reconstructed from energy clusters that are calibrated to the hadronic scale. In order to improve the energy and mass resolution and to reduce the impact of pileup processes and sensitivity to the underlying event these jets are ‘groomed’ with a ‘trimming’ algorithm [176]. In this procedure the jet constituents are reclustered to new subjets using the k_t algorithm [177] with $R = 0.2$. Any subjet that contributes less than 5% to the transverse momentum of the original large- R jet is removed. Afterwards the large- R jet is reconstructed again using the remaining clusters. The energy scale and mass of the trimmed jets are calibrated with correction factors derived from simulations [178]. The jet mass definition is further improved by combining the calorimeter measurements with the information from inner detector tracks, leading to a better resolution at high momenta [179]. Finally, correction factors are derived from a data-to-simulation comparison [174] that was performed on 36 fb^{-1} proton–proton collision data. The relative jet energy resolution was found to range between 10% and 4% for transverse momenta from 200 GeV to 2 TeV. Large- R jets are used in this thesis as basis for the reconstruction of $h \rightarrow b\bar{b}$ and $h \rightarrow \tau^+\tau^-$ candidates.

4.3 Track Jets

Track jets use inner detector tracks as constituents instead of energy deposits in the calorimeter. In comparison to calorimeter jets they benefit from a better spacial resolution. On the other hand, they can only estimate the energy of charged components of a particle decay and show a degrading energy resolution in the high-energy regime. Anti- k_t track jets with a variable radius parameter are employed in this thesis in order to identify jets that contain b hadrons. The radius parameter $R(p_T) = \rho/p_T$ shrinks with increasing momenta [180]. This increases the sensitivity to highly boosted $h \rightarrow b\bar{b}$ decays, where the b hadrons have very low angular separation. The constant parameter ρ determines how fast the jet radius decreases and is set to 30 GeV. This value was found to maximize the sensitivity to $h \rightarrow b\bar{b}$ decays across a wide energy range [24]. The minimum and maximum values of $R_{\min} = 0.02$ and $R_{\max} = 0.4$ are imposed to the radius parameter. They prevent the jet size from growing too large at low momenta and from shrinking below the detector resolution at high momenta.

Track jets can be assigned to a large- R jet with the ghost association method [181, 182]. This allows the use of large- R jets to retrieve the complete kinematic information of a $h \rightarrow b\bar{b}$ decay including charged and neutral decay products, whereas track jets with their good spatial resolution are used to identify b hadrons within the large- R jet.

4.4 b -Tagging

Finding jets that contain b hadrons is one of the key ingredients to identify $h \rightarrow b\bar{b}$ candidates. The Higgs boson kinematics is reconstructed with a large- R jet, while the presence of b hadrons is identified with variable- R track jets [24]. The identification of a b hadron in a track jet is performed with multiple algorithms [183] that utilize impact parameter information, secondary vertex information, as well as a fitting algorithm that aims to reconstruct the complete b hadron decay chain. This exploits the fact that b hadrons have a relatively long lifetime, high mass, and a distinct decay multiplicity. Tracks from b hadron decays tend to have large impact parameters. In many cases displaced secondary vertices can be found along the jet direction. The MV2c10 algorithm [184] combines this information in Boosted Decision Trees (BDT) that were trained to discriminate b -initiated jets from jets initiated by light or c quarks.

A track jet is labeled as *b -tagged* if it fulfills a certain cut requirement on the MV2c10 discriminant score. The requirement used in this thesis provides a b -tagging efficiency of on average 70% in simulated $t\bar{t}$ events, although the efficiency decreases to about 60% at jet momenta above 500 GeV [185]. This requirement provides a rejection factor, which is defined as the inverse rate of mis-identifications in background events, of 300 for jets initiated by light quarks, 36 for hadronically decaying τ leptons and 8.9 for jets initiated by c quarks. The b -tagging efficiency was also measured in a high-purity sample of $t\bar{t}$ events in proton–proton collision data. Scale factors are retrieved from a data-to-simulation comparison. These scale factors, which are close to unity, are applied as weights in simulation to match the tagging efficiency between data and simulation [185].

In this thesis, various event categories are defined based on the number of b -tagged track jets that are associated with a large- R jet. A reconstructed $h \rightarrow b\bar{b}$ candidate is a large- R jet with at least two associated track jets, where the two highest-momentum track jets are b -tagged.

4.5 Electrons

The electron reconstruction is based on a matching of energy clusters in the electromagnetic calorimeter to tracks in the inner detector [186]. The direction of each track is extrapolated to the calorimeter and then geometrically matched to energy clusters. The extrapolation allows a rescaling of the track momentum to improve the track-cluster matching. Clusters that have a matched track are used as seeds for *superclusters*. Nearby clusters that may emerge from electron bremsstrahlung or cluster splittings are added to the supercluster. At this stage, an initial position and energy calibration is applied to the superclusters, followed by another iteration of track matching. Subsequently, the energies of the final electrons are recalibrated, and variables for electron identification are calculated. The electron calibration consists of a simulation-based calibration that brings the energy of the reconstructed electron to the level of the simulated particle. This is followed by energy scale and resolution corrections that were retrieved from $Z/\gamma^* \rightarrow e^+e^- + \text{jets}$ events collected in 81 fb^{-1} of proton-proton collision data [186]. Energy scale corrections are applied to the data whereas energy resolution corrections are applied to simulations.

Electrons are identified with a likelihood-based discriminant that employs electromagnetic shower quantities and combined track-cluster variables. Multiple operating points are provided, delivering average identification efficiencies ranging from 93% for the ‘*Loose*’ operating point to 80% for the ‘*Tight*’ operating point.

The identification efficiencies gradually increase from low to high energies and decrease under high-pileup conditions. Additionally, various isolation criteria are defined to select electrons that are isolated from any other local activities in the detector. The isolation selections utilize cuts on variables that quantify the amount of tracks and energy deposits in the vicinity of an electron. Their efficiencies vary between 99% for the loosest and 90% for the tightest criterion. Efficiency correction factors were measured for the identification and isolation requirements in a data-to-simulation comparison [186].

4.6 Muons

The muon reconstruction is based on a combination of charged particle detection in the inner detector and in the muon spectrometer [187]. Tracks of muons in the inner detector are reconstructed in an analogous manner as described in Section 4.1. The reconstruction of tracks in the muon spectrometer begins with a search for track segments inside each muon chamber. Afterwards, these segments are combined in a global χ^2 fit over all muon spectrometer layers. Muon spectrometer hits that are assigned to a given track but provide a large contribution to the χ^2 value are removed and the track is refitted. A muon track is accepted if the χ^2 result satisfies a selection criterion. In addition, a loose requirement on

the compatibility of the track with the proton–proton interaction point must be fulfilled. Based on a combination of inner detector, calorimeter, and muon spectrometer information, five muon candidate types are defined [188]. A ‘*combined*’ muon has two independently reconstructed tracks, in the inner detector and in the muon spectrometer, both sharing a consistent trajectory. For an ‘*inside-out*’ muon, a track in the inner detector is extrapolated to the muon spectrometer, and a combined track is fitted between both detector components. A ‘*segment-tagged*’ muon has a track in the inner detector and at least one compatible track segment in the muon spectrometer. A ‘*calorimeter-tagged*’ muon has a track in the inner detector that matches to energy deposits of a minimum-ionizing particle in the calorimeter. An ‘*extrapolated*’ muon is reconstructed only based on the muon spectrometer track.

Various identification criteria are defined to distinguish prompt muons from background, which originates, for example, from light hadron decays. The muon identification utilizes quantities like the χ^2 score of the track fit or the number of hits in the inner detector and in the muon spectrometer. In this thesis, the ‘*Loose*’ operating point is used, which incorporates muons of all five reconstruction types. Combined muons have the highest purity and deliver the largest contribution to the Loose muon selection. Inside-out muons increase the sensitivity to low-energy muons. Segment-tagged and calorimeter-tagged muons are restricted to the $|\eta| < 0.1$ region to recover inefficiencies arising from a not fully instrumented muon spectrometer in that region due to cabling and services for the ATLAS detector. Extrapolated muons are employed in the region $2.5 < |\eta| < 2.7$, which is not covered by the inner detector. Additional isolation operating points are provided to select muons that are well separated from other particles. For this purpose, track-based and calorimeter-based isolation variables quantify the energy deposits in cones around the reconstructed muon. The ‘*Loose*’ isolation operating point is utilized for the muon selection in this thesis.

Data samples enriched with events of $Z/\gamma^* \rightarrow \mu^+\mu^- + \text{jets}$ and $J/\psi \rightarrow \mu^+\mu^- + \text{jets}$ are selected from up to 139 fb^{-1} of proton–proton collision data. They are used to derive correction factors on the muon energy scale and resolution [187] and on the reconstruction, identification, and isolation efficiencies [188]. Both efficiencies for the Loose identification and isolation operating points vary with the muon momentum. The identification efficiency ranges between 98% and 99% for muon momenta above 5 GeV. The isolation efficiency reaches 86% to 99% in the same kinematic phase space.

4.7 Missing Transverse Momentum

The conservation of momentum implies that the sum of the transverse momenta of all final state particles should effectively be zero. A deviation from zero in an event implies the presence of neutrinos or possibly new beyond-the-SM particles that are invisible to the detector systems. This imbalance is known as *missing transverse momentum* and is calculated from the negative vectorial sum of the transverse momenta of all final state particles. This is expressed by the event observables of the missing transverse momentum vector $\mathbf{E}_T^{\text{miss}}$, its magnitude E_T^{miss} , and its azimuthal direction ϕ^{miss} [189].

The missing transverse momentum is calculated from two quantities. The *hard term* is

the vectorial sum of the transverse momenta of all calibrated particles that are reconstructed and identified in an event. In this thesis, electrons, muons, and small- R calorimeter jets are considered for this term.² The *soft term* considers reconstructed tracks that are not assigned to any hard object. To reduce pileup contamination, only tracks that are compatible with the main hard-scatter vertex are included in the soft term. Calorimeter signatures of neutral particles are not considered in the soft term as these would suffer from large out-of-time pileup contributions. An ambiguity-resolving procedure prevents a double-counting of detector signatures when combining the $E_{\text{T}}^{\text{miss}}$ contributions.

The accuracy of the hard term solely depends on the reconstruction and calibration of the hard objects. The performance of the soft term can be quantified with events with no expected missing momentum. In such events the soft momentum is expected to be well balanced against the momenta of the hard objects. This is validated in events of $Z/\gamma^* \rightarrow e^+e^- + \text{jets}$ and $Z/\gamma^* \rightarrow \mu^+\mu^- + \text{jets}$ in simulations and in 36 fb^{-1} of proton–proton collision data [190].

² For technical reasons calibrated large- R jets and boosted di- τ objects are currently not included in the $E_{\text{T}}^{\text{miss}}$ calculation. However, their detector signatures would enter as small- R jets into the calculation. Whether the $E_{\text{T}}^{\text{miss}}$ resolution and accuracy would benefit from the inclusion of calibrated large- R jets and boosted di- τ objects would be the subject of future investigations.

Chapter 5

Boosted Di- τ Reconstruction and Identification

The τ lepton is the heaviest lepton with a mass of 1.777 GeV [25]. Due to its short mean life time of 290 fs and proper decay length of only 87.03 μm , most τ leptons decay before reaching the innermost layers of the ATLAS detector. Hence, they can only be observed via their decay products. With a branching ratio of 35%, τ leptons decay into lighter leptons and neutrinos via $\tau^- \rightarrow e^- \bar{\nu}_e \nu_\tau$ or $\tau^- \rightarrow \mu^- \bar{\nu}_\mu \nu_\tau$.¹ Because of their high mass, τ leptons can also decay into final states with hadrons, which occurs with a branching ratio of 65%. The investigation of hadronic decay modes is the main subject of this thesis. The decay products include a τ neutrino and an odd number of charged mesons, whereas 77% of the hadronic decays of τ leptons include one charged meson, denoted as *1-prong*, and 22% include three charged mesons, denoted as *3-prong*. One or more additional neutral mesons are produced in 65% of all hadronic τ decays. The charged and neutral mesons are predominantly pions, whereas other hadrons like kaons are rarely involved. The τ neutrino usually leaves the detector without interaction, so only the visible decay products, denoted as τ_{vis} , can be reconstructed.

The techniques to reconstruct hadronic τ decays are introduced in this chapter. First, the standard procedure for reconstructing individual resolved τ candidates is outlined, emphasizing in particular the shortcomings for the detection of boosted $h \rightarrow \tau^+ \tau^-$ decays. The novel techniques to reconstruct boosted τ pairs, called *boosted di- τ reconstruction*, are introduced afterwards. The performance of the di- τ reconstruction is compared with the standard resolved τ reconstruction. Also, the accuracy and resolution of the di- τ energy reconstruction is reviewed. Dedicated identification techniques are developed to reduce the large background of hadron jets produced by the fragmentation of quarks and gluons. The performance of the identification algorithm as well as the performance of additional track-multiplicity requirements that are utilized in the search for $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ are discussed. Finally, systematic uncertainties on the selection efficiency and energy response are evaluated. The results presented in this chapter are mainly estimated from simulations. A data-driven calibration and validation of those novel techniques is presented in Chapter 8.

¹ Charge conjugate decay modes are implied.

5.1 Resolved τ Reconstruction

The standard procedure to reconstruct hadronic τ decays detects each τ_{vis} object individually. This approach is hereafter referred to as *resolved* τ reconstruction and is particularly performant when the τ leptons are well isolated. A detailed description of the resolved τ reconstruction in ATLAS during Run 1 is given in Reference [191]. The latest developments and improvements during Run 2 are summarized in References [192–195].

The resolved τ reconstruction is seeded by anti- k_t jets with a radius parameter of $R = 0.4$ [191]. The seeding jet is formed from energy clusters calibrated to the hadronic scale and must fulfill the requirements of $p_T > 10$ GeV and $|\eta| < 2.5$. The primary vertex with the highest p_T -weighted fraction of all tracks within a $\Delta R < 0.2$ cone around the seeding-jet direction is identified as the origin of the τ candidate. The main hard-scatter vertex² of an event is not necessarily the origin vertex of a τ candidate, although especially in the high-energy regime they often coincide. The τ vertex is used to correct the η and ϕ direction of the τ candidate. Boosted decision trees are utilized for the τ track selection by considering the track momentum, the number of hits in the inner detector, and their impact parameters relative to the τ vertex. A τ candidate is required to have either one or three associated tracks. An independent algorithm called Tau Particle Flow [195] aims to reconstruct individual charged and neutral hadrons of the τ decay and can therefore be used to classify a τ candidate based on its most likely decay mode.

The energy of a τ candidate is calculated from the vectorial sum of the energy clusters within a $\Delta R < 0.2$ cone around the reconstructed τ direction. Furthermore, a τ specific energy calibration is applied that subtracts potential pileup contributions and uses a boosted regression tree with Tau Particle Flow information to bring the reconstructed energy close to the energy of the visible τ decay products in simulations. After calibration, a τ candidate is required to have a $p_T > 20$ GeV and $|\eta| < 2.5$. Candidates in the barrel-endcap transition region, $1.37 < |\eta| < 1.52$, are excluded due to a poor calorimeter instrumentation in this area.

At this stage, the τ reconstruction provides very little discrimination against the large background of quark- or gluon-initiated jets. These backgrounds are rejected with multivariate classifiers in a dedicated identification step. In Run 1 to early Run 2, a BDT classifier was used [192], which was recently superseded by a recurrent neural network (RNN) [194]. These classifiers utilize various discriminating variables, which are known for their good background suppression, mostly based on the distribution and energies of tracks and energy deposits in the calorimeter. Additionally, the RNN employs low-level information of individual tracks and energy clusters. Finally, correction factors on the identification efficiency and energy calibration are derived from proton–proton collision data [193].

The standard resolved τ reconstruction is well performing as long as the τ decay is isolated. However, the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal processes that are considered in this thesis can lead to a small spatial separation between two τ leptons. Figure 5.1 shows the angular distance between the visible decay products of two τ decays at generator level

² The main hard-scatter vertex is identified by using all tracks of an event (see Section 4.1) while for the τ vertex only those tracks in the vicinity of the τ candidate are considered.

in $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ decays with resonance masses m_X from 1 TeV to 3 TeV. With increasing masses m_X , the Lorentz boost of the Higgs bosons increases, which finally leads to a decreasing spatial distance between the two τ leptons. The minimal distance that the standard τ reconstruction is able to resolve is given by the radius parameter $R = 0.4$ of the seeding jet of the τ candidate. As described in Section 4.2, the anti- k_t algorithm collects energy deposits with distances smaller than R into one jet. In practice, this means that two τ leptons with a distance smaller than 0.4 are reconstructed as only one jet and subsequently as only one τ candidate. As can be seen in Figure 5.1, a sizable fraction of $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal events show τ lepton distances smaller than this 0.4 threshold, especially when m_X is above 1.2 TeV. Although the most noticeable loss in sensitivity in this region arises from the τ reconstruction, there are additional effects from selection and calibration procedures that are employed after the reconstruction step, i.e., the τ track selection, energy calibration, and identification. These can also be corrupted by additional tracks and energy deposits of a second nearby τ lepton.

In the following section, the novel di- τ reconstruction techniques are introduced, which aim to recover the sensitivity to events with a boosted pair of τ leptons. Its performance is compared to the standard resolved τ reconstruction.

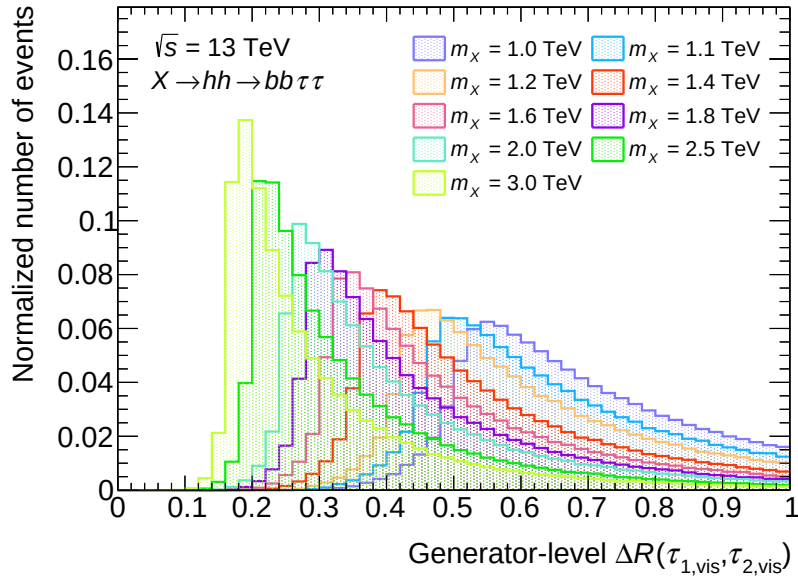


Figure 5.1: Distribution of the angular distance $\Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}})$ between the visible decay products of the two τ decays at generator level in simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events with resonance masses m_X from 1 TeV to 3 TeV.

5.2 Boosted Di- τ Reconstruction

The boosted di- τ reconstruction aims to reconstruct the hadronic decay products of a pair of τ leptons produced by the decay of a boosted massive particle. The massive particle may be a Higgs boson, a Z boson, or potentially a BSM particle that can decay into a τ pair. The di- τ reconstruction follows an approach similar to the techniques already developed

for the $h \rightarrow b\bar{b}$ reconstruction in the sense that it is seeded by a large- R jet, followed by a detection of smaller subjets containing the τ decay products. The calorimeter information of the seeding jet and its subjets is combined with inner detector information from tracks and vertices. Before going into the details of the di- τ reconstruction, a schematic representation of a typical di- τ candidate is shown Figure 5.2. Different regions are defined inside of a di- τ candidate during reconstruction. The *core cone* and the *subjet cone* are the cones with $\Delta R < 0.1$ and $\Delta R < 0.2$ around a subjet direction, respectively. The *isolation region* is the $\Delta R < 1.0$ cone around the seeding-jet direction under exclusion of the subjet cones. These regions are used to differentiate energy deposits and tracks and they become particularly useful for a later background separation.

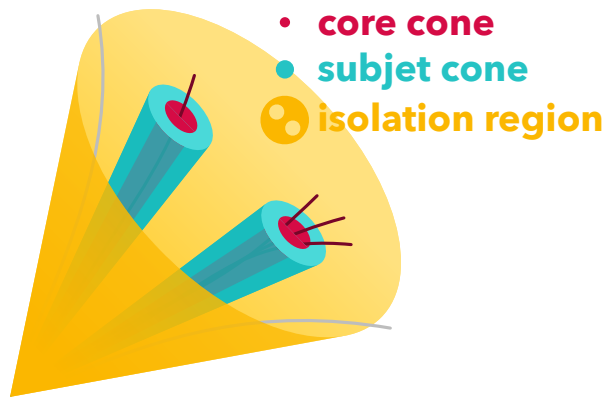


Figure 5.2: Schematic representation of a reconstructed di- τ object. The yellow cone indicates the seeding jet. The blue cones indicate the subjets. A di- τ candidate may have multiple subjets, but the decay products of the pair of τ leptons are expected to be contained within the two highest- p_T subjets. A di- τ candidate is divided into different regions. The core and subjet cones are cones around the subjet axes with radii of 0.1 and 0.2, respectively. The isolation region is a cone with radius 1.0 around the seeding-jet direction without the subjet cones. Tracks are indicated by the bend lines. They are identified as core, subjet, or isolation tracks, depending on their location.

5.2.1 Seeding Jet and Subjet Reconstruction

A di- τ candidate is seeded by an anti- k_t jet with a radius parameter of $R = 1.0$. Energy clusters that are calibrated to the hadronic scale are used as jet constituents.³ The radius parameter was chosen sufficiently high in order to obtain a large isolation region, which is beneficial for the later suppression of quark- and gluon-initiated jet background. This background is expected to leave more energy deposits in the isolation region, whereas genuine τ pairs are expected to have a distinct two-subjet signature. Additionally, the large radius provides enough space to have a transition region where both, the resolved τ and the boosted di- τ reconstruction, are sensitive. The large- R jet must have a $p_T > 300$ GeV and $|\eta| < 2.5$. The requirement on the transverse momentum is primarily employed to save

³ In contrast to the large- R jets, that are used for the $h \rightarrow b\bar{b}$ selection, no trimming algorithm is applied here. The di- τ kinematics are constructed from the two highest- p_T subjets. This paradigm provides sufficient protection against pileup and reduces sensitivity to the underlying event.

disk space during central ATLAS sample production. It was found to have a minor impact on the efficiency of the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal process, whereas the ubiquitous quark- and gluon-initiated jet background can be reduced drastically.

The subjets are reconstructed from the constituents of the seeding jet by using the anti- k_t algorithm with a radius parameter of $R = 0.2$. The decay products of a typical hadronic τ decay are expected to be well contained within $\Delta R < 0.2$. A similar cone size is already established in the resolved τ reconstruction, e.g., in the determination of the resolved τ energy. Alternative subjet clustering algorithms like k_t [177] and Cambridge-Aachen [196] were tested, but no improvements in terms of selection efficiencies were found. Hence, the anti- k_t algorithm is chosen in correspondence with the resolved τ reconstruction. Each subjet is required to have a $p_T > 10$ GeV and must contain at least one track within the subjet cone. The subjet p_T requirement was chosen rather low to have room for potential enhancements in a subsequent calibration or in further selection optimizations. The track selection criteria are detailed in the following section. A valid di- τ candidate must have at least two subjets. After ordering the subjets in p_T , the di- τ kinematics are reconstructed from the vectorial sum of the four-momenta of the leading and subleading subjet.

5.2.2 Track and Vertex Association

The track and vertex selection follows the example of the resolved τ reconstruction in early Run 2.⁴ An initial set of tracks that geometrically match the seeding jet is selected with the following requirements: the track p_T must exceed 1 GeV, it must have at least two hits in the pixel detector and a total of at least seven hits in the pixel and SCT detectors. The vertex with the highest track p_T fraction is selected as production vertex of the di- τ candidate. The track p_T fraction is defined as the p_T sum of tracks that are assigned to a vertex divided by the p_T sum of all tracks in the di- τ seeding jet. The location of the selected vertex is used to correct the axes of the tracks. Afterwards, additional impact parameter criteria are applied to the tracks: $|d_0| \leq 1.0$ mm and $|z_0 \sin \theta| \leq 1.5$ mm. The parameter d_0 is the closest distance of a track to the di- τ vertex in the transverse plane, z_0 is the closest distance along the longitudinal axis, and θ is the polar angle of a track. The remaining tracks are categorized as *core tracks*, *subjet tracks*, or *isolation tracks*, depending on their respective locations within the di- τ candidate.

5.2.3 Reconstruction Performance

The efficiency of the di- τ reconstruction is tested on simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events. A di- τ candidate is considered to be correctly reconstructed if the two leading subjets respectively match, within a distance of $\Delta R < 0.2$, to the simulated visible τ decay products. The di- τ reconstruction efficiency is the fraction of events in which the di- τ is correctly reconstructed.⁵ This is shown in Figure 5.3 as a function of the distance $\Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}})$

⁴ The latest τ reconstruction employs a multi-variate track selection [194] in favor of the simpler early Run 2 cut-based track selection [193]. An adaptation of the di- τ track selection to these latest developments might be beneficial for future performance improvements.

⁵ Acceptance cuts, if used for the efficiency calculation in the subsequent figures, are indicated in the figures.

between the visible decay products of the two τ leptons at generator level. For this purpose, a signal sample with a resonance mass of $m_X = 2$ TeV is chosen as a benchmark, as it covers a large ΔR range. Figure 5.3 also shows the efficiency of the resolved τ reconstruction, in this case defined as the fraction of events that include at least two reconstructed τ candidates that each match within $\Delta R < 0.2$ to the generated visible τ decay products. In this efficiency, the resolved τ candidates are required to have at least one associated τ track.⁶ The resolved reconstruction efficiency decreases sharply at $\Delta R = 0.4$ when the two τ decays are so close that they merge into the same small- R seeding jet. In the region of $0.2 < \Delta R < 0.4$, the di- τ reconstruction provides the largest gain in sensitivity. At even smaller distances the boosted di- τ subjects merge and the efficiency decreases.

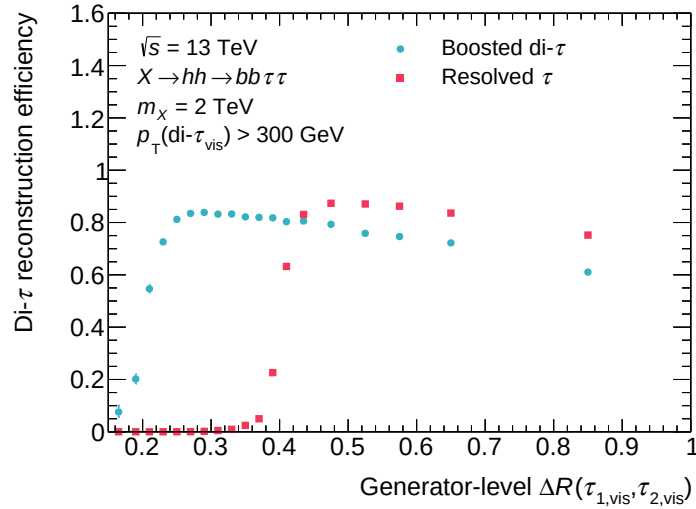


Figure 5.3: Efficiency to reconstruct a boosted pair of hadronically decaying τ leptons as boosted di- τ object, shown as blue circles, and as resolved τ objects, shown as red squares, as a function of the angular distance $\Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}})$ between the visible decay products of the two τ decays at generator level. The efficiencies are computed in simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events with a resonance mass of 2 TeV. The statistical uncertainties are shown as vertical error bars.

Other sources of inefficiencies, besides the merging of seeding jets and subjets, are explained in the following. The di- τ seeding jet must exceed the $p_T > 300$ GeV threshold. The impact of this requirement depends on the signal kinematics. It is almost negligible for the $m_X = 2$ TeV sample, but leads to small inefficiencies at $m_X = 1$ TeV. A subjet may not be reconstructed because the τ decay products are too soft. In the investigated range of signal masses, this happens rather rarely and can only be observed at the edge cases of the kinematic phase space. One of those cases is having high ΔR values in an $m_X = 2$ TeV signal sample. Those events tend to have a large momentum imbalance between the τ leptons, making the subleading τ lepton less likely to exceed the required p_T threshold. This can be seen in the efficiency slope towards high ΔR values in both the resolved τ and boosted di- τ efficiencies. Moreover, a boosted di- τ subjet must contain at least one track. That means inefficiencies in the track selection can lead to subjets not being recognized. Inefficiencies

⁶ The requirement is employed to the resolved τ candidates to have a fair comparison to the boosted di- τ reconstruction, which also requires at least one track per subjet at this stage. Typically a stricter requirement of exactly one or three associated tracks is employed for the resolved τ reconstruction.

in the track selection also occur in the resolved reconstruction, although it can be noted that the multi-variate track selection used in the resolved case is more efficient than the cut-based di- τ track selection. Finally, the boosted reconstruction considers only the two leading subjets to determine whether a di- τ candidate is correctly reconstructed. This leads to a loss in efficiency if, for example, a subjet from pileup has a higher energy than one of the τ leptons.⁷ These events are considered to be not correctly reconstructed because the di- τ calibration and identification build upon the assumption that the leading subjets contain the τ leptons. The resolved τ reconstruction, on the other hand, can reconstruct more than two τ candidates per event and all candidates are considered in the efficiency calculation. This increases the chance of finding the correct τ pair among all candidates. Any reconstructed candidate that does not match to a simulated τ decay might be rejected by the subsequent τ identification.

Figure 5.4(a) shows the reconstruction efficiency as a function of the momentum $p_{T,\text{vis}}$ of the visible decay products of the τ pair at generator level. The di- τ reconstruction efficiency reaches a plateau when the visible momentum exceeds the seeding jet p_T requirement of 300 GeV. The efficiency of the resolved reconstruction decreases with $p_{T,\text{vis}}$ as boosted topologies become more likely at high momenta. The di- τ reconstruction efficiency is very stable with respect to the number of pileup interactions μ , as can be seen in Figure 5.4(b). The chance to incorrectly reconstruct one of the two leading subjets slightly increases with the number of pileup interactions, leading to a small efficiency decrease under high-pileup conditions.

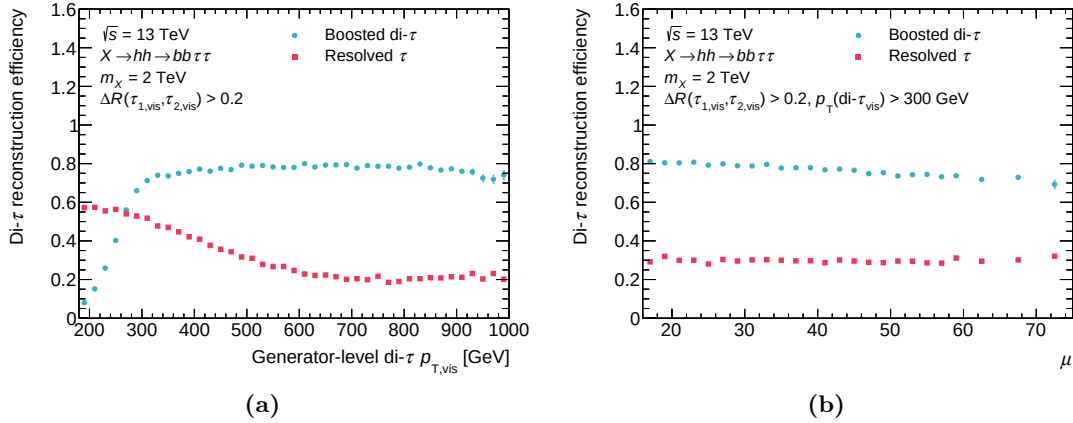


Figure 5.4: Efficiency to reconstruct a boosted pair of hadronically decaying τ leptons as boosted di- τ object (blue circles) and as resolved τ objects (red squares) as a function of (a) the momentum $p_{T,\text{vis}}$ of the visible decay products of the τ pair at generator level and (b) the number of pileup interactions μ . The efficiencies are computed in simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events with a resonance mass of 2 TeV. The statistical uncertainties are shown as vertical error bars.

⁷ An efficiency loss of about 10% is found, although the exact size of the effect depends on the signal kinematics. It could be subject of future studies to investigate whether this effect can be mitigated with a subjet selection that is sensitive to subjets from high-energy pileup. For example, properties like the number and energy of associated tracks could be used to suppress subjets from pileup.

5.3 Di- τ Energy Response

In this section, the energy response of the reconstructed di- τ candidate is discussed. The constituents of the di- τ seeding jet and its subjets are energy clusters that are calibrated to the hadronic scale with the local hadronic cell weighting scheme [173]. The reconstructed di- τ four-momentum is calculated from the vectorial sum of the four-momenta of the two leading subjets. To determine the energy accuracy and resolution, the energy E^{reco} of the reconstructed di- τ candidate is compared to the energy $E_{\text{vis}}^{\text{true}}$ of the visible decay products of the τ pair at generator level.

The accuracy is determined from the ratio $E^{\text{reco}}/E_{\text{vis}}^{\text{true}}$. The $E^{\text{reco}}/E_{\text{vis}}^{\text{true}}$ distribution is fitted with a Gaussian function in different regions of $p_{\text{T,vis}}$ and η_{vis} .⁸ The energy accuracy is then computed from the mean value of these Gaussian fits. This is shown in Figure 5.5. Only correctly reconstructed di- τ candidates are used for this purpose. A signal simulation with $m_X = 2$ TeV is used to illustrate the results, but these results are also representative of other resonance masses. It can be seen that the energy accuracy is very close to unity, with deviations below 4%. At transverse momenta below 300 GeV, the reconstructed energy tends to be overestimated. This is an artifact of the $p_{\text{T}} > 300$ GeV requirement on the seeding jet in the di- τ reconstruction. In events where the simulated momentum of the τ pair is below this threshold, but only di- τ candidates are reconstructed whose seeding jets exceed the threshold, a bias for overestimated energies arises. Near the barrel-endcap transition region, $1.37 < |\eta| < 1.52$, the di- τ energy tends to be underestimated due to the poor detector instrumentation in that region.

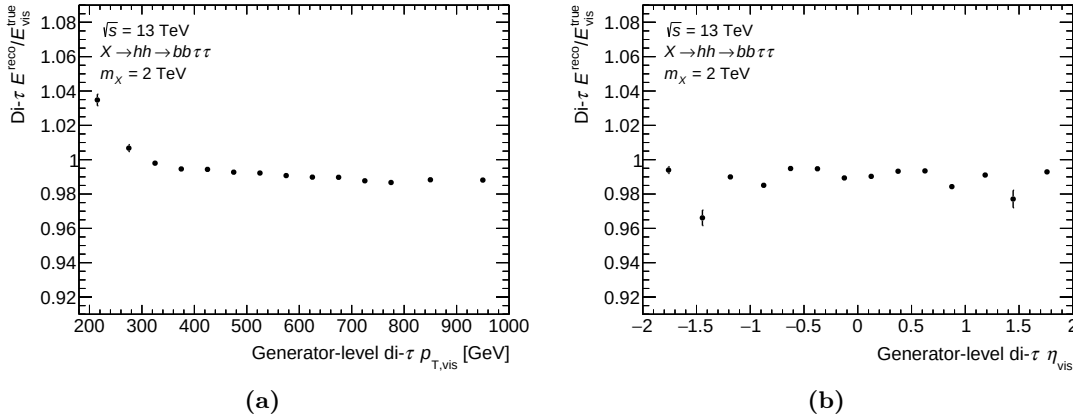


Figure 5.5: Energy accuracy as a function of (a) the momentum $p_{\text{T,vis}}$ and (b) the pseudo-rapidity η_{vis} of the visible decay products of the τ pair at generator level. The energy accuracy is computed in simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events with a resonance mass of 2 TeV. The statistical uncertainties are shown as vertical error bars.

The di- τ energy resolution is determined from the ratio $(E^{\text{reco}} - E_{\text{vis}}^{\text{true}})/E_{\text{vis}}^{\text{true}}$. Again, these distributions are fitted with Gaussian functions in various regions of $p_{\text{T,vis}}$ and η_{vis} . The resolution is given by the standard deviation of the fitted curve. The results are

⁸ The fit range is constrained to one standard deviations below and above the mean value of the distribution. This prevents a bias due to not Gaussian shaped tails of the distributions.

presented in Figure 5.6. As expected from the energy determination in the calorimeters, the resolution steadily improves with increasing momenta. It is found to range between 2% and 6%, except for the barrel-endcap transition region where the resolution reaches only approximately 7.5%.

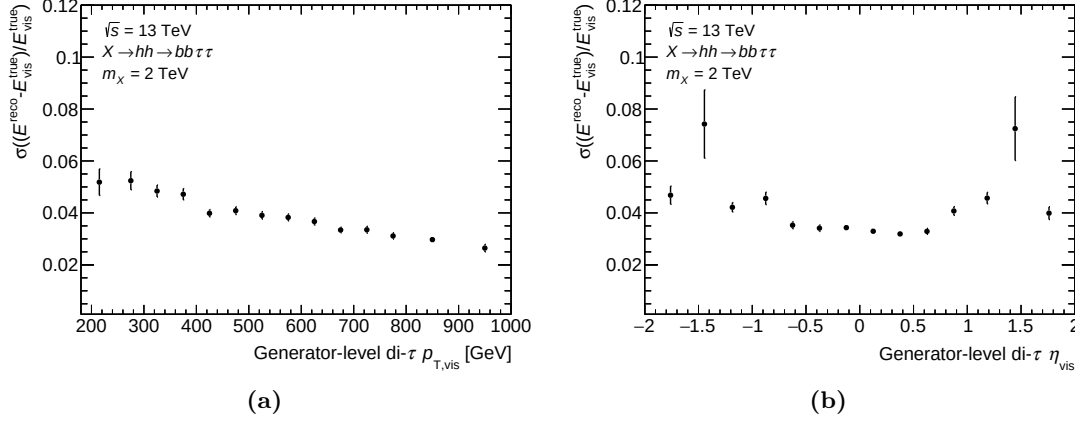


Figure 5.6: Energy resolution as a function of (a) the momentum $p_{T,\text{vis}}$ and (b) the pseudo-rapidity η_{vis} of the visible decay products of the τ pair at generator level. The resolution is computed from the standard deviation σ of the $(E^{\text{reco}} - E_{\text{vis}}^{\text{true}})/E_{\text{vis}}^{\text{true}}$ distribution in simulated $X \rightarrow hh \rightarrow bb\tau^+\tau^-$ events with a resonance mass of 2 TeV. The statistical uncertainties are shown as vertical error bars.

Based on the comparison between reconstructed and simulated energies, it is possible to derive energy calibration factors to further improve the accuracy and resolution of the visible energy. However, when using the di- τ reconstruction techniques in a data analysis, the effective energy resolution is much more limited by the resolution loss due to the missing neutrino energies. Therefore, further corrections of the visible energy of di- τ candidates are not applied. A validation of the di- τ energy response in proton-proton collision data is presented in Chapter 8.

5.4 Di- τ Identification

The reconstruction algorithm aims to find boosted τ pairs with high efficiency. However, at this stage, it provides little rejection against background processes, in particular quark- or gluon-initiated jets that are produced in proton-proton collisions with high cross section. The distinction between di- τ candidates from signal processes and di- τ candidates from quark- or gluon-initiated jets is performed with a dedicated *di- τ identification* algorithm. A signal di- τ has typically two high-energetic subjects with a small number of associated high-momentum tracks. The di- τ isolation region is expected to contain only a small amount of tracks and energy deposits in the calorimeter. The jets produced by particle showers of hadronizing quarks and gluons have typically a broad detector signature with multiple subjects and a large number of low-momentum tracks. These characteristics are quantified in a set of identification variables that are processed in a BDT classifier.

5.4.1 Training Event Selection

The training of the BDT classifier is performed on $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ samples for signal and events dominated by quark- and gluon-initiated jets recoiled by the ATLAS experiment as a background. The four- τ final state is chosen as signal process as it doubles the number of available di- τ candidates in the training. Simulations with graviton masses of 1.50 TeV, 1.75 TeV, 2.00 TeV, 2.25 TeV and 2.50 TeV are combined to form the signal training set. Equal signal cross sections are assumed when forming the training set to not introduce a bias to a certain signal hypothesis. Only correctly reconstructed di- τ candidates are considered for the signal training set. The background training set is selected from 3.2 fb^{-1} of proton-proton collision data that has been recorded by the ATLAS experiment in 2015. The events are selected using small- R jet triggers with transverse energy thresholds between 100 GeV and 400 GeV and have to contain at least one reconstructed di- τ candidate. These events are known to be dominated by multi-jet events with quark- and gluon-initiated jets. The contamination of this background training set by events with genuine boosted τ pairs, e.g., from $Z/\gamma^* \rightarrow \tau^+\tau^- + \text{jets}$ or even $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal, are found to be negligible.

After selection, more than 0.3 million signal di- τ candidates and 13 million background candidates are available for the training of the di- τ identification. Half of the signal and half of the background is used in the BDT training, the other half for performance evaluation purposes. The signal events are reweighted to the same pileup profile as the 2015 data. Furthermore, the signal and background events are reweighted such that the di- τ p_T spectra become flat. This compensates for p_T dependencies of the identification variables and prevents the training from focusing only on a certain kinematic phase space. Figure 5.7 shows the di- τ p_T distribution in signal and background before and after the p_T -reweighting. It can be seen that the p_T distribution of the signal before reweighting is significantly harder than the p_T distribution of the background sample. After reweighting, both become flat over a large momentum range. However, a flat momentum distribution cannot be sustained indefinitely because the required event weights would grow too large at high p_T and would make it susceptible to statistical fluctuations. Hence, a phase-out term is applied above 1 TeV, resulting in an exponential decrease in the p_T spectrum at very high momenta.

5.4.2 Identification Variables

A set of identification variables is defined in order to quantify the differences between di- τ objects from signal and from quark- or gluon-initiated jets. These variables exploit, for example, the ratios of energy deposits in the core cone $\Delta R < 0.1$ compared to the energy deposits in the subjet cone $\Delta R < 0.2$, the number of subjet tracks, or the angular distance of tracks to the subjet direction. Some of those variables have a correspondence to resolved τ identification variables. In the case of the di- τ identification such variables are defined individually for the leading and subleading subjets. There are also variables that exploit the specific decay topology of a boosted τ pair, for example, that there are typically two pronounced subjets and a small number of tracks and energy deposits in the isolation region.

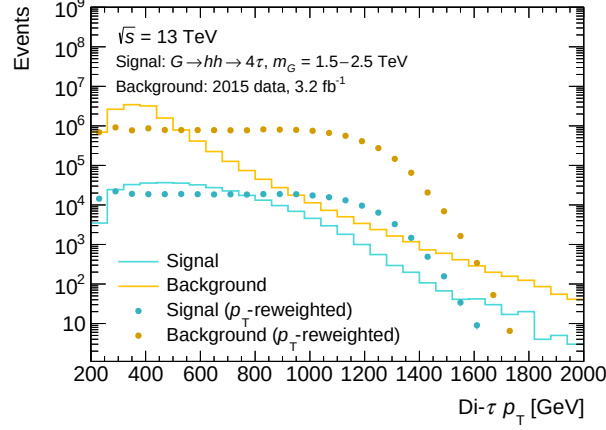


Figure 5.7: Distribution of the reconstructed di- τ p_T in signal (blue) and background (yellow). The histograms represent the p_T distribution before reweighting. The markers show the distributions after applying the p_T -reweighting. The p_T -reweighting achieves a flat p_T spectrum until 1 TeV. Beyond 1 TeV, a phase-out term is applied in order to prevent large weights and statistical fluctuations at very high momenta from dominating the training procedure. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

From initially 51 potential identification variables, the set is reduced, based on their discrimination performance and correlation. The final set of 17 identification variables is listed in Table 5.1. It is found that the training performance is improved when a logarithm is applied to identification variables with large tails. The absolute value is taken for identification variables that show a symmetric distribution around zero. The distributions of the identification variables are shown in Figures 5.8 to 5.17.

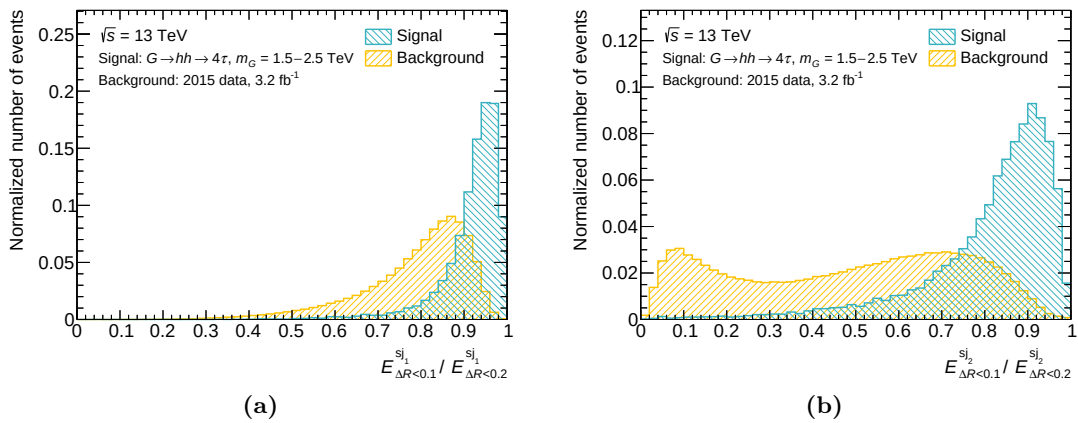


Figure 5.8: Distribution of the ratio of the energy deposited in the core cone to that in the subjet cone for (a) the leading subjet and (b) the subleading subjet. The energy deposits in the signal tend to be more collimated, resulting in distributions close to one. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

Table 5.1: Formulas and descriptions of the variables used in the di- τ identification.

Variable	Description
$E_{\Delta R < 0.1}^{\text{sj}_1} / E_{\Delta R < 0.2}^{\text{sj}_1}$ and $E_{\Delta R < 0.1}^{\text{sj}_2} / E_{\Delta R < 0.2}^{\text{sj}_2}$	Ratio of the energy deposited in the core cone to that in the subjet cone for the leading and subleading subjects, respectively (see Figure 5.8)
$(p_T^{\text{sj}_1} + p_T^{\text{sj}_2}) / p_T^{\text{seed}}$ and $p_T^{\text{sj}_2} / p_T^{\text{seed}}$	Ratio of the scalar sum of the two leading subjects p_T to the di- τ seeding jet p_T and ratio of the p_T of the subleading subject to the di- τ seeding jet p_T (see Figure 5.9)
$n_{\text{tracks}}^{\text{subjects}}$ and $n_{\text{tracks}}^{\text{sj}_1}$	Number of tracks within all subjects and within the leading subject (see Figure 5.10)
$\log(m_{\Delta R < 0.1}^{\text{tracks, sj}_1})$ and $\log(m_{\Delta R < 0.1}^{\text{tracks, sj}_2})$	Logarithms of the invariant mass of the core tracks in the leading and subleading subject, respectively (see Figure 5.11)
$\log(m_{\Delta R < 0.2}^{\text{tracks, sj}_1})$ and $\log(m_{\Delta R < 0.2}^{\text{tracks, sj}_2})$	Logarithms of the invariant mass of the tracks within the leading and subleading subject, respectively (see Figure 5.12)
$\Delta R_{\text{max}}(\text{track, sj}_1)$ and $\Delta R_{\text{max}}(\text{track, sj}_2)$	Maximum separation of a track from its associated subjet axis in the leading and subleading subject, respectively (see Figure 5.13)
$\sum [p_T^{\text{track}} \Delta R(\text{track, sj}_2)] / \sum p_T^{\text{track}}$	Sum of ΔR between tracks within the subleading subject and its axis, weighted by track- p_T (see Figure 5.14)
$\sum [p_T^{\text{iso-track}} \Delta R(\text{iso-track, sj})] / \sum p_T^{\text{iso-track}}$	Sum of ΔR between subjet axis and isolation tracks that are within $0.2 < \Delta R < 0.4$, weighted by track- p_T (see Figure 5.15)
$\log(\sum p_T^{\text{iso-tracks}} / p_T^{\text{seed}})$	Logarithm of the ratio of the scalar sum of isolation tracks p_T to the di- τ seeding jet p_T (see Figure 5.16)
$\log(d_{0,\text{lead-track}}^{\text{sj}_1})$ and $\log(d_{0,\text{lead-track}}^{\text{sj}_2})$	Logarithms of the closest distance in the transverse plane between the primary vertex and the highest- p_T track within the leading and subleading subject, respectively (see Figure 5.17)

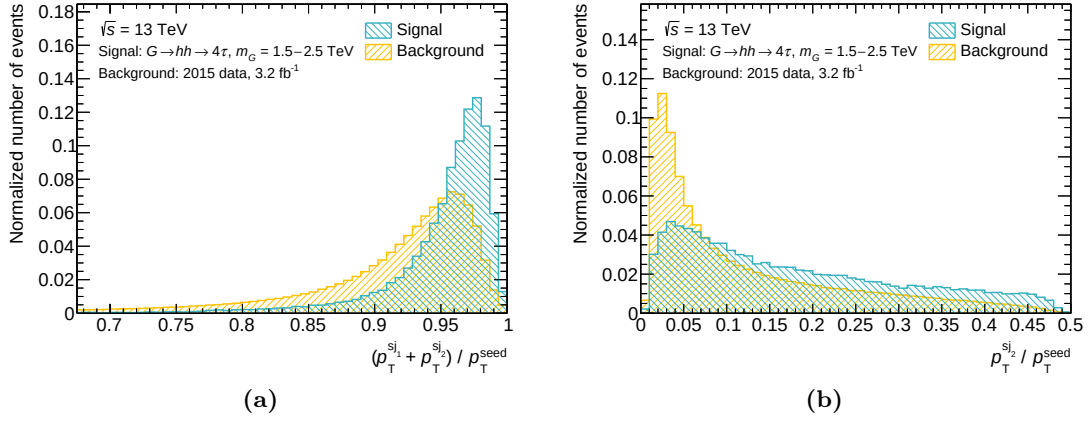


Figure 5.9: Distribution of (a) the ratio of the scalar sum of the two leading subjects p_T to the di- τ seeding jet p_T and (b) the ratio of the p_T of the subleading subject to the di- τ seeding jet p_T . In signal, the majority of energy deposits is contained within the leading and subleading subjects, resulting in distributions with higher values than in background events. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

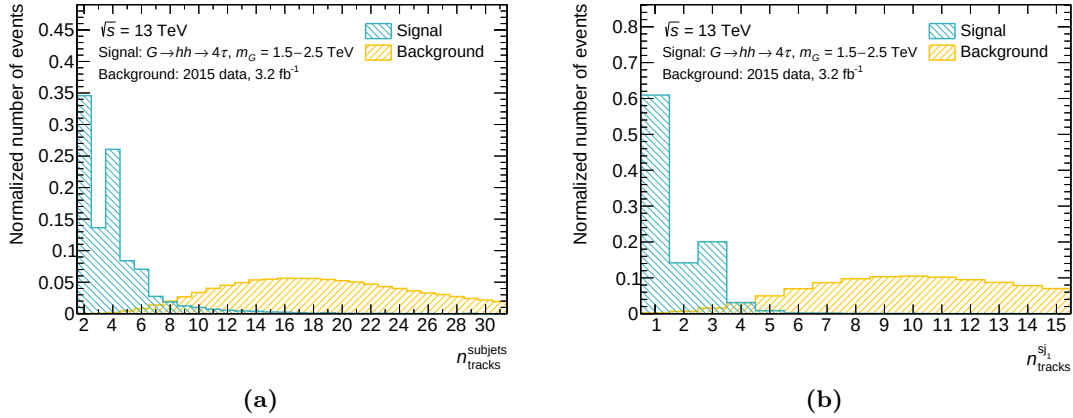


Figure 5.10: Distribution of the number of tracks (a) within all subjects and (b) within the leading subject. The track-multiplicity in signal subjects is mostly one or three. Quark- and gluon-initiated jets tend to have significantly higher track-multiplicities. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

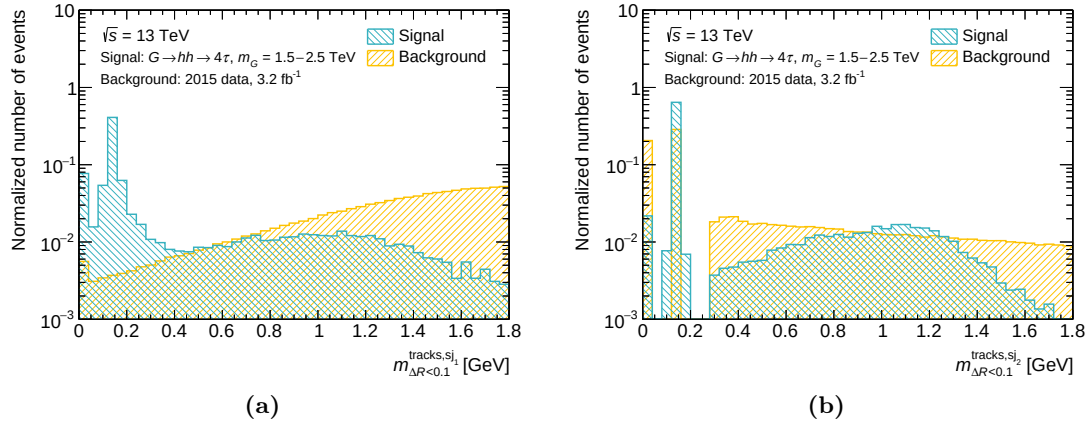


Figure 5.11: Distribution of the invariant mass of the core tracks in (a) the leading and (b) the subleading subjet. The first peak at zero corresponds to di- τ candidates with no core tracks in a subjet. The second peak at approximately the mass of a charged pion corresponds to candidates with one core track. The third peak in signal corresponds to candidates with three core tracks and reflects the invariant mass of a τ lepton without neutral mass components. The signal dataset consists of simulated $G \rightarrow hh \rightarrow 4\tau$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

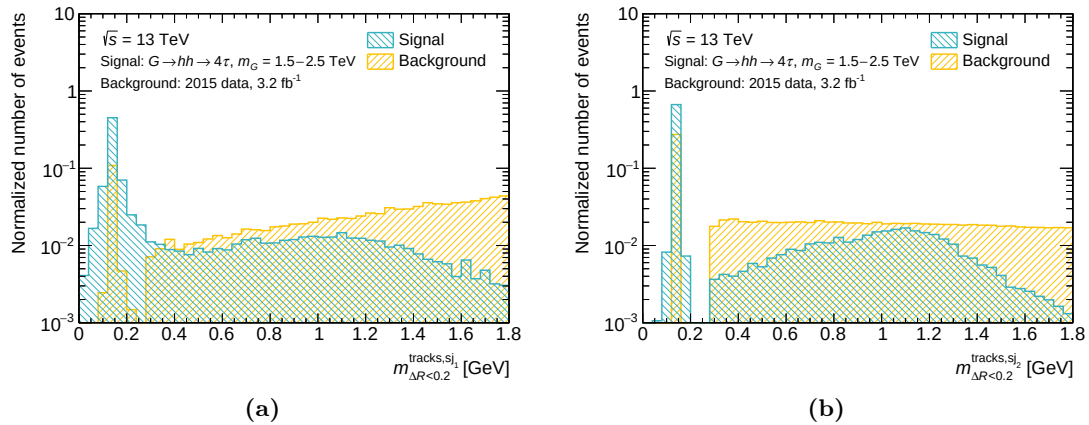


Figure 5.12: Distribution of the invariant mass of the tracks within (a) the leading and (b) the subleading subjet. The first peak at approximately the mass of a charged pion corresponds to candidates with one subjet track. The second peak in signal corresponds to candidates with three tracks and reflects the invariant mass of a τ lepton without neutral mass components. The signal dataset consists of simulated $G \rightarrow hh \rightarrow 4\tau$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

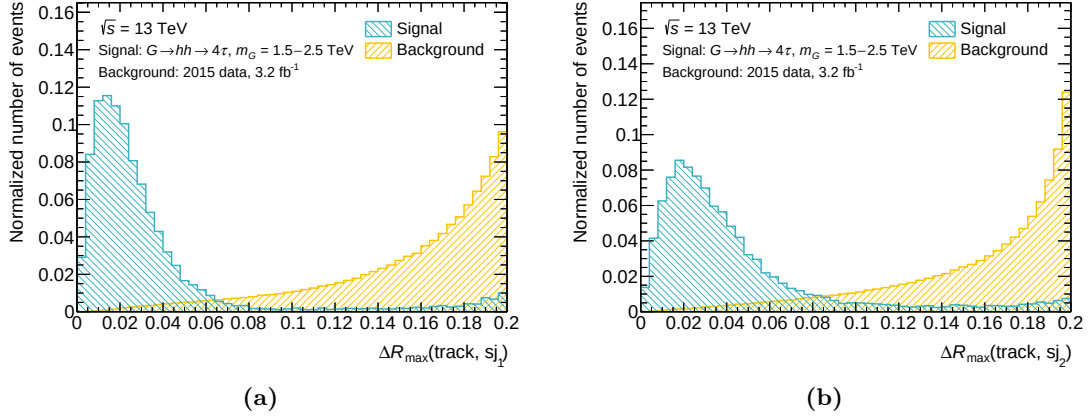


Figure 5.13: Distribution of the maximum separation of a track from its associated subjet axis in (a) the leading and (b) the subleading subjet. The tracks in signal tend to be more collimated, resulting in distributions close to zero. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

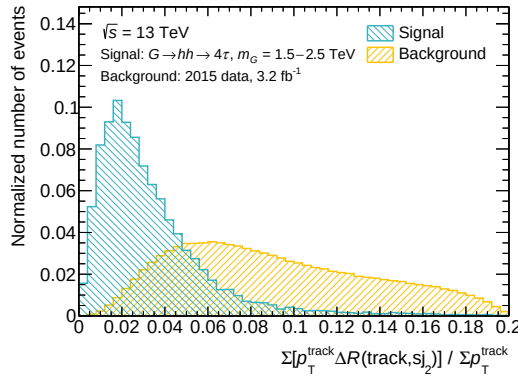


Figure 5.14: Distribution of the sum of ΔR between tracks within the subleading subjet and its axis, weighted by track- p_T . The tracks in signal tend to be more collimated, resulting in distributions close to zero. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

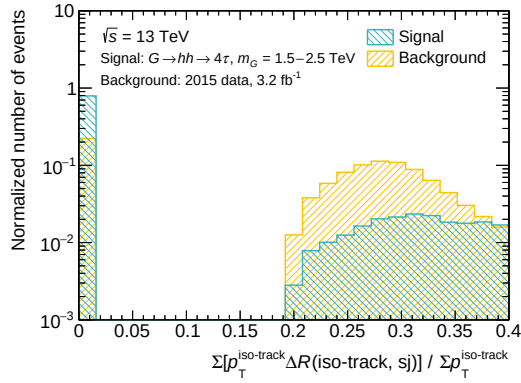


Figure 5.15: Distribution of the sum of ΔR between subjet axis and isolation tracks, weighted by track- p_T . Only isolation tracks within $0.2 < \Delta R < 0.4$ around a subjet are considered. The first peak corresponds to di- τ candidates without such isolation tracks, which are more common in signal than in background events. In background, a subjet is typically too small to contain a full quark- or gluon-initiated jet. Therefore, the isolation tracks are often distributed closely around a subjet. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

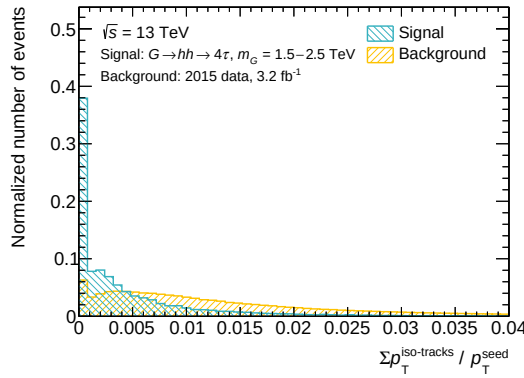


Figure 5.16: Distribution of the ratio of the scalar sum of isolation tracks p_T to the di- τ seeding jet p_T . In signal, there are typically very few and low- p_T isolation tracks. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

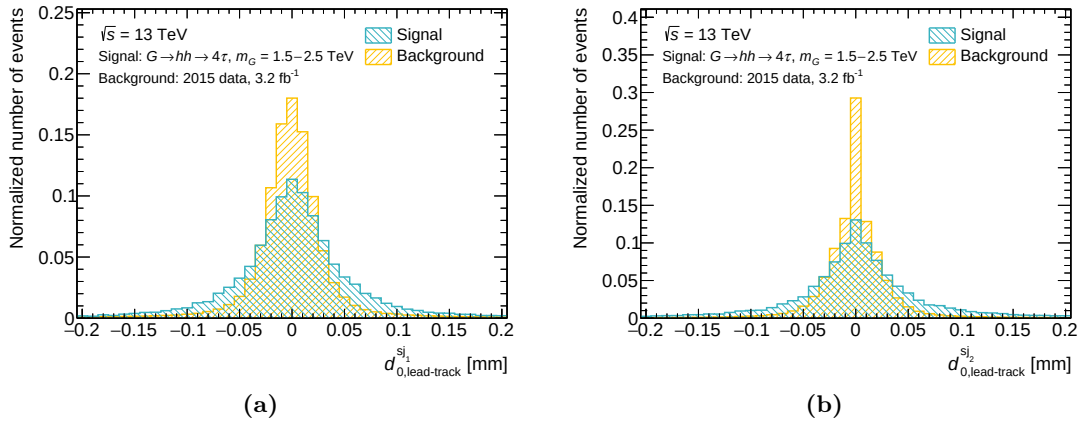


Figure 5.17: Distribution of the closest distance d_0 in the transverse plane between the primary vertex and the highest- p_T track within (a) the leading and (b) the subleading subjet. The d_0 distributions in signal tends to be wider than in background, due to the considerable decay length of a τ lepton. The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

5.4.3 Identification Training

The BDT training is performed with the TMVA toolkit [197]. The BDT classifier consists of multiple binary decision trees. In this training, a maximum number of 150 trees is chosen. Each decision tree is grown during training by finding the identification variable and the corresponding cut value that provides the best separation between signal and background. The separation is determined with the Gini index, $p \cdot (1 - p)$, where p is the signal purity, i.e., the ratio of signal events to all events that pass the cut. Up to 300 possible cut values are examined per identification variable. After finding the best initial cut, the training sample is split into two nodes containing events that passed or failed the criterion, respectively. This procedure is repeated iteratively until a stop condition is fulfilled. In this training, this is the case when a maximum tree depth of eight is reached or the number of events in a node falls below 0.5% of the initial training sample size. The final leaf nodes are identified as either signal- or background-like, depending on their signal purity.

The so-called boosting procedure modifies the event weights before training the subsequent decision tree. By doing so, it enhances the statistical stability and discrimination performance of the classifier. In the di- τ identification, the AdaBoost (adaptive boosting) algorithm [198] is employed with a boosting parameter of $\beta = 0.2$. Events that are misclassified in the previous decision tree get an enhanced weight in the training of the subsequent tree. After training, the final BDT discriminant score is computed from a weighted average over the classification results of all decision trees. A high BDT score indicates a signal-like signature, and a low value indicates a background-like signature, as can be seen in Figure 5.18.

The training parameters, i.e., the maximum number of trees, the number of possible cut values per variable, the stop conditions for tree growing, and the boosting algorithm have been varied and tuned in multiple trainings in order to achieve a high separation performance

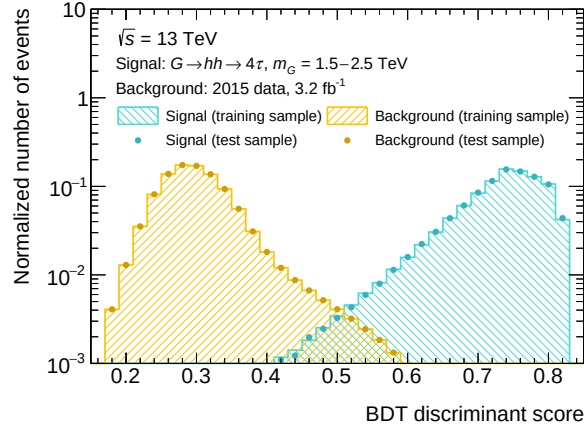


Figure 5.18: Distribution of the BDT discriminant score for signal (blue) and background (yellow). No signs of overtraining are observed in the comparison between training sample (histogram) and test sample (markers). The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data. Half of the events are employed in the BDT training, the other half is used for performance evaluation.

while avoiding overtraining. Overtraining describes the effect of a classifier having too many degrees of freedom and thereby becoming sensitive to statistical fluctuations of the training dataset. No signs of overtraining are observed in the di- τ identification as this would become manifest in differences between the BDT responses of the training dataset and the independent test dataset in Figure 5.18.

5.4.4 Identification Performance

The performance of the di- τ identification is determined by the identification efficiency, which is defined as the fraction of reconstructed di- τ candidates that meet a given cut on the BDT score. Due to the continuous BDT discriminant score, any cut value can be chosen that provides the desired signal efficiency and background rejection. The relation between signal and background efficiency in the di- τ identification is illustrated in Figure 5.19. In a preliminary study, a BDT score cut of 0.72 was found to provide the highest signal sensitivity against multi-jet background events in a search for $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$. This operating point corresponds to a signal efficiency of more than 60% and a background rejection, i.e., an inverse background efficiency, of approximately 10^4 . This means on average one out of 10^4 reconstructed di- τ candidates from quark- or gluon-initiated jets is misidentified as a genuine boosted τ pair. This operating point is used in the following to illustrate the di- τ identification performance. The absolute values in terms of signal and background efficiencies would be different at other operating points, but the general qualitative behavior is similar.

Figure 5.20 shows the di- τ identification efficiency in simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events with $m_X = 2 \text{ TeV}$ as a function of the generator-level di- τ $p_{T,\text{vis}}$ and the number of pileup interactions μ . The identification efficiency increases with transverse momentum until it reaches a plateau at 300 GeV. It shows a low dependence on the number of pileup

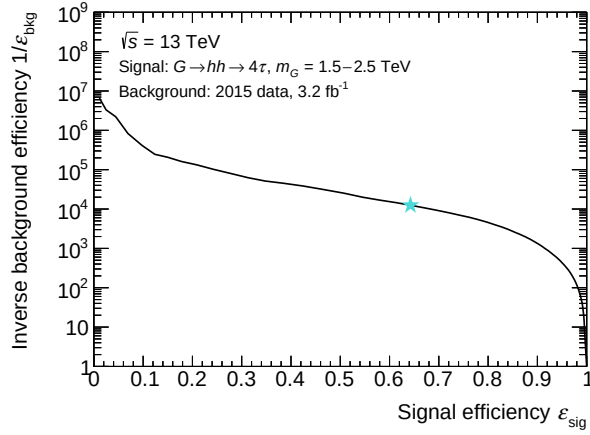


Figure 5.19: Inverse background efficiency as a function of signal identification efficiency. The blue star represents the chosen operating point at a signal efficiency of more than 60% and an inverse background efficiency of approximately 10^4 . The signal dataset consists of simulated $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ events with resonance masses between 1.5 TeV and 2.5 TeV. The background dataset consists of 3.2 fb^{-1} of ATLAS data.

interactions. Only a slight efficiency decrease towards high μ values can be seen. The efficiency that a background event passes the di- τ identification is shown in Figure 5.21 as a function of the reconstructed di- τ p_T and μ . This figure is based on half of the 2015 data that was not used for BDT training. The background efficiency reaches a plateau at transverse momenta above approximately 400 GeV. The pileup dependency is difficult to assess with this background sample, due to the limited statistics that comes with the high background rejection and the limited pileup profile in 2015 data. Nevertheless, no strong pileup dependency is observed in the μ range investigated. This was also confirmed in an investigation of multi-jet simulations, which provide a larger pileup range.

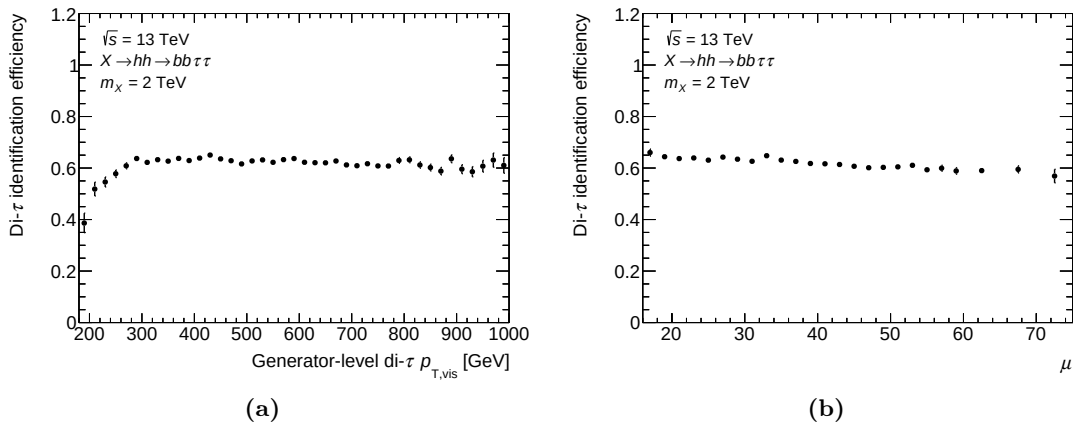


Figure 5.20: Di- τ identification efficiency as a function of (a) the momentum $p_{T,\text{vis}}$ of the visible decay products of the τ pair at generator level and (b) the number of pileup interactions μ . The efficiencies are computed in simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events with a resonance mass of 2 TeV. The statistical uncertainties are shown as vertical error bars.

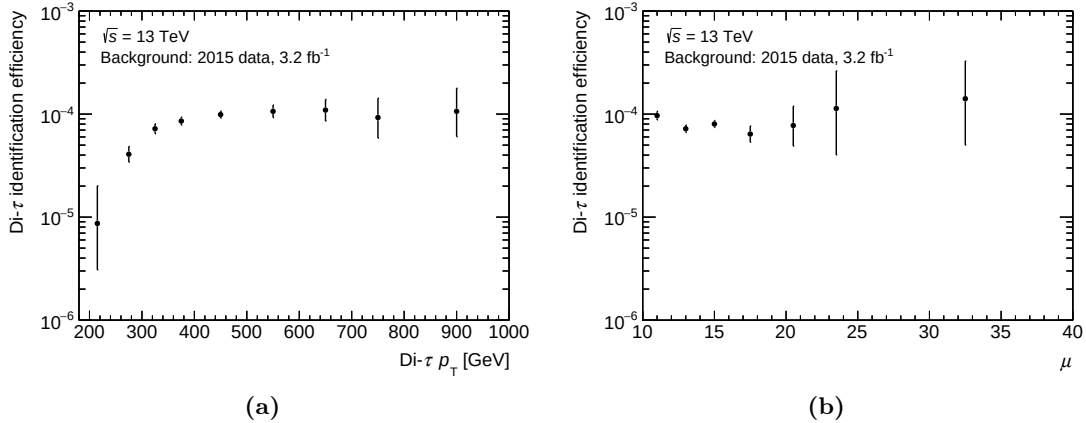


Figure 5.21: Efficiency for background events to pass the di- τ identification as a function of (a) the reconstructed di- τ momentum p_T and (b) the number of pileup interactions μ . The background dataset consists of 3.2 fb^{-1} of ATLAS data. The statistical uncertainties are shown as vertical error bars.

5.5 Track-Multiplicity Selection

The large majority of hadronically decaying τ leptons produce one or three charged pions. Thus, it is expected that a di- τ subjet originating from a τ lepton contains one or three tracks. This is already considered in di- τ identification variables that count the track-multiplicity. However, it was found that a tighter requirement than the one imposed by the BDT is beneficial in a data analysis searching for new physics. For this purpose, the two leading di- τ subjects are required to have exactly one or three associated core tracks. This further increases the rejection of quark- and gluon-initiated jets and enables a reliable determination of the τ lepton charge. The τ lepton charges are utilized in the region definitions of the data analysis described in the following chapters. Regions where the two leading di- τ subjects have opposite-sign charges are enriched with events with genuine boosted τ pairs. Regions where the subjects have same-sign charges are enriched with multi-jet background and are used to estimate and validate this background. Figure 5.22 shows the efficiency of the tight track-multiplicity requirement, computed after the di- τ identification, as a function of the generator-level di- τ $p_{T,\text{vis}}$ and the number of pileup interactions μ . There is a small dependency on p_T , which is mainly caused by 3-prong τ decays. At high momenta, the typical track distances decrease, making it more likely that one of the tracks is not reconstructed because it shares too many inner detector hits with a nearby track. The number of pileup interactions in an event does not affect the track-multiplicity selection.

5.6 Systematic Uncertainties from Simulation Variations

In this section, systematic uncertainties for the di- τ algorithms are presented. These are extracted from a set of systematically varied Monte Carlo simulations. A data-based calibration is presented in Chapter 8, giving an additional source of systematic uncertainties. It can already be noted that the data-based systematic uncertainties are dominant due to the

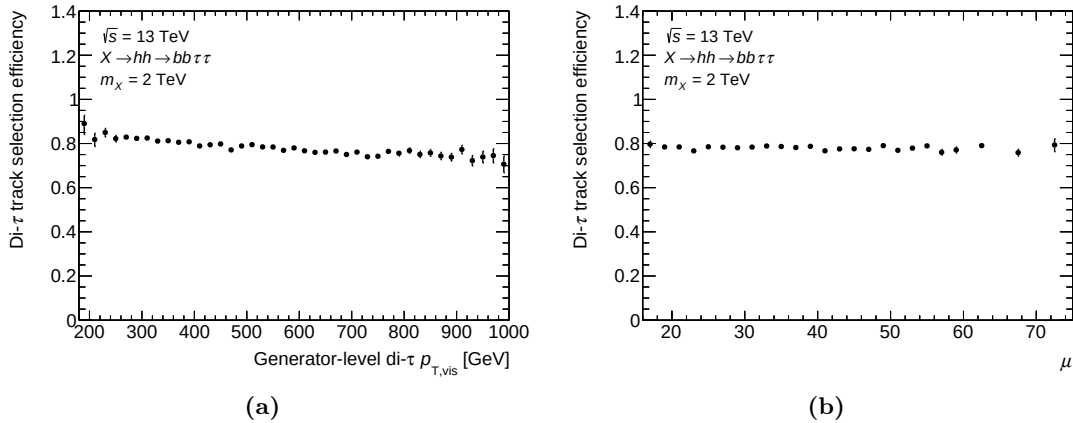


Figure 5.22: Efficiency of the tight track-multiplicity requirement as a function of (a) the momentum $p_{T,\text{vis}}$ of the visible decay products of the τ pair at generator level and (b) the number of pileup interactions μ . The efficiencies are computed in simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events with a resonance mass of 2 TeV. The statistical uncertainties are shown as vertical error bars.

limited data statistics and due to uncertainties on the background estimation. Nevertheless, the systematic uncertainties from simulation variations, as they are presented here, are still considered because they allow for an investigation of potential systematic uncertainties with high statistics and can cover kinematic regions of phase space that are not accessible by a data-based calibration.⁹ Systematic uncertainties on the reconstruction and identification efficiencies and on the energy response are derived in this section.

The systematic uncertainties are estimated with a set of $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ simulations with graviton masses ranging from 1 TeV to 5 TeV. The systematic variations alter properties of the GEANT4 detector model and thereby influence the simulated particle propagation and interactions with the detector material. The variations are chosen in accordance with what is used for the uncertainty estimation of the resolved τ reconstruction efficiency. Each of them uses the same events at matrix element level in order to avoid statistical fluctuations dominating the estimate of the systematic uncertainty. In one variation an alternative physics list is used. The physics lists provide the energy-dependent models and cross sections that are employed in GEANT4 to simulate particle showers and interactions of various particle types with the detector material [199]. Here, the default FTFP_BERT physics list is changed to QGSP_BIC. Both methods differ primarily in the modeling of inelastic hadronic interactions.¹⁰ This variation impacts the energy-related selection cuts in the di- τ reconstruction, the di- τ energy response, as well as variables used in the di- τ identification. Additionally, there are three variations of the inner detector model that predominantly affect the track reconstruction as well as the identification variables that utilize tracks. In these variations, the passive material is increased by 30% in the Insertable B-layer, by 50% in the pixel detector PP0 service region, and finally by 5% in all

⁹ These are regions of very high momenta, that are generally less populated in data, and regions where the di- τ algorithms are particularly less efficient, e.g., at very low or high ΔR between the τ leptons.

¹⁰ The following models are used depending on the energy scale and the types of interacting particles [199]: the Fritiof (FTF) model [200, 201], the Quark–Gluon String (QGS) model [202, 203], the Bertini (BERT) cascade model [204] and the Binary cascade (BIC) model [205].

inner detector layers.

The systematic uncertainties are retrieved in various kinematic regions of phase space. The sensitivity of the di- τ reconstruction depends on the spatial separation of the τ leptons and their respective momenta. The systematic uncertainties may differ between regions where the di- τ reconstruction is more or less sensitive. For this reason, three categories of angular distance $\Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}})$ between the visible τ decay products at generator-level are considered:

$$\begin{aligned} \text{low-}\Delta R : \quad & \Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}}) < 0.2, \\ \text{medium-}\Delta R : \quad & 0.2 < \Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}}) < 1.0, \\ \text{high-}\Delta R : \quad & 1.0 < \Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}}). \end{aligned}$$

Furthermore, the most sensitive kinematic region, medium- ΔR , is separated into additional categories of the transverse momentum of the leading τ , $p_T(\tau_{1,\text{vis}})$, and subleading τ , $p_T(\tau_{2,\text{vis}})$, at generator level:

$$\begin{aligned} \text{low-}p_T^{\tau_1} : \quad & p_T(\tau_{1,\text{vis}}) < 200 \text{ GeV}, \\ \text{high-}p_T^{\tau_1} : \quad & 200 \text{ GeV} < p_T(\tau_{1,\text{vis}}), \\ \text{low-}p_T^{\tau_2} : \quad & p_T(\tau_{2,\text{vis}}) < 20 \text{ GeV}, \\ \text{medium-}p_T^{\tau_2} : \quad & 20 \text{ GeV} < p_T(\tau_{2,\text{vis}}) < 50 \text{ GeV}, \\ \text{high-}p_T^{\tau_2} : \quad & 50 \text{ GeV} < p_T(\tau_{2,\text{vis}}). \end{aligned}$$

These regions are chosen based on the di- τ reconstruction efficiency and the requirement to have sufficient statistics in all regions.

5.6.1 Efficiency Uncertainties

The selection efficiency, i.e., the efficiency to correctly reconstruct and identify a boosted pair of τ leptons, is evaluated in all systematically varied Monte Carlo samples and compared to the nominal sample, which uses the same GEANT4 settings as the standard ATLAS sample production. The uncertainty on the selection efficiency, $\Delta\epsilon_{\text{var}} = |\epsilon_{\text{nom}} - \epsilon_{\text{var}}|$, is evaluated from the efficiency difference between the nominal sample and a systematically varied sample. The total uncertainty $\Delta\epsilon$ and the corresponding fractional uncertainty $\Delta\epsilon/\epsilon_{\text{nom}}$ are derived from the four variation uncertainties. None of the variations stands out particularly in terms of their contribution to overall uncertainty. On average, the variation of the physics list has a slightly higher impact compared to the three configuration variations of the inner detector. Table 5.2 lists the nominal selection efficiencies and the total uncertainties in the different kinematic regions. The fractional uncertainties range between 0.4% and 21%. The uncertainties are generally small in those regions where the di- τ reconstruction and identification algorithms are most sensitive but increase in regions of low momenta or low or high ΔR , respectively.

Table 5.2: Nominal selection efficiencies ε_{nom} , total efficiency uncertainties $\Delta\varepsilon$, and fractional efficiency uncertainties $\Delta\varepsilon/\varepsilon_{\text{nom}}$ in different kinematic regions. The uncertainties are derived from a set of systematically varied $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ simulations with resonance masses between 1 TeV and 5 TeV.

Region			ε_{nom}	$\Delta\varepsilon$	$\frac{\Delta\varepsilon}{\varepsilon_{\text{nom}}}$
	low- ΔR		0.0059	0.0006	9.8%
medium- ΔR	low- $p_{\text{T}}^{\tau_1}$	low- $p_{\text{T}}^{\tau_2}$	0.014	0.002	14.9%
medium- ΔR	high- $p_{\text{T}}^{\tau_1}$	low- $p_{\text{T}}^{\tau_2}$	0.132	0.006	4.3%
medium- ΔR	low- $p_{\text{T}}^{\tau_1}$	medium- $p_{\text{T}}^{\tau_2}$	0.034	0.003	8.0%
medium- ΔR	high- $p_{\text{T}}^{\tau_1}$	medium- $p_{\text{T}}^{\tau_2}$	0.396	0.005	1.4%
medium- ΔR	low- $p_{\text{T}}^{\tau_1}$	high- $p_{\text{T}}^{\tau_2}$	0.286	0.017	6.0%
medium- ΔR	high- $p_{\text{T}}^{\tau_1}$	high- $p_{\text{T}}^{\tau_2}$	0.557	0.002	0.4%
	high- ΔR		0.0037	0.0008	21.0%

5.6.2 Energy Response Uncertainties

A systematic uncertainty on the energy response is determined from the same systematic variations and in the same kinematic regions as for the efficiency uncertainties. Here, the transverse momentum distribution is compared between the nominal and the systematically varied samples. The di- τ p_{T} is highly correlated to the energy and is an important observable in the application of the di- τ tagger in searches for new physics. For the comparison between nominal and variation samples the transverse momentum of di- τ candidates is transformed as $p_{\text{T}} \mapsto (1 + \alpha) \cdot p_{\text{T}}$. For each variation, a momentum shifting parameter α is determined that leads to the best agreement with the nominal p_{T} distribution. Their agreement is evaluated with a χ^2 function:

$$\chi^2(\alpha) = \sum_i \frac{(n_i^{\text{nom}} - n_i^{\text{var}}(\alpha))^2}{n_i^{\text{nom}}},$$

where the number of events in bin i of the p_{T} distribution is given by n_i^{nom} for the nominal distribution and by $n_i^{\text{var}}(\alpha)$ for the distribution of the alternative sample. The value α that leads to the smallest χ^2 and thereby to the best agreement can be identified as a fractional uncertainty on the di- τ p_{T} . The total fractional uncertainty $\Delta p_{\text{T}}/p_{\text{T}}$ is determined from a quadratic error propagation over the fractional uncertainties of all four variations. Table 5.3 summarizes the results in the various kinematic regions. The total uncertainties range from 0.6% to 3.2%. As expected, the main contribution comes from the variation of the physics list.

Table 5.3: Fractional uncertainty on the transverse di- τ momentum $\Delta p_T/p_T$ in different kinematic regions. The uncertainties are derived from a set of systematically varied $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ simulations with resonance masses between 1 TeV and 5 TeV.

Region			$\frac{\Delta p_T}{p_T}$
	low- ΔR		2.1%
medium- ΔR	low- $p_T^{\tau_1}$	low- $p_T^{\tau_2}$	1.2%
medium- ΔR	high- $p_T^{\tau_1}$	low- $p_T^{\tau_2}$	0.6%
medium- ΔR	low- $p_T^{\tau_1}$	medium- $p_T^{\tau_2}$	1.4%
medium- ΔR	high- $p_T^{\tau_1}$	medium- $p_T^{\tau_2}$	0.7%
medium- ΔR	low- $p_T^{\tau_1}$	high- $p_T^{\tau_2}$	1.0%
medium- ΔR	high- $p_T^{\tau_1}$	high- $p_T^{\tau_2}$	1.0%
	high- ΔR		3.2%

Chapter 6

Event Selection and Categorization

This chapter describes the common event selection criteria that are applied in the data-driven di- τ calibration and in the search for $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$. The initial event cleaning step makes sure that the events were recorded under proper collider and detector conditions. An overlap removal ensures that detector signatures are not double-counted by multiple reconstructed physics objects. This is followed by the preselection, which ensures that a trigger has fired and that the selected events have a common signature of a di- τ candidate and a recoiling large- R jet. In the events selected for di- τ calibration, a large- R jet recoils against a Z boson, providing the τ pair with a substantial Lorentz boost. In the search for $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$, the recoiling jet is used to reconstruct the $h \rightarrow b\bar{b}$ decay. Finally, the events are categorized into different regions that are used for background estimation, validation, di- τ calibration, or as a $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region.

6.1 Event Cleaning and Overlap Removal

The data events must be recorded under good detector conditions, i.e., all detector components were working stably. As mentioned in Section 3.3, this is confirmed for events collected in the Good Run Lists that are centrally provided by the ATLAS collaboration. The Good Run Lists used in this analysis and their respective integrated luminosities can be found in Appendix A. To avoid contaminations of non-collision backgrounds, e.g., from calorimeter noise, beam halo, or cosmic rays, events are rejected if they contain a small- R jet with $p_T > 20$ GeV that does not meet the loose quality criteria described in Reference [206]. Additionally, events must have at least one vertex with at least two associated tracks with $p_T > 500$ MeV.

The overlap removal procedure ensures that the same detector signatures are not double-counted by multiple reconstructed objects. The procedure applied in this thesis follows the ATLAS recommendations for analyses with boosted topologies. The exact requirements are summarized in Table 6.1. Overlapping electrons, muons or jets are removed, depending on their distances, transverse momenta, or whether they share an inner detector track. In general, reconstructed objects that are expected to have a high purity, like muons or electrons, are favored over lower-purity objects like jets. When an electron and a muon share the same inner detector track the electron is removed, except when the muon is of

type calorimeter-tagged. Calorimeter-tagged muons usually have a low purity. Small- R jets are removed if their angular distance to an electron or muon is smaller than $\Delta R = 0.2$. Electrons and muons with distances of $0.2 < \Delta R < 0.4$ to one of the remaining small- R jets are removed if their transverse momentum is small as defined in Table 6.1. The remaining electrons are given priority over large- R jets. Finally, all small- R jets are removed if they overlap with a large- R jet.

There are additional overlap removal requirements that are specific to this analysis. Those are discussed in the following sections. For the selection of boosted $h \rightarrow b\bar{b}$ candidates, only large- R jets with a separation $\Delta R > 1.0$ from the selected di- τ candidate are considered. During preselection, events with electrons or muons are vetoed. Hence, no overlap removal between di- τ candidates and light leptons is needed in this thesis.

Table 6.1: Criteria to reject a reconstructed physics object against another nearby object. The overlap removal ensures that a single detector signature is not used to reconstruct multiple objects. Only objects that pass the preceding overlap removal criterion are considered in the subsequent steps.

Reject	Against	Criteria
electron	electron	shared inner detector track, reject lower- p_T electron
muon	electron	shared inner detector track and muon type is calorimeter-tagged
electron	muon	shared inner detector track
small- R jet	electron	$\Delta R < 0.2$
electron	small- R jet	$\Delta R < \min(0.4, 0.04 + 10 \text{ GeV}/p_T(e))$
small- R jet	muon	$\Delta R < 0.2$ and jet has less than 3 associated tracks
small- R jet	muon	jet has less than 3 associated tracks and one is shared with muon
muon	small- R jet	$\Delta R < \min(0.4, 0.04 + 10 \text{ GeV}/p_T(\mu))$
large- R jet	electron	$\Delta R < 1.0$
small- R jet	large- R jet	$\Delta R < 1.0$

6.2 Event Preselection

The overarching objective of the preselection is to select events with a common topology, i.e., with a boosted di- τ candidate, a recoiling jet, and a certain amount of missing transverse momentum. To calculate a reliable E_T^{miss} direction, it is required that it amounts to more than 10 GeV. Events that contain an electron or muon that meets the requirements of Chapter 4 are vetoed. This achieves orthogonality against other $X \rightarrow hh$ searches with electrons or muons in their final states. Furthermore, the veto of events with light leptons effectively reduces the boosted $Z/\gamma^* \rightarrow e^+e^- + \text{jets}$ background, which has a very similar detector signature as boosted $Z/\gamma^* \rightarrow \tau^+\tau^- + \text{jets}$ events. Additional requirements on the trigger selection, the reconstructed di- τ , and the large- R jet are described in the following sections.

6.2.1 Trigger Selection

At least one high-energy large- R jet must be found by the trigger system in an event. The L1 trigger threshold on the large- R jet E_T is 100 GeV. The unprescaled HLT thresholds have increased over the time of data taking from 360 GeV to 460 GeV. For each run number, the lowest-threshold, unprescaled trigger is chosen. The trigger thresholds and their contribution to the pre-selected data are given in Table 6.2. To ensure a constant trigger efficiency, an offline p_T requirement is imposed on the highest- p_T large- R jet in an event. The offline p_T must exceed the trigger threshold by 40–50 GeV, depending on the actual trigger. The 50 GeV requirement is applied to triggers that ran predominantly in the years 2015 and 2016, while for 2017 and 2018 a 40 GeV increase in threshold is sufficient as those triggers received an improved large- R jet energy calibration.

Table 6.2: Trigger thresholds of the L1 and the HLT, and the requirements on the offline p_T of the highest- p_T large- R jet in an event. The percentages indicate the contribution of each trigger to the total number of pre-selected data events.

L1 [GeV]	HLT [GeV]	Offline p_T [GeV]	Fraction of pre-selected events
100	360	410	6.3%
100	400	450	12.0%
100	420	460	22.4%
100	440	480	24.5%
100	460	500	34.8%

6.2.2 Di- τ Selection

In addition to the requirements listed in Chapter 5, further selection criteria are defined for the di- τ candidates. These are introduced to further reduce background contaminations and to enable a background estimation strategy. Also, kinematic regions where large efficiency changes occur are discarded as these are typically difficult to model in simulations.

Each event needs to contain at least one reconstructed di- τ candidate. The requirement on the di- τ p_T is raised to 300 GeV in order to cope with the efficiency turn-on seen in Figure 5.4(a). The transition regions between the barrel and the end-cap calorimeters are excluded from the di- τ selection by requiring a di- τ pseudorapidity of $|\eta| < 1.37$ or $1.52 < |\eta| < 2.0$. In this way, di- τ candidates with poor energy resolution are excluded from the selection. In order to reduce the contribution of multi-jet background, a di- τ candidate must contain at most 3 subjets, the p_T threshold for the two leading subjets is raised to 50 GeV, and the distance between them is required to be less than $\Delta R = 0.8$. The latter requirement also ensures that the energy deposits of the subjets are fully contained within the seed jet cone.

The two leading subjets are required to contain exactly one or three core tracks. The charges q^{sj1} and q^{sj2} are determined from the sum of the charges of those tracks for the leading and subleading subjet, respectively. The di- τ charge product, $Q = q^{\text{sj1}} \cdot q^{\text{sj2}}$, is

required to be ± 1 . Opposite-sign ($Q = -1$) di- τ candidates are used for the signal and validation regions, whereas same-sign ($Q = +1$) di- τ candidates are used for control regions enriched with multi-jet background, as further explained in Section 6.3. In the rare cases where multiple di- τ candidates in an event fulfill the above requirements, the candidate with the highest transverse momentum is selected.

6.2.3 Large- R Jet Selection

The large- R jet that is selected in addition to the di- τ candidate can have two purposes. In the data-driven di- τ validation, it serves as a recoil jet against a Z boson to ensure that the τ pair is sufficiently boosted. In the search for $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ final states, it is used to reconstruct the $h \rightarrow b\bar{b}$ decay.

Only large- R jets with $p_T > 300$ GeV, $|\eta| < 2.0$, and a mass of $m_J > 50$ GeV are considered. The b -tagging is performed on the two leading track jets that are assigned to a large- R jet. The number of b -tagged track jets inside large- R jets, $N_{b\text{-tag}}$, can be zero, one or two. Accordingly, they are referred to as either 0-, 1-, or 2- b -tagged in the following. Events that contain additional b -tagged large- R jets, except the one selected, are discarded to ensure orthogonality against a $X \rightarrow hh \rightarrow b\bar{b}b\bar{b}$ search. The selected large- R jet must be well separated from the di- τ candidate with an angular distance of $\Delta R > 1.0$. If multiple large- R jets fulfill those requirements, the jet with the highest momentum is the selected.

6.3 Event Categorization

After the aforementioned preselection, the events are categorized into different regions for background estimation and validation, for the data-driven di- τ validation, and for the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ search. All regions and their respective usage is summarized in Table 6.3.

The di- τ charge product Q is used to categorize the events as same-sign (SS, $Q = +1$) or opposite-sign (OS, $Q = -1$) regions. The SS regions are enriched with multi-jet (MJ) background and are used for computing fake-factors (FF) and their systematic uncertainties. Details on the multi-jet background estimation with fake-factors are given in Chapter 7.

OS regions are enriched with genuine boosted τ pairs and are divided into 0-, 1-, or 2- b -tag regions based on the number of b -tags, $N_{b\text{-tag}}$. With an increasing $N_{b\text{-tag}}$ the sensitivity to a $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal increases and the expected background yields decrease.

The angular distance $|\Delta\varphi|$ between the di- τ candidate and the missing transverse momentum is used to further discriminate between events with genuine boosted τ pairs and multi-jet background. The 0- and 1- b -tag regions with $|\Delta\varphi| > 1$ are enriched with multi-jet events and are used to validate the aforementioned multi-jet background estimate. The 0- and 1- b -tag regions with $|\Delta\varphi| < 1$ are enriched with events with a boosted Z boson decaying into a pair of τ leptons. Those regions are used for the di- τ calibration and validation. Details on the data-driven di- τ calibration can be found in Chapter 8. The 2- b -tag and $|\Delta\varphi| < 1$ region serves as a signal region for the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ search.

This analysis is presented in Chapter 9.

Additional requirements are set for the signal region to further increase the signal sensitivity. The visible hh mass m_{hh}^{vis} is defined as the invariant mass of the di- τ candidate and the recoiling large- R jet system. Based on m_{hh}^{vis} , three signal subregions are defined: an m_{hh}^{vis} -inclusive, an $m_{hh}^{\text{vis}} > 900$ GeV, and an $m_{hh}^{\text{vis}} > 1200$ GeV subregion. Which signal subregion is employed depends on the signal hypothesis investigated. The threshold increases with increasing signal mass hypothesis. Furthermore, the mass of the large- R jet must be compatible with the Standard Model Higgs boson mass, i.e., $60 \text{ GeV} < m_J < 160 \text{ GeV}$, to suppress background processes. On the other hand, the 1- b -tag di- τ validation region may have a considerable contamination from $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events where one of the b hadrons is not identified. To prevent this contamination the m_J mass window requirement is inverted and the m_{hh}^{vis} must be lower than 1500 GeV in that region.

Table 6.3: Event selection regions and their respective usage for background estimation, validation, di- τ calibration, or as $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region. After preselection, the events are categorized based on the di- τ charge product Q , the number of b -tags, $N_{b\text{-tag}}$, the angular distance $\Delta\varphi$ between the di- τ candidate and the missing transverse momentum, the large- R jet mass m_J , and the visible hh mass m_{hh}^{vis} . The signal region is divided into three m_{hh}^{vis} subregions that are used depending on the signal hypothesis investigated.

Region	Usage	Q	$N_{b\text{-tag}}$	$ \Delta\varphi $	m_J [GeV]	m_{hh}^{vis} [GeV]
FF SS 0- b -tag	Fake-factor computation	+1	0	–	–	–
FF SS 1- b -tag	Fake-factor uncertainty	+1	1	–	–	–
FF SS 2- b -tag	Fake-factor uncertainty	+1	2	–	–	–
FF OS 0- b -tag	Fake-factor uncertainty	–1	0	–	–	–
MJ 0- b -tag	Multi-jet validation	–1	0	> 1	–	–
MJ 1- b -tag	Multi-jet validation	–1	1	> 1	–	–
Z 0- b -tag	Di- τ calibration	–1	0	< 1	–	–
Z 1- b -tag	Di- τ validation	–1	1	< 1	< 60 or > 160	< 1500
Signal region	$X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ search	–1	2	< 1	> 60 and < 160	$> [-, 900, 1200]$

Chapter 7

Background Estimation

A reliable estimate of the Standard Model background processes is crucial for the di- τ calibration as well as for the search for new physics. In this thesis, the estimate of most of the SM background processes is based on the prediction from Monte Carlo simulations. For the di- τ calibration, high- p_T Z bosons, typically produced in association with light quarks or gluons, provide the largest source of genuine boosted pairs of τ leptons. An additional small contribution comes from di-boson production processes with one Z boson decaying into a τ pair. Background processes with W boson or top quark decays may produce a single genuine τ lepton, which, in combination with secondary energy deposits from quark- or gluon-jets, underlying event, or pileup, can be misidentified as a boosted di- τ . The background contribution from multi-jet events with quark- or gluon-initiated jets being misidentified as a boosted di- τ is estimated with a dedicated data-driven technique. In the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region, the production of a single Z boson in association with heavy-flavor quarks, especially with two b quarks, is the most dominant background. Also the production of a Higgs boson in association with a Z boson can produce the same final state as the signal process.

This chapter introduces the setup of Monte Carlo generators that are used to simulate the SM background processes. These processes, as well as the object and event selections, are subject to systematic uncertainties that quantify potential differences between data and simulations. Those are introduced in the following. Afterwards, the data-driven multi-jet estimation is introduced. It is derived and validated in different regions enriched with multi-jet background events. The background process of a Z boson produced in association with heavy-flavor quarks receives a dedicated correction. It is measured in a control region with Z bosons decaying into an electron or muon pair. Finally, an uncertainty on the top quark background in the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region is estimated. It covers the limited amount of simulated top background events in the signal region.

7.1 Background Monte Carlo Samples

All the background predictions considered, except for multi-jet events, are retrieved from Monte Carlo simulations. These include the production of a single Z or W boson, di-boson production, the production of a Higgs boson in association with a Z boson as well as top

quark productions. The setup used to generate these processes is described in the following.

The production of a single Z boson in association with jets (Z +jets) and of a single W boson in association with jets (W +jets) is simulated with SHERPA 2.2.1 [207]. The matrix element calculation is performed with the Comix [208] and OPENLOOPS 1 [209–211] libraries. Final states with up to two jets are generated at next-to-leading order (NLO) accuracy and final states with up to four jets are generated at leading order (LO) accuracy. The matrix elements are matched to the SHERPA parton shower [212] with the MEPS@NLO prescription [213–216]. The NNPDF3.0NNLO set [217] is used as parton distribution function. The events are normalized to a next-to-next-to-leading order (NNLO) cross section prediction [218]. The Z +jets events are categorized as ‘*light-flavor*’ (Z +lf) or ‘*heavy-flavor*’ (Z +hf) events based on the quark flavor of the associated jet production. The W +jets events are not further divided into these categories as their overall background contribution is anyway small. The categorization is based on a geometrical matching between generator-level hadrons with at least 5 GeV and reconstructed track jets. If a b hadron is found within a jet, it is labeled as a b jet. If this is not the case, but it contains a c hadron, it is labeled as a c jet. The remaining jets are labeled as light (l) jets. An event is categorized as Z +hf event if the two track jets that are used for b -tagging are labeled as bb , bc , bl , or cc jets. The remaining events are categorized as Z +lf events.

The di-boson processes ZZ , WZ , and WW are simulated with the POWHEGBOX 2 generator [219–221] at NLO accuracy in QCD. Singly resonant amplitudes are considered, as well as interferences from Z/γ^* and same lepton final state combinations. The parton shower, underlying event, and the hadronization are simulated with PYTHIA 8.186 [136]. Their phenomenological parameters are adjusted to the AZNLO tune [222]. The CT10 [223] and CTEQ6L1 [224] PDF sets are used to simulate the hard scattering and the parton shower, respectively. Decays of b and c hadrons are modeled by the EVTGEN 1.2.0 program [132].

The production of a Higgs boson in association with a Z boson is simulated with POWHEG-BOX 2 [219–221]. The calculation is performed with the MiNLO [225] prescription and the GoSAM package [226] at NLO accuracy for Zh final states with up to one additional jet. The loop-induced $gg \rightarrow Zh$ production is simulated separately at LO accuracy. The events are generated with the NNPDF3.0NNLO set [217] and are reweighted to the PDF4LHC15NLO set [227]. Parton shower and non-perturbative effects are simulated with PYTHIA 8.212 [130] with the AZNLO tune [222] and the CTEQ6L1 [224] PDF set. The $q\bar{q}/qg \rightarrow Zh$ prediction is normalized to cross sections calculated at NNLO accuracy in QCD with NLO electroweak corrections [228–234] and the $gg \rightarrow Zh$ events are normalized to cross sections calculated at NLO with soft-gluon resummation up to next-to-leading-logarithm accuracy in QCD [235–237]. The cross sections and decay branching ratios are calculated with HDECAY [86–89] and PROPHECY4F [90–92]. Decays of b and c hadrons are modeled by the EVTGEN 1.2.0 program [132].

The top quark background is simulated with POWHEG-BOX 2 [219–221] and consists of contributions from $t\bar{t}$ pair production [238], production of a single top quark in the s -channel [239] and in the t -channel [240], as well as Wt production of a top quark in association with a W boson [241]. The events are generated at NLO accuracy in QCD

with the NNPDF3.0NLO set [217]. For the $t\bar{t}$ production, a resummation damping factor h_{damp} that controls high- p_T radiations is set to $1.5 \cdot m_{\text{top}}$ [242]. Single top s -channel and Wt productions are evaluated in the five-flavor scheme, whereas the t -channel is computed in the four-flavor scheme. The parton shower and non-perturbative effects are modeled with PYTHIA 8.230 [130] using the A14 tune [131] and the NNPDF2.3LO set [129]. Decays of b and c hadrons are modeled by EVTGEN 1.6.0 [132]. The $t\bar{t}$ production cross section is calculated using TOP++2.0 [243–249] at NNLO accuracy in QCD including a soft-gluon resummation of next-to-next-to-leading logarithms. The single-top production cross sections are calculated with HATHOR 2.1 [250, 251] at NLO accuracy in QCD, and the Wt cross section is calculated at NLO accuracy in QCD including next-to-next-to-leading logarithmic soft-gluon terms [252, 253].

The multi-jet background estimate is extracted from ATLAS data. However, in one study preparatory to the data-driven method, multi-jet simulations were used to estimate the respective contributions of quark- and gluon-initiated jets. These events are simulated at LO accuracy using PYTHIA 8.186 [136] and the NNPDF2.3LO set [129] for the matrix element di-jet production as well as for the parton shower and non-perturbative effects. The generator parameters are adjusted to the A14 tune [131].

Pileup effects are simulated with PYTHIA 8.186 [136] in all of the aforementioned processes. The original hard-scattering event is overlaid with simulated inelastic proton–proton collision events by using the NNPDF2.3LO set [129] and the A3 tune [137]. The simulated events are weighted in such a way that they resemble the pileup profile of the ATLAS data. The detector response is simulated with a model [138] of the ATLAS detector in the GEANT4 program [139].

7.2 Systematic uncertainties

Processes derived from Monte Carlo simulations are subject to systematic uncertainties that quantify potential differences between ATLAS data and simulations. In particular uncertainties related to large- R jets, di- τ candidates, the b -tagging procedure, the missing transverse momentum, electrons and muons, the pileup modeling, and the integrated luminosity are discussed in the following.

One of the most dominant systematic uncertainties in simulated events arise in this thesis from the large- R jet energy scale and resolution, as well as from the jet mass scale and resolution. A variation of the jet energy or mass results in a varying event yield due to the selection criteria imposed on the jets in an event. The large- R jet systematic uncertainties were evaluated in a comparison between proton–proton collision data and simulation [174] in events where the large- R jet recoils against a reference object with a well-known energy. Such a reference object can be either a photon, a Z boson decaying into light leptons, or a system of small- R jets. Additionally, multiple variations of the simulation model were considered in the determination of the large- R jet uncertainties.

Systematic uncertainties on the di- τ reconstruction and identification efficiency as well as on the di- τ energy response are derived from systematic variations of the simulation model. These are described in Section 5.6. Additional uncertainties arising from the

data-driven di- τ calibration are determined and discussed in Chapter 8.

The b -tagging efficiencies were measured in $t\bar{t}$ events in ATLAS data and simulations [185]. The efficiency correction factors obtained from this measurement are subject to uncertainties related to the normalization and modeling of the $t\bar{t}$ simulations, as well as to experimental uncertainties in the measurement and the available statistics. An additional extrapolation uncertainty is considered for b -tagged jets with p_T beyond the kinematic regime to which the data-based calibration is sensitive.¹ A similar procedure was pursued to derive uncertainties on the rates at which light-flavor jets [254] and c jets are misidentified as b jets.

The missing transverse momentum is computed from a hard term, originating from reconstructed and calibrated particle objects in an event, and a soft term that considers tracks not assigned to any hard objects. The calibration of hard objects and their respective uncertainties have a direct impact on the E_T^{miss} result. Uncertainties on the soft term are estimated from the E_T^{miss} modeling in simulated events with a Z boson decaying into light leptons in comparison with ATLAS data [190]. Multiple MC generators and parton shower models were considered in this comparison and in the systematic uncertainty estimation.

Uncertainties related to electrons and muons are only relevant in a control region that is used for Z +hf background estimation. The uncertainties concern the reconstructed energy, as well as the efficiencies of the trigger, reconstruction, identification, and isolation criteria. These are derived from measurements with $Z/\gamma^* \rightarrow e^+e^-$ +jets and $Z/\gamma^* \rightarrow \mu^+\mu^-$ +jets [186–188]. In all other regions, events with light leptons are discarded and their systematic uncertainties were found to be negligible.

An uncertainty on the pileup modeling aims to cover differences in the visible inelastic proton–proton cross section between data and the predictions of the A3 tune that is used for the pileup simulation. In the ATLAS collaboration, it was found that the prediction of the A3 tune is 3% larger than the value measured in data with an estimated uncertainty of 4%. This is accounted for by varying the number of pileup interactions accordingly when determining the event weights that reweight the MC pileup profile to data. Finally, the simulated event yields are scaled to the integrated luminosity of the combined 2015–2018 data of 139 fb^{-1} with an uncertainty of 1.7% [164].

There are additional systematic uncertainties that arise from the background estimation procedures that are employed in this thesis. This concerns in particular the data-driven estimation of the multi-jet background and the Z +hf and top background estimation, which are detailed in the following sections.

7.3 Multi-Jet Background

The multi-jet background originates from quark- or gluon-initiated jets that are misidentified as di- τ candidates. Despite the large discrimination power of the di- τ identification algorithm against this background, it still accounts for one of the largest backgrounds in the di- τ calibration and in the search for resonant Higgs boson pair production. This background is typically difficult to model in simulations. In particular the exact shower shapes that lead

¹ Additional uncertainties on the b -tagging efficiency in the high- p_T regime were evaluated in simulations with systematically varied MC generator settings [185].

to jets being misidentified as di- τ objects are difficult to simulate and the prediction of the large cross section comes with large uncertainties in the relevant phase space. The di- τ identification is also sensitive to differences between data and simulations regarding the ratio between quark- and gluon-induced jets and their flavor composition. In addition, it is not feasible to generate a multi-jet sample that provides a sufficient number of events that would pass the high rejection power of the di- τ identification.

For those reasons a data-driven method is developed that employs a ‘fake factor’ (FF) approach. The fake factors are measured in a region enriched with multi-jet background and are calculated from the ratio of events where respectively the di- τ candidate passes or fails the identification criterion. To predict the multi-jet background in a region of interest, i.e., a validation or signal region, the fake factors are applied as a weight to events that fail the identification requirement. The measurement of the fake factors and their uncertainties, as well as a validation of the multi-jet background estimate, is given in the following sections.

7.3.1 Fake Factor Measurement

The fake factors are measured in the ‘FF SS 0- b -tag’ region and are defined as

$$FF = \frac{N_{\text{pass}}(\text{data}) - N_{\text{pass}}(\text{MC})}{N_{\text{fail}}(\text{data}) - N_{\text{fail}}(\text{MC})},$$

where N_{pass} and N_{fail} are the number of events where the di- τ candidate passes or fails the identification requirement, respectively. The ‘FF SS 0- b -tag’ region has still a small contribution of other background processes that are estimated from MC simulations. These are subtracted from data so that only the multi-jet background component is measured. The number of multi-jet background events $N_{\text{multi-jet}}$ that would pass the di- τ identification in a region of interest is then estimated by weighting the fail category events with the fake factor:

$$N_{\text{multi-jet}} = FF \cdot (N_{\text{fail}}(\text{data}) - N_{\text{fail}}(\text{MC})).$$

A di- τ candidate passes the identification requirement when it has a BDT discriminant score larger than 0.72, as introduced in Chapter 5. In order to be counted in the fail category the di- τ candidate must have a BDT score between 0.4 and 0.72. The lower cut on the BDT score is introduced to obtain a stable ratio of di- τ candidates from quark- or gluon-initiated jets. As can be seen in Figure 7.1, di- τ candidates with low BDT discriminant scores originate predominantly from gluon-initiated jets, whereas high BDT values are dominated by quark-initiated jets. The fragmentation of quarks produces jets that are more collimated and have a signature that is more often misidentified as hadronic τ decays. The ratio between quark- and gluon-initiated jets stabilizes at a BDT score of approximately 0.4. By removing di- τ candidates with lower BDT values, the composition of quark- and gluon-initiated jets in the fail category is close to the pass category.

The nominal fake factors are presented in Figure 7.2 as a function of di- τ p_T . A parameterization in di- τ p_T was found to be beneficial for the multi-jet modeling for two reasons: the background efficiency varies with the momentum, as already explained in Chapter 5, and the momentum distribution slightly changes between the region where

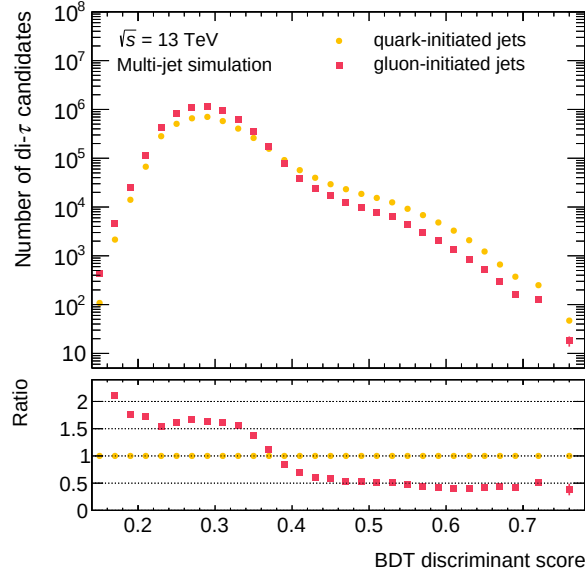


Figure 7.1: Distribution of the BDT discriminant score for quark-initiated (yellow circles) and gluon-initiated (red squares) jet background in a multi-jet simulation sample. Gluon-initiated jets are the predominant background at low BDT score values, whereas high BDT score values are dominated by quark-initiated jets. Their ratio stabilizes at BDT score values above 0.4.

the fake factors are measured and those regions of interest where they are applied. The p_T bins have been chosen in order to closely resemble the changes in efficiency while still maintaining reasonable statistics. Parameterizations other than di- τ p_T were tested, e.g., di- τ η , subjet p_T , and track-multiplicities, but those did not change the multi-jet prediction results.²

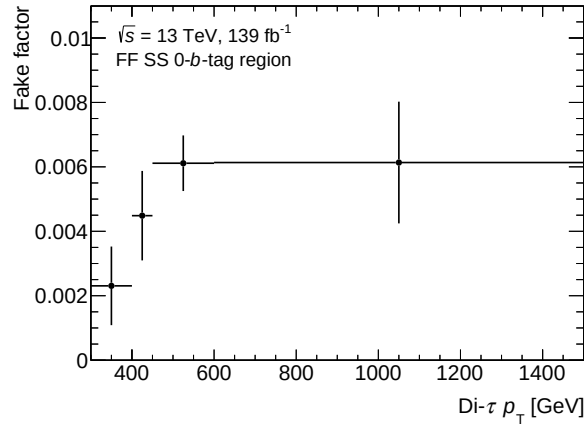


Figure 7.2: Fake factors measured in the ‘FF SS 0- b -tag’ region as a function of di- τ p_T . The statistical uncertainties are shown as vertical lines. The horizontal lines indicate the bin widths.

² No significant fake factor dependency on di- τ η was found. The subjet p_T is highly correlated with the di- τ p_T , so no significant improvements were found in the modeling results. The fake factors vary with the number of tracks. However, it was found that the track-multiplicity distributions do not change between the regions of fake factor measurement and application. Therefore, track-multiplicity-inclusive fake factors were found to be sufficient. Finer parameterizations led primarily to an increase in statistical uncertainties.

The nominal fake factors are measured in a same-sign and 0- b -tag region. However, the regions of interest in which the multi-jet background contributions are estimated are opposite-sign regions and have partially higher numbers of b -tags. The transitions from same-sign to opposite-sign and to a higher number of b -tags are covered by the following systematic fake factor uncertainties.

The uncertainty on the sign transition is computed from the difference between nominal same-sign fake factors and those from an opposite-sign region, i.e., from the difference between ‘FF SS 0- b -tag’ and ‘FF OS 0- b -tag’ regions. Those are shown in Figure 7.3(a). The differences yield to uncertainties between 2% and 30% depending on the di- τ p_T .

The b -tag transition is accounted for by measuring the fake factors in ‘FF SS 1- b -tag’ and ‘FF SS 2- b -tag’ regions. Due to the limited data statistics in those regions, only a p_T inclusive fake factor is computed. These are presented in Figure 7.3(b). The largest difference to the p_T -inclusive fake factor from the ‘FF SS 0- b -tag’ region is considered as a systematic uncertainty. In this case, this is the difference between the 0- b -tag and the 1- b -tag fake factor, yielding to an uncertainty of 42%.

The systematic uncertainties listed in Section 7.2 are also considered in the fake factor measurement and their application, although their influence is small as they only affect the MC subtraction.

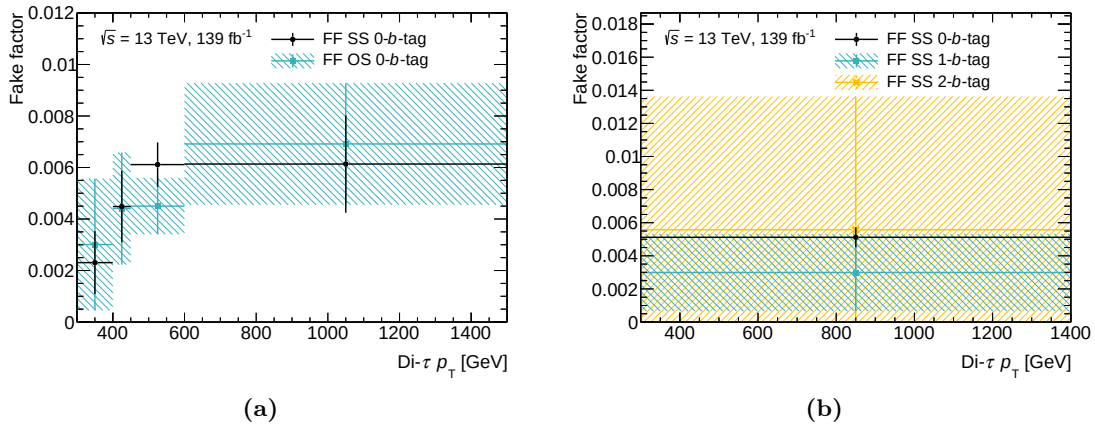


Figure 7.3: Fake factors used to estimate the systematic uncertainties on the sign-transition (a) and b -tag-transition (b). The statistical uncertainties are shown as vertical lines and hatched boxes. The horizontal lines indicate the bin widths. (a): Nominal fake factors from ‘FF SS 0- b -tag’ region (black circles) and fake factors from ‘FF OS 0- b -tag’ region (blue squares) as a function of di- τ p_T . (b): p_T -inclusive fake factors from ‘FF SS 0- b -tag’ (black circles), ‘FF SS 1- b -tag’ (blue squares), and ‘FF SS 2- b -tag’ (yellow crosses) regions.

7.3.2 Multi-Jet Background Validation

The results of the fake factor approach are validated in two regions enriched with multi-jet background events. The ‘MJ 0- b -tag’ region, defined in Table 6.3, has an opposite-sign di- τ candidate, a recoiling large- R jet with no b -tags, and an angular distance $|\Delta\varphi| > 1$ between the di- τ candidate and the missing transverse momentum directions. The latter requirement effectively reduces processes with a genuine pair of τ leptons in the final state.

In Figures 7.4(a)-7.4(e), a set of event observables in the ‘MJ 0- b -tag’ region is presented, i.e., the mass and momentum of the di- τ candidate and of the recoiling large- R jet, as well as the visible hh mass m_{hh}^{vis} , which is defined as the invariant mass of the two-body system of the di- τ candidate and the recoiling large- R jet. In general, a good agreement between the multi-jet prediction and the measured data is found in that region.

The selection of the ‘MJ 1- b -tag’ region differs from the aforementioned region only by the b -tag requirement. It is used to investigate multi-jet processes with heavy-flavor quarks. With the more stringent b -tag requirement, the available data statistics is strongly suppressed. This allows only for an investigation of the total inclusive event yield in this region, as illustrated in Figure 7.4(f). It shows a discrepancy between the observed data yield and the multi-jet prediction. Based on this non-closure, an additional systematic uncertainty of 50% is applied on the multi-jet background yields in all regions with at least one b -tag.

7.4 Z + Heavy Flavor Background

The Z +hf background becomes prominent in regions with at least one b -tag. Especially in the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region, it is the dominant background process. The shape of this background is estimated from simulations. A normalization correction is derived from a comparison between simulations and ATLAS data. Previous analyses, e.g., the search for Higgs boson pair production in resolved $b\bar{b}\tau^+\tau^-$ final states [5] and the observation of $h \rightarrow b\bar{b}$ decays and Vh production with the ATLAS detector [255], have shown that the production of Z bosons in association with heavy-flavor quarks is underestimated in SHERPA simulations.

The Z +hf normalization correction is derived in a region that is from here on referred to as ‘ Z + hf’ control region. Events with $Z \rightarrow \ell^+\ell^-$ decays, where ℓ denotes an electron or muon, are used for this purpose. The correction is applicable to $Z \rightarrow \tau^+\tau^-$ decays, as the Z +hf production is independent of the Z decay mode. Electrons and muons provide clean signatures and their selection efficiencies are well measured by the ATLAS collaboration. The event selection is adapted from a measurement of $h \rightarrow b\bar{b}$ production in association with a vector boson at high transverse momentum [256], whereas changes to the selection strategy are made in order to bring the kinematic phase space in agreement with the signal region of this thesis.

The selected events must pass a single lepton trigger. The single electron E_T thresholds range between 24 GeV and 140 GeV, and the single muon E_T thresholds range between 20 GeV and 50 GeV. There must be at least two leptons with same flavor in an event, where each of the leptons is required to have a $p_T > 7$ GeV and to fulfill the requirements of the loose identification and isolation operating points. The combined dilepton mass must be in the range $81 \text{ GeV} < m_{\ell\ell} < 101 \text{ GeV}$, i.e., be compatible with the mass of a Z boson. Their combined transverse momentum is required to be $p_{T,\ell\ell} > 300 \text{ GeV}$. The events must contain at least one large- R jet with two associated b -tagged track jets, a transverse momentum $p_{T,J} > 250 \text{ GeV}$, and a mass $m_J > 50 \text{ GeV}$. The same b -tagging procedure as in the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region is applied.

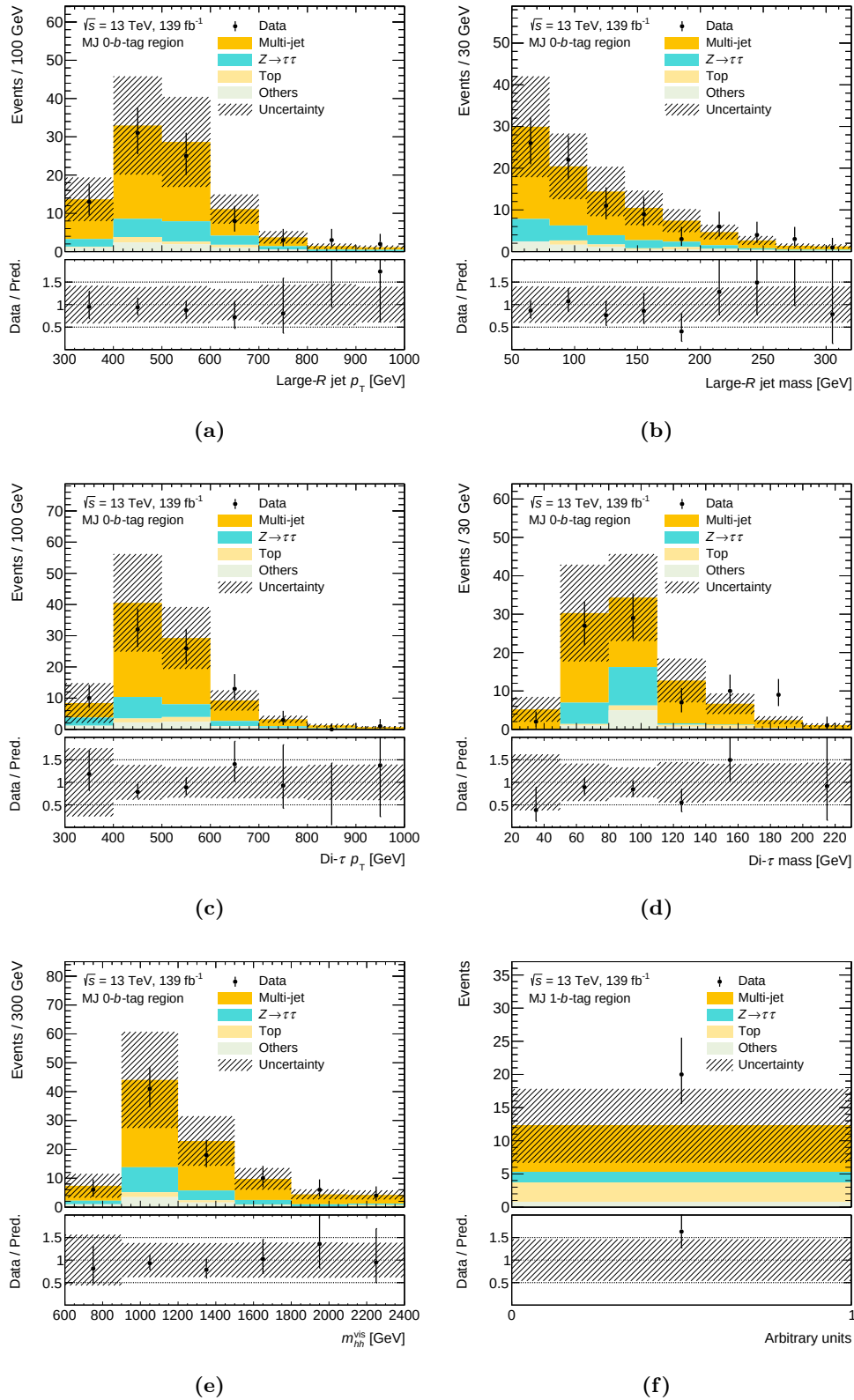


Figure 7.4: Distributions of the large- R jet p_T (a), large- R jet mass (b), di- τ p_T (c), di- τ mass (d), and m_{hh}^{vis} (e) in the ‘MJ 0- b -tag’ region, as well as the overall event yield in the ‘MJ 1- b -tag’ region (f). The lower panels show the ratio between measured data and predicted total background yields. The combined statistical and systematic uncertainties of the background prediction are represented by the hatched bands.

Table 7.1: Event yields in the ‘Z + hf’ control region. The event yields are given for various processes and for the total sum of predicted events including statistical uncertainties, as well as measured data yield.

Process	Event Yield
Z+hf	149.80 ± 2.50
Z+lf	7.09 ± 0.97
Zh	11.03 ± 0.04
Others	26.17 ± 0.86
Sum of events	194.09 ± 2.82
Data	226

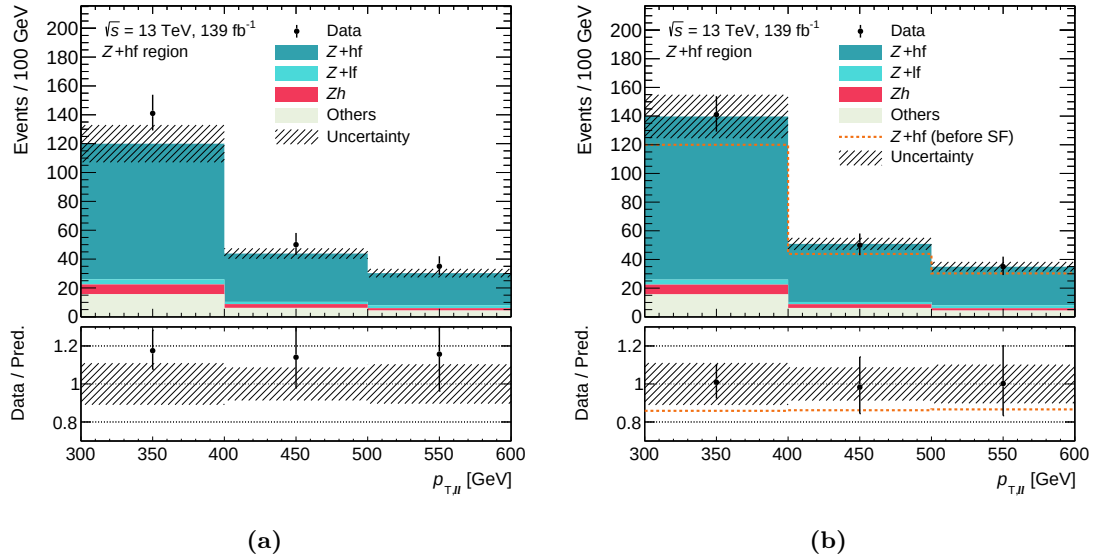


Figure 7.5: Distributions of the combined dilepton transverse momentum $p_{T,\ell\ell}$ in the ‘Z + hf’ control region before (a) and after (b) Z+hf correction. The combined statistical and systematic uncertainties of the background prediction are represented by the hatched bands. The orange line in (b) indicates the background prediction before Z+hf correction.

The event yields in the ‘ $Z + \text{hf}$ ’ control region are summarized in Table 7.1. This is also depicted in Figure 7.5(a) as a function of $p_{T,\ell\ell}$. It can be seen that the MC prediction consistently underestimates the measured data yields. For this reason, a correction factor f_{hf} is extracted from this region to correct the $Z + \text{hf}$ normalization. It is defined as the ratio of measured to predicted $Z + \text{hf}$ event yields:

$$f_{\text{hf}} = \frac{N(\text{data}) - N(\text{MC, not } Z + \text{hf})}{N(\text{MC, } Z + \text{hf})},$$

where the number of background events that are not from $Z + \text{hf}$ production are estimated from simulations and are subtracted from the data yield. This results in a correction factor of

$$f_{\text{hf}} = 1.21 \pm 0.10 (\text{stat}) \pm 0.12 (\text{syst}).$$

The statistical uncertainty comes from the limited number of Monte Carlo events and the limited data. The systematic uncertainty includes the systematic variations detailed in Section 7.2. This correction factor is applied as weight to all $Z + \text{hf}$ events in this thesis. The $p_{T,\ell\ell}$ distribution after $Z + \text{hf}$ correction is depicted in Figure 7.5(b), showing a good agreement between the corrected MC prediction and data.

7.5 Top Background

The top background is estimated from Monte Carlo simulations. The largest contribution to the top background yield comes from $t\bar{t}$ production, which is generally among the backgrounds with the highest production cross section and whose MC sample has the largest statistics of all simulation samples used in this thesis. Nevertheless, no MC events pass the final selection cuts of the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region. To ensure that the $t\bar{t}$ yield in the signal region is not underestimated by a lack of MC statistics, an upper limit on the uncertainty of the yield is estimated and explained in the following. In all other regions, the top background yields are taken directly from simulations.

A top quark typically decays into a W boson and a b quark. The W boson then further decays with a branching ratio of about 67% into a pair of quarks or with respective branching ratios of about 11% into an electron, a muon, or a τ lepton and the corresponding neutrino [25]. Typically, $t\bar{t}$ events with high-energy final state products show a back-to-back topology. This makes it unlikely that more than one b hadron of the top decay is contained within a single large- R jet. Indeed, the highest contributions from top background are found in the 1- b -tag validation regions. Moreover, the amount of $t\bar{t}$ events that produce a genuine boosted τ pair is very minor, allowing the di- τ identification to reduce this background even further. In the 2- b -tag signal region, before m_J and m_{hh}^{vis} cuts are applied, the top background yields to 0.12 predicted events in 139 fb^{-1} , but zero MC events meet the $60 \text{ GeV} < m_J < 160 \text{ GeV}$ requirement. Under this circumstance, standard procedures that apply a percentage uncertainty to the background yield are not applicable. Instead, a conservative uncertainty estimate is applied. One can identify the top yield prior to the final cuts as an upper boundary on the final top yield. This results in an estimated top

background yield of $N = 0_{-0}^{+0.12}$ in the signal region after all cuts are applied.

Other approaches have been tested by also considering the background reduction power of the m_J and m_{hh}^{vis} cuts. The efficiencies of the mass cuts are estimated in regions with higher top background statistics, i.e., a 1- b -tag region and a region with an inverted di- τ identification criterion. With the mass cut efficiencies considered, the upper uncertainty on the top yield is reduced by between 42% and 88%.³ It is found that neither the conservative uncertainty estimate nor the reduced uncertainties have a noticeable impact on the resulting limit. Hence, the $+1\sigma$ uncertainty of 0.12 events is considered for the top background yield in the signal region.

³ The reduction of the top background varies depending on the m_{hh}^{vis} requirement applied. The signal subregions are either m_{hh}^{vis} -inclusive or have a 900 GeV or 1200 GeV cut applied.

Chapter 8

Data-Driven Di- τ Calibration

In this chapter the calibration of the di- τ algorithms with 139 fb^{-1} of proton–proton collision data is presented. Before the di- τ algorithms can be employed in a search for new physics, they must be validated on a known Standard Model process. This is done in a control region, orthogonal to the signal region, where the new physics is not expected to contribute. Here, this is the ‘ Z 0- b -tag’ control region, which is enriched with genuine boosted τ pairs from decays of boosted Z bosons. First, the predicted yield of events where a genuine τ pair is correctly reconstructed and identified by the di- τ algorithms in simulations is compared to data. Secondly, a normalization correction and related uncertainties are retrieved from the ‘ Z 0- b -tag’ control region. Finally, the di- τ energy response is validated in the same region.

8.1 ‘ Z 0- b -tag’ Control Region

The ‘ Z 0- b -tag’ control region is an opposite-sign region as it can be expected from $Z \rightarrow \tau^+\tau^-$ decays. A 0- b -tag region is used as it provides more events than any regions with higher b -tag counts. It also provides a negligible contamination with $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal events. The angular distance between the di- τ candidate and the missing transverse momentum is required to be $|\Delta\varphi| < 1$, i.e., they must point into similar directions.

Distributions of the di- τ p_T and mass can be seen in Figure 8.1. The event selection in this region aims to achieve a large contribution of events where the di- τ candidate matches to a genuine τ pair in simulation.¹ Such di- τ candidates are referred to as ‘*true di- τ* ’ in the following. The contribution of events with a true di- τ in this control region is 67%. The di- τ mass distribution shows a pronounced Z mass peak, although below the nominal Z resonance mass, which is due to the missing energy of the neutrinos of the τ decays. With an additional di- τ mass window cut between 30 GeV and 90 GeV, the contribution of true di- τ events can be increased to 76%. Of those true di- τ events 93% originate from Z +jets events, 5.8% from di-boson events, 1.0% from Vh , and 0.3% from $t\bar{t}$ decays. Compared to Z +jets the contribution of di-boson and Vh events is small due to their lower production cross section. The $t\bar{t}$ process has a large cross section and a decently high branching ratio to

¹ As introduced in Chapter 5, a di- τ candidate is considered to match to a genuine τ pair if the two leading subjects have each a distance of $\Delta R < 0.2$ from the simulated visible τ decay products.

have two hadronic τ decays in the final state. However, these would typically be produced in a back-to-back topology, so there is a small probability to obtain a narrow boosted pair of τ leptons from a $t\bar{t}$ decay.

In Figure 8.1 it can be seen that regions with a high contribution of true di- τ events are slightly overestimated by the Monte Carlo predictions. Regions where other background processes dominate, such as in the high di- τ mass tail, appear to be correctly modeled. Hence, the normalization of true di- τ events in simulations is calibrated with a normalization scale factor in the following section.

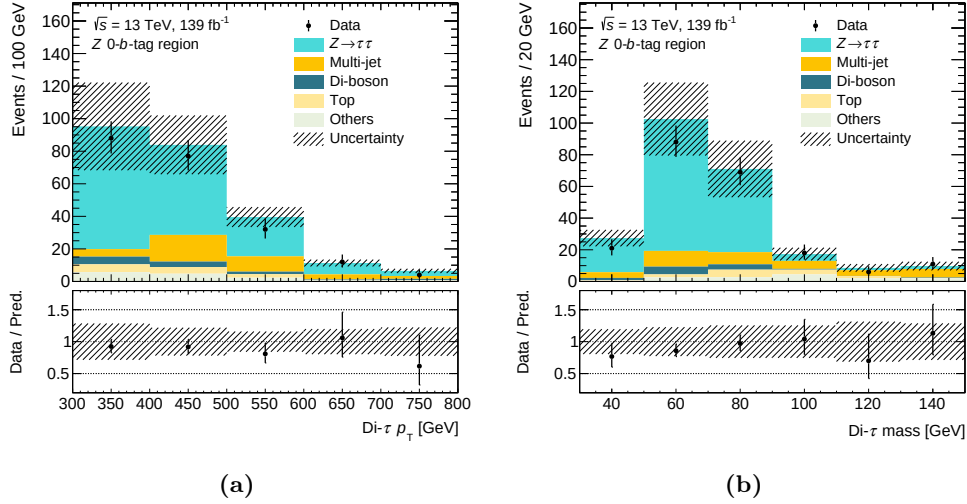


Figure 8.1: Distributions of the di- τ p_T (a) and mass (b) in the ‘Z 0-b-tag’ region. Events outside the displayed range are added to the first or last bin respectively. The lower panels show the ratio between measured data and predicted total background yields. The combined statistical and systematic uncertainties of the background prediction are represented by the hatched bands.

8.2 Di- τ Event Normalization Calibration

A calibration of the normalization of true di- τ events is important for its application in a search for new physics. It ensures that the expected background yield as well as the yield of a potential new signal is well predicted in simulations.

For a better distinction between true di- τ events and other backgrounds, a new grouping of the processes is introduced: ‘true di- τ ’, ‘multi-jet’, and ‘others’. The true di- τ category includes events where a boosted τ pair is correctly recognized, predominantly from $Z \rightarrow \tau^+\tau^-$ decays. The multi-jet process is unchanged from before and includes the data-driven estimate of misidentified quark- and gluon-initiated jets. The ‘others’ category includes the simulation-based backgrounds that do not contain a genuine pair of τ leptons, as well as a small fraction of events where a final state τ pair exists but is not correctly detected by the di- τ algorithms. A normalization calibration is only retrieved for true di- τ events. A calibration of events where a di- τ candidate is mis-identified is not considered, as it would strongly depend on the underlying background process, and at this point there is no indication that such a correction is necessary. These backgrounds appear to be correctly

predicted by simulations, as can be seen in the high mass tail in Figure 8.1(b) and in the background validation regions of the previous chapter.

Table 8.1: Event yields in the ‘ Z 0- b -tag’ control region. The event yields are given for various processes and for the total sum of predicted events with statistical uncertainties, as well as the measured data yield.

Process	Event Yield
True di- τ	154.0 ± 3.0
Multi-jet	21.1 ± 0.3
Others	27.7 ± 2.4
Sum of events	202.8 ± 3.8
Data	178

The normalization correction is determined in the ‘ Z 0- b -tag’ control region with an additional di- τ mass window cut between 30 GeV and 90 GeV, which further increases the purity of true di- τ events. The event yields in this region are summarized in Table 8.1. It can be seen that the expected event yield slightly overestimates the measured data yield. The normalization of true di- τ events is corrected with the following scale factor:

$$SF = \frac{N(\text{data}) - N(\text{non-di-}\tau)}{N(\text{true di-}\tau)} = 0.84 \pm 0.09 \text{ (stat)} \begin{smallmatrix} +0.14 \\ -0.13 \end{smallmatrix} (Z\text{-modelling}) \begin{smallmatrix} +0.19 \\ -0.20 \end{smallmatrix} \text{ (syst)},$$

which is in the following applied as a weight to all simulated events that contain a true di- τ . The uncertainties on the scale factor consider the limited statistics of data and simulations, an uncertainty on the Z boson modeling in simulations, and systematic uncertainties on the background estimation. These are discussed in the following paragraphs. A set of event observables after application of the normalization correction in the ‘ Z 0- b -tag’ region are shown in Figures 8.2(a)-8.2(e). The distributions generally show a good agreement between prediction and observed data. No significant dependency of the scale factor with respect to any of those observables is found. For this reason, and in order to preserve statistics, the scale factor is derived inclusively. The scale factor is also validated in the independent ‘ Z 1- b -tag’ region. This is shown in Figure 8.2(f). The ‘ Z 1- b -tag’ validation region differs from ‘ Z 0- b -tag’ by the requirement on the number of b -tags and by additional requirements on the large- R jet mass m_J and the visible, hypothetical hh mass m_{hh}^{vis} to reduce signal contamination, i.e., $m_J < 60$ GeV or $m_J > 160$ GeV and $m_{hh}^{\text{vis}} < 1500$ GeV. Although only a limited number of data events is available in this region, a good agreement between the corrected prediction and the measured data yield is found.

The statistical uncertainty on the scale factor of about 11% considers the limited number of data events, as well as the limited number of events available for the true di- τ and background predictions. The main impact on the statistical uncertainty arises from the limited number of data events, for which a Poisson probability distribution is assumed.

The Z -modeling uncertainty contains a 5% uncertainty on the Z +jet production cross section [257] as well as uncertainties on the acceptance and efficiency of the event selection in this analysis. These are summarized in Table 8.2. The uncertainties on the acceptance times

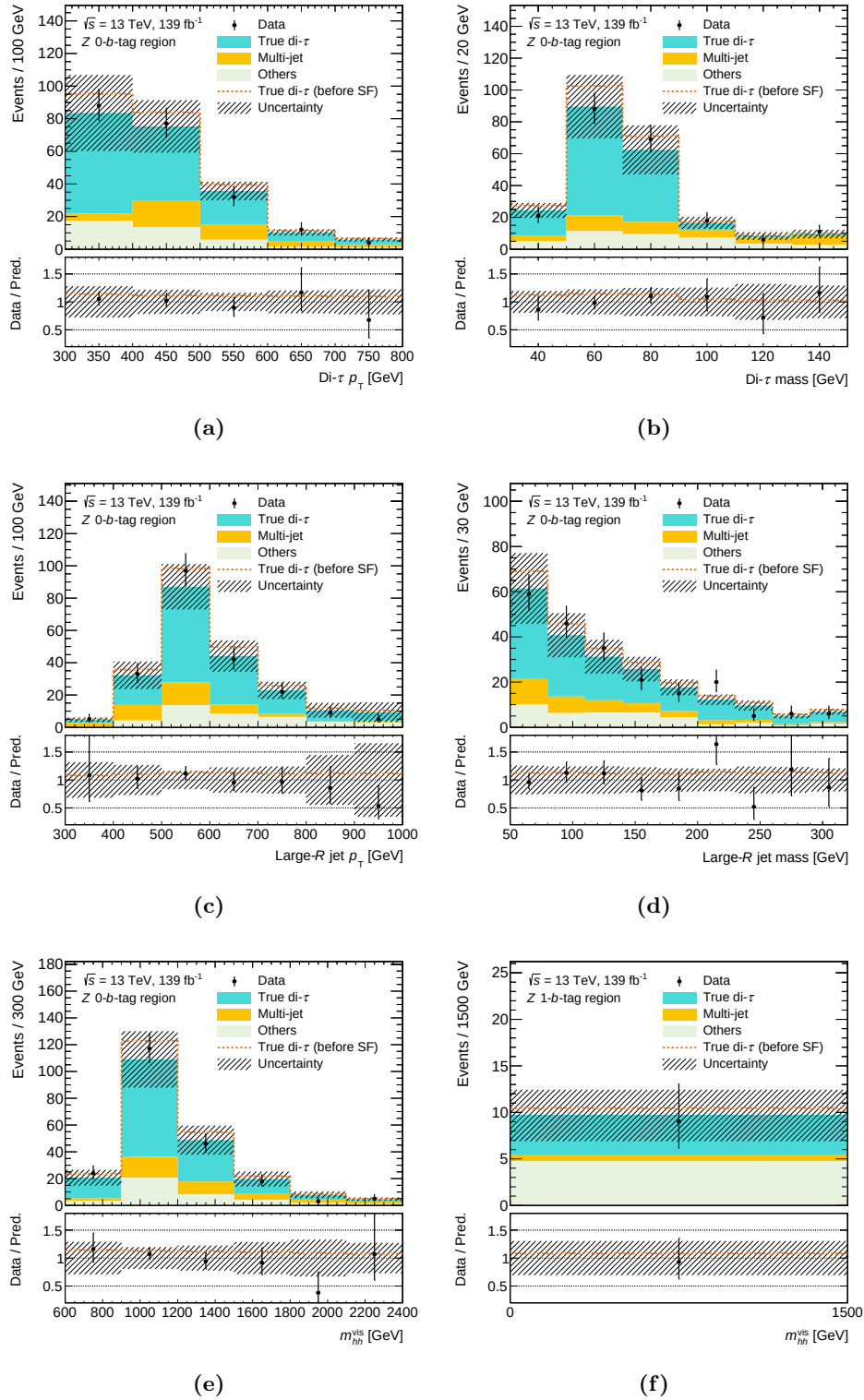


Figure 8.2: Distributions of the $\text{di-}\tau$ p_T (a), $\text{di-}\tau$ mass (b), large- R jet p_T (c), large- R jet mass (d), and m_{hh}^{vis} (e) in the ‘ Z 0- b -tag’ region, as well as the overall event yield in the ‘ Z 1- b -tag’ region (f). The hatched orange line represents the event yield before the application of the normalization scale factor. Events outside the displayed range are added to the first or last bin respectively, except in Figure (f) where $m_{hh}^{\text{vis}} < 1500$ GeV is part of the event selection to suppress potential $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal. The lower panels show the ratio between measured data and predicted total background yields. The combined statistical and systematic uncertainties of the background prediction are represented by the hatched bands.

efficiency are measured at generator level by considering multiple systematic variations of the SHERPA event generation. Further details on the motivation for the following variations and their implementation in SHERPA can be found in Reference [258]. Uncertainties due to missing higher-order contributions are determined from variations of the QCD renormalization and factorization scales by factors of 0.5 and 2. An uncertainty on the matching between matrix element and parton shower is evaluated by changing the nominal 20 GeV matching scale to 15 GeV or 30 GeV. The scale used for the resummation of soft gluon emission is varied by factors of 0.5 and 2. An uncertainty on the PDF set is determined by evaluating the standard deviation of the acceptance times efficiency in 100 PDF replicas provided by the NNPDF3.0NNLO set.² In addition, an uncertainty on the PDF choice is estimated with the alternative sets CT14nnlo [259] and MMHT2014nnlo [135]. An uncertainty related to the choice of the value of the strong coupling constant $\alpha_S(m_Z^2)$ is derived by varying its nominal value of 0.118 by ± 0.001 . For each $\alpha_S(m_Z^2)$ value, the corresponding NNPDF3.0NNLO variant is used. The aforementioned uncertainties are combined via quadratic error propagation to a total Z -modeling uncertainty of +15.1% and -16.0%.

Table 8.2: Z -modeling uncertainties of the di- τ normalization correction. The quoted up and down uncertainties are relative to the correction scale factor.

Variation	Uncertainty	
Renormalization and factorization scales	+12.9%	-14.9%
Matrix element matching	+5.1%	-1.4%
Cross section	+5.0%	-5.0%
PDF choice	+2.0%	-2.0%
Resummation scale	+2.0%	-1.2%
Strong coupling constant	+1.2%	-1.2%
PDF replicas	+0.9%	-0.9%
Combined	+15.1%	-16.0%

The systematic uncertainty on the normalization correction arises from background modeling uncertainties and instrumental uncertainties that are detailed in Sections 7.2 and 7.3. Their impacts on the scale factor calculation are summarized in Table 8.3. The largest influence has the large- R jet calibration, which impacts the selection of the recoiling large- R jet in true di- τ events and other simulated background processes. The second largest uncertainty is related to the estimation of multi-jet background events, which are the biggest source of misidentified di- τ candidates in the ‘ Z 0- b -tag’ region. The systematic uncertainties are combined via quadratic error propagation to a total uncertainty of +22.2% and -24.1%.

² The PDF replicas are produced from fits to pseudo data, whereas the pseudo data itself is generated from the nominal NNPDF set. This is further detailed in Reference [217].

Table 8.3: Systematic uncertainties of the di- τ normalization correction. The quoted up and down uncertainties are relative to the correction scale factor.

Source	Uncertainty	
Large- R jet calibration	+20.0%	−21.9%
Multi-jet background estimation	+9.3%	−9.9%
MC based di- τ calibration	+1.0%	−1.0%
Luminosity and pileup	+1.8%	−1.8%
Flavor-tagging calibration	+0.8%	−1.0%
Missing transverse energy calibration	+0.2%	−0.5%
Combined	+22.2%	−24.1%

8.3 Di- τ Energy Calibration

The di- τ energy is computed from the two leading subjects, which consist of calibrated energy clusters in the calorimeter. A good agreement between the reconstructed di- τ energy and the energy of the visible decay products of the τ pair is already shown in Section 5.3 based on simulations. In Section 5.6, uncertainties on the di- τ energy are derived from systematic variations of the parameters of the Monte Carlo event generator. Finally, a validation of the di- τ energy in this section shows consistent results between simulation and data. A large difference between the energy responses in simulations and data would introduce a bias that might require corrections. It must be noted, however, that the search for new physics presented in this thesis is far less sensitive to a shift in the di- τ energy scale than to the variation of the event normalization that was introduced in the previous section.

Data and simulations are compared in the ‘ Z 0- b -tag’ control region in multiple event observables that are correlated with the di- τ energy. In particular, the distributions of the di- τ p_T and mass can be seen in Figures 8.2(a) and 8.2(b). It is found that simulation and data agree very well and that any small deviations in the event distributions are sufficiently covered by the estimated systematic uncertainties. For that reason, it is concluded that neither a data-driven correction of the di- τ energy, nor additional uncertainties on the di- τ energy response are required.

Chapter 9

Search for Resonant Higgs Boson Pair Production

In this chapter the search for resonant Higgs boson pair production in the fully-hadronic $b\bar{b}\tau^+\tau^-$ final state is presented. A summary of the selection requirements in the signal region is given, with emphasis on the signal acceptance and efficiency of the most important requirements. An uncertainty on the modeling of the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ simulation is estimated. As no significant deviations between the expected SM background processes and data are observed in the signal region, exclusion limits on the signal production are derived. For this purpose, a statistical analysis based on a profile-likelihood ratio is employed.

9.1 Signal Region

The $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region utilizes the same event preselection as most control and validation regions, as described in Chapter 6. This primarily includes an E_T^{miss} cut, a trigger preselection, and a veto against events with electrons or muons. Events of the signal region must contain a di- τ candidate whose two highest- p_T subjects have charges of opposite signs. The angular distance between the di- τ candidate and the E_T^{miss} direction is required to be $|\Delta\varphi| < 1$, i.e., the di- τ candidate and the missing transverse momentum point into similar directions. At least one of the large- R jets in the event must have a p_T high enough to exceed the trigger thresholds. One large- R jet must have two associated b -tagged track jets and must have a distance $\Delta R > 1.0$ to the di- τ candidate.

The acceptance times efficiency to select an $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal event, where both τ leptons decay hadronically, is depicted in Figure 9.1. This is shown for the nine considered signal hypotheses with resonance masses m_X from 1 TeV to 3 TeV at different stages of the event selection. The acceptance times efficiency of the preselection ranges between 20% and 60%, whereas the low- m_X signals are most limited by the trigger acceptance. After preselection, the di- τ selection shows efficiencies between 20% and 30%. The highest selection efficiency is found for signal samples with m_X of about 2 TeV. The signals with resonance masses from 1 TeV to 1.4 TeV have a small fraction of events where the distance between the τ leptons is too large to be reconstructed as a boosted di- τ candidate, whereas the 3 TeV signal has a fraction of events with τ distances too low to be resolved by the

di- τ subset reconstruction.¹ The efficiency of the large- R jet selection strongly depends on the signal m_X , with values ranging between 20% for 1 TeV and almost 80% for the 3 TeV signal. The signals with the lowest masses are particularly limited by the trigger dependent large- R jet p_T requirement. Finally, the categorization of events into the signal region shows efficiencies between 20% and 30% after the previous selection stages. Here, the most limiting factor is the efficiency of the 2- b -tag requirement. This final selection stage also includes requirements on the mass m_J of the selected large- R jet and the visible hh mass m_{hh}^{vis} . These are further discussed in the following.

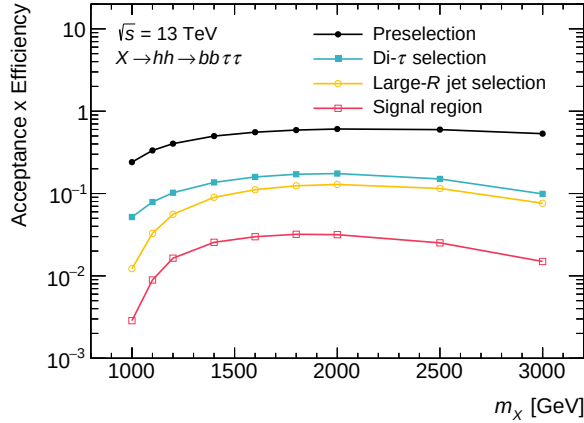


Figure 9.1: Acceptance times efficiency to select an $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal event with a fully hadronic τ pair decay as a function of the resonance mass m_X , shown at different stages of the event selection.

The m_J and m_{hh}^{vis} requirements are applied to further reduce the background contributions while maintaining almost the same signal efficiency. The m_J and m_{hh}^{vis} distributions of all signal hypotheses considered are depicted in Figure 9.2. It can be seen that the m_J distributions peak similarly at the mass of the SM Higgs boson. Only the 1 TeV and 1.1 TeV signal distributions are slightly shifted towards higher m_J masses. This is a bias caused by the large- R jet trigger selection, as jets with higher energies have typically higher masses, and such events have generally a greater chance of being accepted. On the other hand, the signal hypotheses with high resonance masses m_X are less effected by the trigger acceptance and consequently do not show such a bias. With a m_J requirement of $60 \text{ GeV} < m_J < 160 \text{ GeV}$ an efficiency of about 90% is achieved in all signal samples. The m_{hh}^{vis} distributions strongly depend on the resonance masses m_X . The mean value of the distributions is typically about three-quarters of the m_X due to the lack of neutrino energy. Based on m_{hh}^{vis} , the signal region is divided into three subregions. No m_{hh}^{vis} cut is considered in the search for signals with resonance masses of up to 1.4 TeV. A $m_{hh}^{\text{vis}} > 900 \text{ GeV}$ cut is applied in the search for resonance masses in the range from 1.6 TeV to 2.0 TeV. For the highest considered resonances of 2.5 TeV and 3 TeV, a requirement of $m_{hh}^{\text{vis}} > 1200 \text{ GeV}$ is imposed. Efficiencies of more than 99% are achieved in all signal samples with these m_{hh}^{vis} requirements. The m_J and m_{hh}^{vis} requirements, like all other selection cuts, were determined

¹ The limitations of the di- τ reconstruction are already discussed in Chapter 5. The distribution of the distances between τ leptons for all signal masses is shown in Figure 5.1.

during a time when the signal region was still blinded, so that the data eventually observed could not influence decision making. The cuts on m_J and m_{hh}^{vis} are chosen only based on the signal samples, because the background template is assessed to be too statistically limited to evaluate its m_J and m_{hh}^{vis} distributions in a fine binning. Therefore, a further tuning of these cuts is omitted to avoid being sensitive to statistical variations in the background estimate.²

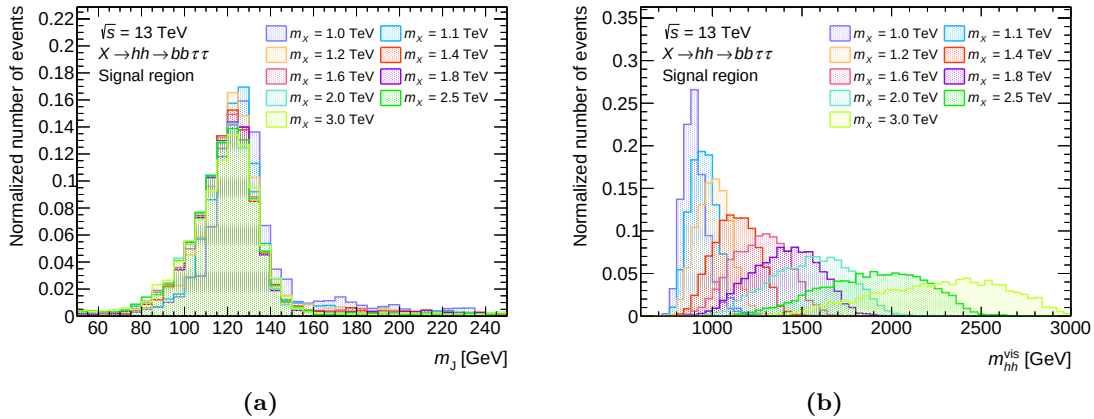


Figure 9.2: Distributions of the large- R jet mass m_J (a) and the visible hh mass m_{hh}^{vis} (b) of simulated $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ events with resonance masses m_X from 1 TeV to 3 TeV in the signal region.

Other mass requirements were tested, such as a cut on the range of the di- τ mass, as well as mass definitions that take E_T^{miss} into account. A di- τ mass requirement was found to give no significant improvements, as the most dominant background from $Z \rightarrow \tau^+\tau^-$ decays has, given the loss in energy and resolution due to the τ neutrinos, a fairly similar mass distribution as the $h \rightarrow \tau^+\tau^-$ decay in the signal process. This is in contrast to the requirement on m_J , which is sensitive to the mass of the b pair and was found to improve the results. In the signal process, the b quarks are produced via a $h \rightarrow b\bar{b}$ decay, while in the dominant background of a Z boson produced in association with two b quarks, the b quarks are produced non-resonantly, hence, there is a large difference between the m_J distributions of the signal and background processes. An inclusion of E_T^{miss} into the definitions of the di- τ and hh masses leads to a more accurate reconstruction of the masses of the SM Higgs boson and the heavy signal resonance. A more accurate mass reconstruction allows for more stringent mass requirements in the event selection. However, their distributions tend to be significantly wider due to the additional E_T^{miss} resolution. No significant changes in the final results are found when using these alternative mass definitions.

Figure 9.3 shows the m_{hh}^{vis} distribution in the signal region. No significant deviation between the expected SM background and data is observed. Hence, exclusion limits on the resonant production of a pair of SM Higgs bosons are derived in this chapter. Two example signal hypotheses are shown in Figure 9.3. Their production cross sections are

² A tuning of these cuts based on signal significance, which also considers the expected background yields, might be beneficial in future iterations of this analysis. However, this would require better background statistics, either by producing more background simulations or by loosening other selection requirements.

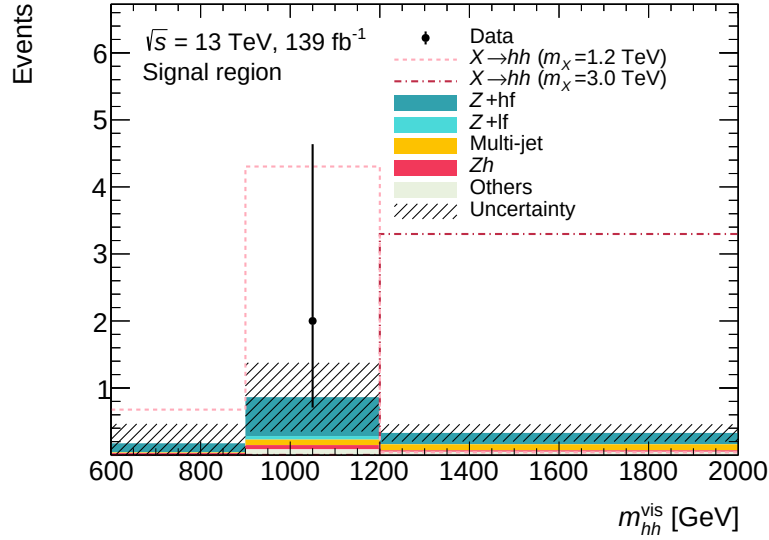


Figure 9.3: Distribution of the visible hh mass m_{hh}^{vis} in the signal region. Events outside the displayed range are added to the first or last bin respectively. The combined statistical and systematic uncertainties of the background prediction are represented by the hatched band. The production cross sections of the 1.2 TeV and 3.0 TeV signal hypotheses are scaled to the values of the expected exclusion limits.

scaled to the values of the expected exclusion limits. The data and background yields in the three signal subregions are summarized in Table 9.1. The $Z+\text{hf}$ production with a Z boson decaying into a boosted τ pair is the dominant background process. Multi-jet events are the second leading background. Its relative contribution to the total background increases in the subregions with more stringent m_{hh}^{vis} requirements. Two events with the signature being searched for are found in data. Both were recorded in the 2018 data takings with reconstructed visible hh masses of 1012 GeV and 1114 GeV. Event displays of those two events are shown in Figure 9.4.

Table 9.1: Event yields in the three signal subregions with different m_{hh}^{vis} requirements. The event yields are given for various processes and for the total sum of predicted events with statistical uncertainties, as well as the measured data yield.

Process	Event Yields		
	m_{hh}^{vis} -inclusive	$m_{hh}^{\text{vis}} > 900 \text{ GeV}$	$m_{hh}^{\text{vis}} > 1200 \text{ GeV}$
$Z+\text{hf}$	0.89 ± 0.25	0.75 ± 0.21	0.17 ± 0.05
Multi-jet	0.18 ± 0.03	0.17 ± 0.03	0.09 ± 0.02
Zh	0.11 ± 0.01	0.09 ± 0.01	$0.02 \pm -$
$Z+\text{lf}$	0.05 ± 0.05	0.05 ± 0.05	$-$
Others	0.13 ± 0.05	0.13 ± 0.05	0.05 ± 0.03
Sum of events	1.37 ± 0.26	1.19 ± 0.23	0.33 ± 0.07
Data	2	2	0

The systematic uncertainties that are introduced in the previous chapters are considered here as well. Their impact on the SM background yields are shown in Table 9.2. Among the

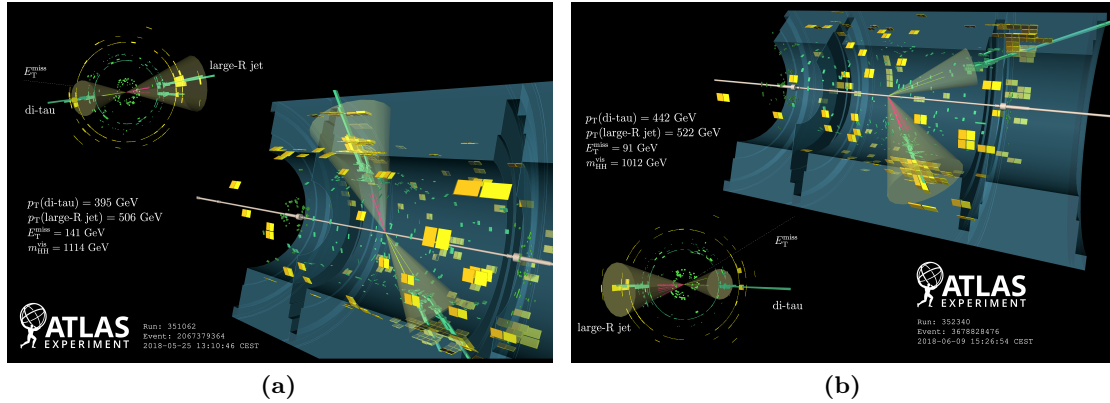


Figure 9.4: Event displays of the two events observed in Run 2 proton–proton collision data that satisfy all selection requirements of the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region. The values of the reconstructed momenta of the di- τ candidate and the large- R jet, the missing transverse momentum E_T^{miss} , and the visible hh mass m_{hh}^{vis} are given in the figures. [11]

largest uncertainties on the total background yield are the uncertainties related to the large- R jet and di- τ calibrations. The uncertainties related to the multi-jet background estimate become more prominent in the $m_{hh}^{\text{vis}} > 1200$ GeV subregion, as the relative contribution of this background increases. Also the upper uncertainty on the top background yield becomes more dominant with more stringent m_{hh}^{vis} requirements. Although the absolute value of the top background uncertainty stays the same in all subregions, its relative contribution increases when the total background yield gets close to zero.³

Table 9.2: Systematic uncertainties on the expected background in the three signal subregions with different m_{hh}^{vis} requirements. The quoted up and down uncertainties are relative to the total expected background yields.

Source	Uncertainty					
	m_{hh}^{vis} -inclusive		$m_{hh}^{\text{vis}} > 900$ GeV		$m_{hh}^{\text{vis}} > 1200$ GeV	
Large- R jet calibration	+19%	−14%	+36%	−16%	+19%	−19%
Di- τ calibration	+19%	−20%	+21%	−19%	+15%	−16%
Multi-jet background estimation	+10%	−10%	+11%	−11%	+21%	−21%
Top background estimation	+9%	−0%	+10%	−0%	+36%	−0%
Z +hf background estimation	+8%	−8%	+8%	−8%	+7%	−7%
Flavor-tagging calibration	+7%	−6%	+7%	−7%	+7%	−7%
Luminosity and pileup	+2%	−10%	+2%	−12%	+5%	−2%
E_T^{miss} calibration	+0.01%	−0.01%	+0.02%	−0.01%	+0.03%	−0.04%
Combined	+32%	−30%	+46%	−31%	+50%	−34%

³ As mentioned in Section 7.5, the top background uncertainty has no significant impact on the limit results. In the m_{hh}^{vis} -inclusive and $m_{hh}^{\text{vis}} > 900$ GeV subregions it is small compared to other uncertainties. In the $m_{hh}^{\text{vis}} > 1200$ GeV subregion it becomes dominant, but large uncertainties on a background expectation close to zero have only minor impact on the exclusion limit, as further discussed in Section 9.4.

9.2 Signal Acceptance Uncertainties

The systematic uncertainties that are applied to the background simulations are also considered for the signal samples. An additional uncertainty is applied to the signal process, which takes into account the modeling of the signal kinematics and missing higher-order contributions in the signal simulation. Different variations of the parameters of the MC are evaluated, regarding their influence on the signal acceptance times efficiency. This is assessed in a generator-level analysis that emulates the event selection of the signal region. A generator-level analysis is employed here as the full detector simulation and object reconstruction with all generator parameter variations would be too computationally intensive.

The generator-level event selection is introduced in the following. Signal events that contain a simulated electron with $p_T > 7$ GeV and $|\eta| < 2.47$ or muon with $p_T > 7$ GeV and $|\eta| < 2.7$ are vetoed. The event must have an $E_T^{\text{miss}} > 10$ GeV, which is calculated from the simulated neutrinos in the event. The two highest- p_T τ leptons must be of opposite charge, each having a $p_{T,\text{vis}} > 50$ GeV, and a combined di- τ $p_{T,\text{vis}} > 300$ GeV. Their pseudorapidity must be in the range $|\eta| < 1.37$ or $1.52 < |\eta| < 2.0$ and their angular distance is required to be in the range $0.2 < \Delta R < 0.8$. These quantities follow the di- τ selection cuts of the signal region, but are in this case calculated from the simulated decay products of the hadronic τ decay, except the neutrinos. Large- R jets are reconstructed from the simulated particles as well. There must be at least one large- R jet with $p_T > 500$ GeV in an event. This emulates the cut that ensures a constant trigger efficiency. While the data analysis includes multiple triggers and p_T thresholds, here, due to the lack of trigger simulation at generator level, only the p_T threshold with the largest contribution to the signal region is considered. Finally, an event must contain at least one large- R jet with a transverse momentum $p_T > 300$ GeV, a pseudo-rapidity $|\eta| < 2.0$, a mass in the range $60 < m_J < 160$ GeV, and a distance $\Delta R > 1.0$ to the simulated di- τ direction.

The efficiencies of the b -tagging and the di- τ reconstruction, identification, and track selection are difficult to incorporate in a generator-level analysis, especially considering the multi-variate selection requirements. By assigning constant b -tagging and di- τ efficiencies, the acceptance times efficiency, $A \times \varepsilon$, measured in Figure 9.1 with the full detector simulation is sufficiently reproduced. Potential changes of the b -tagging and di- τ efficiencies with respect to MC generator variations are already considered in their respective systematic uncertainties.

The fractional uncertainty $\Delta(A \times \varepsilon)/(A \times \varepsilon)$ is derived from the difference between an alternative MC generator setting and the nominal MC simulation divided by the nominal acceptance times efficiency. A total uncertainty is computed via quadratic error propagation. The results are summarized in Table 9.3. The following variations have been agreed on within the ATLAS collaboration and follow the recommendations in Reference [227]. Uncertainties due to missing higher-order calculations in QCD are determined from variations of the renormalization and factorization scales by factors of 0.5 and 2. Here, the largest difference to the nominal acceptance times efficiency is considered as uncertainty.⁴ An uncertainty related

⁴ The fully anti-correlated variations, where one scale is varied up by a factor of 2 while the other is

Table 9.3: Uncertainties of the signal acceptance times efficiency. The quoted uncertainties are relative to the nominal acceptance times efficiency.

Variation	Uncertainty								
	1.0 TeV	1.1 TeV	1.2 TeV	1.4 TeV	1.6 TeV	1.8 TeV	2.0 TeV	2.5 TeV	3.0 TeV
Ren. and fact. scales	0.6%	0.2%	0.8%	0.6%	1.0%	0.5%	0.5%	0.6%	0.7%
Strong coupling	0.5%	0.2%	0.3%	0.1%	0.3%	0.04%	0.1%	0.6%	0.3%
PDF replicas	1.0%	0.6%	0.6%	0.5%	0.4%	0.3%	0.3%	0.2%	0.3%
PDF choice	0.6%	0.4%	0.8%	0.5%	0.7%	0.6%	0.1%	0.4%	0.3%
Parton-shower	24.0%	1.1%	3.1%	3.5%	2.4%	4.1%	4.0%	3.2%	2.3%
Combined	24.0%	1.3%	3.3%	3.6%	2.8%	4.1%	4.1%	3.3%	2.4%

to the strong coupling constant $\alpha_S(m_Z^2)$ is derived by changing the nominal value of 0.130 to 0.119. For both values, the corresponding variant of the PDF set is used. An uncertainties on the PDF set is determined by evaluating the standard deviation of the acceptance times efficiency in 100 PDF replicas provided by the nominal NNPDF2.3LO [129] set. The acceptance times efficiency is also evaluated with two alternative PDF sets, CT14llo [259] and MMHT2014lo68cl [135], with the largest deviation from the nominal value being considered as uncertainty on the PDF choice. Finally, an uncertainty related to the parton shower and hadronization is determined. For this purpose, the simulation of the parton shower and non-perturbative contributions is performed with PYTHIA 8.235 [130] using the A14 [131] tune instead of with the nominal HERWIG 7.1.3 [133, 134] generator. The NNPDF2.3LO set and the same matrix-element simulations from MADGRAPH are used in both cases. The most dominant difference between HERWIG and PYTHIA is found in the modeling of the high-energy tails of the jet distributions. The 1 TeV signal sample is affected most, because the $p_T > 500$ GeV requirement on the leading large- R jet strongly cuts into the signal acceptance. Hence, the high-energy tails become relevant for this sample. An uncertainty of 24% is found for the 1 TeV signal sample and uncertainties between 1% and 4% are found for the other signals. The total uncertainties are primarily affected by the parton shower and hadronization uncertainties, since most of the other variations result in uncertainties below 1%.

9.3 Statistical Analysis

As no significant deviations between the expected SM background and data are observed, exclusion limits are derived on the production of a scalar resonance X that further decays into two SM Higgs bosons. For this purpose, two hypotheses are tested. The hypothesis H_0 assumes a $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal that is produced in addition to the known SM background. This is tested against the background-only hypothesis H_1 . The formalism and design of the statistical analysis is outlined in the following. The exclusion limit results are presented afterwards.

The following descriptions are based on References [260, 261], as well as on the technical documentations of the HistFitter [262], HistFactory [263], RooStats [264], RooFit [265],

varied down by a factor of 0.5 at the same time, are not considered as they are expected to overestimate the uncertainty.

and ROOT [266] packages that are used to construct the statistical tests and for the interpretation of their results.

9.3.1 Statistical Analysis Method

The statistical analysis that is employed in this thesis evaluates the level of incompatibility of the signal plus background hypothesis with the observed data. For this purpose, the hypotheses H_0 and H_1 are generalized by introducing a signal strength factor μ , so that

$$\nu = \mu \cdot \nu_{\text{sig}} + \nu_{\text{bkg}},$$

where ν is the total number of expected events and ν_{sig} and ν_{bkg} are the number of expected signal and background events, respectively. The signal strength is defined to be $\mu \geq 0$. This means that the signal process is expected to be produced in addition to the known SM background without interference effects that would reduce the yields of the known background processes. The $\mu = 1$ case corresponds to the signal plus background hypothesis H_0 at a given signal cross section and $\mu = 0$ corresponds to the background-only hypothesis H_1 . The statistical tests are performed individually for each signal mass m_X .

9.3.2 The Likelihood Function

A parametric model is developed with a likelihood function that quantifies the probability to observe n events in data under the assumption of a certain signal strength μ . Observable quantities, like the number of data events n , are denoted in the following with Roman letters, whereas model parameters, like the expected number of events ν , are denoted with Greek letters. The likelihood function is given with

$$L(\mu, \boldsymbol{\theta}) = \mathcal{P}_{\text{SR}}(n, \mu, \boldsymbol{\theta}) \cdot \mathcal{C}(\boldsymbol{\theta}). \quad (9.1)$$

Here, the experiment is assumed to be over, and the number of data events n is treated as a fixed constant. Hence, the likelihood function only depends on the signal strength μ and a set of nuisance parameters $\boldsymbol{\theta}$. The signal strength is the parameter of interest. The nuisance parameters affect the model, e.g., by introducing uncertainties on the expected event yields, but their estimation is not of main interest. The term $\mathcal{P}_{\text{SR}}$ describes the probability to observe n events in the signal region for a given signal strength and a set of nuisance parameters. The nuisance parameters are typically constrained by auxiliary measurements. The auxiliary measurements are quantified by probability density functions in the term $\mathcal{C}$.

The probability to obtain n events if the mean expected number is ν is described by the Poisson formula $\text{Pois}(n | \nu) = \nu^n \exp(-\nu) / n!$.⁵ This gives for $\mathcal{P}_{\text{SR}}$ in Equation 9.1 with

⁵ In some cases, the Poisson distribution must be evaluated for non-integer values, e.g., when event numbers are varied by uncertainties. For these cases, the ROOT package provides an approximation of the Poisson distribution that replaces the factorial with a Gamma function [262].

$\nu = \mu \cdot \nu_{\text{sig}} + \nu_{\text{bkg}}$ expected events in the signal region:

$$\mathcal{P}_{\text{SR}}(n, \mu, \boldsymbol{\theta}) = \text{Pois}(n | \nu). \quad (9.2)$$

In the literature [260–262], this formula is typically given for binned distributions, thus resulting in a product over the number of events in each bins. The product is omitted here because the signal subregions in this thesis provide only a single event number. Analogue to $\mathcal{P}_{\text{SR}}$, additional factors $\mathcal{P}_{\text{CR}}$ can be defined to consider the number of events in dedicated control regions. Those can be introduced to Equation 9.1 as additional factors.

The expected number of events ν not only depends on the signal strength μ , but is also varied by the nuisance parameters $\boldsymbol{\theta}$. In this thesis, variations due to statistical and systematic uncertainties are considered. For this purpose, the set of nuisance parameters $\boldsymbol{\theta} := (\boldsymbol{\alpha}, \gamma)$ is split into a set of nuisance parameters $\boldsymbol{\alpha}$ related to systematic uncertainties and a nuisance parameter γ related to the statistical uncertainty. Consequently, the expected event number can be written as

$$\nu(\boldsymbol{\alpha}, \gamma) = \gamma \cdot \eta(\boldsymbol{\alpha}) \cdot \nu^0, \quad (9.3)$$

where the nominal event prediction ν^0 is varied by scaling factors γ and $\eta(\boldsymbol{\alpha})$. The scaling factors reflect that the true event number may differ from its estimate by some amount. Analogously, the term $\mathcal{C}$ in Equation 9.1 is factorized into

$$\mathcal{C}(\boldsymbol{\alpha}, \gamma) = \mathcal{C}_{\text{stat}}(\gamma) \cdot \prod_{p \in \text{Syst}} \mathcal{C}_{\text{syst}}(\alpha_p),$$

with terms $\mathcal{C}_{\text{stat}}$ and $\mathcal{C}_{\text{syst}}$ that describe the probability distributions for statistical and systematic uncertainties, respectively.

The expected number of events is derived from simulations or from a data-driven background prediction. In both cases, the samples used for these predictions have only a finite size, so their predictions are subject to statistical fluctuations that must be accounted for in the likelihood function. Barlow and Beeston [267] proposed to model the statistical fluctuations with a Poisson distribution and to introduce a nuisance parameter for each process. However, as this would result in a large number of nuisance parameters, a simplified version is employed, with only one parameter γ that is associated with the total statistical uncertainty δ [262]. This leads to

$$\mathcal{C}_{\text{stat}}(\gamma) = \text{Pois}(m | \gamma\tau),$$

where m is the number of events in the sample used for the event prediction and the parameter $\tau = (\nu/\delta)^2$ is chosen in a such a way that γ is a factor of about 1.

For the systematic uncertainties, it is reasonable to assume that they are distributed according to a Gaussian probability function $\text{Gaus}(x | \mu, \sigma) = (2\pi\sigma^2)^{-1/2} \exp(-(x - \mu)^2/2\sigma^2)$. Let α_p be the nuisance parameter to a given systematic uncertainty parameter p that is constrained by an auxiliary measurement a_p . Furthermore, let α_p be scaled in a way that

$\alpha_p = 0$ corresponds to the nominal value and $\alpha_p = \pm 1$ corresponds to the $\pm 1\sigma$ variations. Then, the probability distribution for the systematic uncertainties is given with

$$\mathcal{C}_{\text{syst}}(\alpha_p) = \text{Gaus}(a_p | \alpha_p, 1).$$

It must be noted that this term only describes the probability of a value α_p to occur. The actual effect of an α_p to the event yield is evaluated in the interpolation and extrapolation scheme, which is detailed in the following.

From the previous considerations and equation 9.3, it follows for a sample s and a systematic uncertainty parameter p that the nominal event yield ν_s^0 of a sample is varied by the scaling factors γ and $\eta_{sp}(\alpha_p)$. The effect of a systematic uncertainty is presented here separately for individual samples, since a systematic variation can have different effects on different physical processes. Furthermore, let $\eta_{sp}^0 := \eta_{sp}(\alpha_p = 0) = 1$ be the nominal scaling factor, and let $\eta_{sp}^\pm := \eta_{sp}(\alpha_p = \pm 1)$ scale the event yields to their $\pm 1\sigma$ predictions, as they are given by the auxiliary measurements. The objective below is to develop a continuous model $\eta_{sp}(\alpha_p)$ that interpolates between the given values η_{sp}^0 and $\eta_{sp}^\pm$ and extrapolates beyond. This is achieved by multiplying the nominal event yields ν_s^0 with interpolation and extrapolation functions η :

$$\nu(\boldsymbol{\alpha}, \gamma) = \gamma \sum_{s \in \text{Sample}} \nu_s^0 \prod_{p \in \text{Syst}} \eta_{sp}(\alpha_p, \eta_{sp}^+, \eta_{sp}^-),$$

where η describes a polynomial interpolation and an exponential extrapolation:

$$\eta(\alpha, \eta^+, \eta^-) = \begin{cases} (\eta^+)^{\alpha} & \text{if } \alpha \geq 1, \\ 1 + \sum_{i=1}^6 c_i \alpha^i & \text{if } |\alpha| < 1, \\ (\eta^-)^{-\alpha} & \text{if } \alpha \leq -1. \end{cases}$$

The coefficients c_i of the 6th-order polynomial interpolation are given by boundary conditions on $\eta_{sp}(\alpha_p)$ and its first and second derivatives at the points $\alpha_p = \pm 1$. The extrapolations to values $\alpha_p \geq 1$ and $\alpha_p \leq -1$ are performed with exponential functions. This method can handle asymmetric uncertainties due to the separate treatment of η_{sp}^+ and η_{sp}^- . An illustration of the interpolation and extrapolation scheme is shown in Figure 9.5. Comparisons between various schemes can be found in Reference [263]. Obviously, there is an ambiguity in the choice of the interpolation and extrapolation functions. However, the chosen approach has some conceptual advantages over simpler methods like a linear interpolation and extrapolation. It ensures $\eta(\alpha) \geq 0$, which prevents an extrapolation to unphysical negative event yields. Also, the interpolation avoids discontinuities in the first and second derivatives, which is beneficial for subsequent numerical minimization and the fit stability.

In summary, the likelihood function is given by

$$L(\mu, \boldsymbol{\alpha}, \gamma) = \text{Pois}(n | \nu(\boldsymbol{\alpha}, \gamma)) \cdot \text{Pois}(m | \gamma\tau) \cdot \prod_{p \in \text{Syst}} \text{Gaus}(a_p | \alpha_p, 1). \quad (9.4)$$

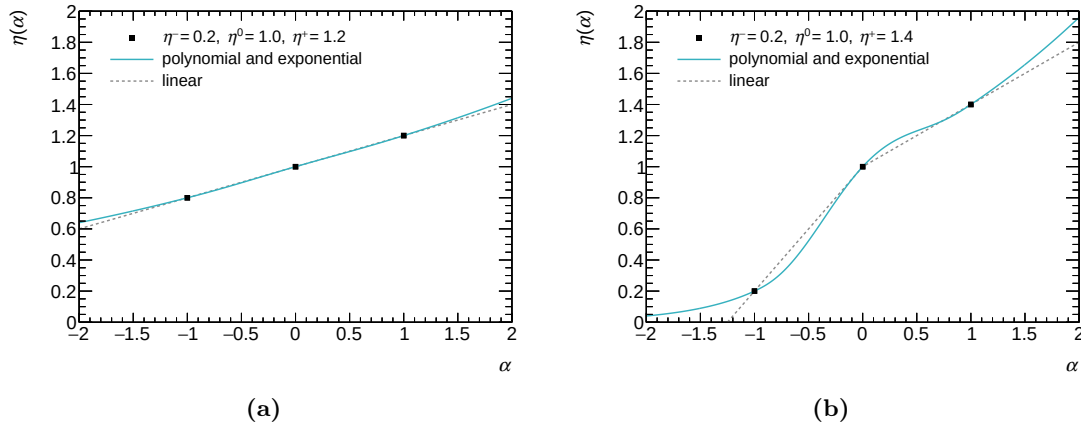


Figure 9.5: Illustrations of the polynomial interpolation and exponential extrapolation scheme (solid blue line) in comparison to a piecewise linear interpolation and extrapolation (dashed gray line) as a function of the nuisance parameter α for two different sets of scaling factors η^+ , η^0 , η^- (black squares).

9.3.3 The Test Statistic

In the following, a test statistic $\tilde{q}_\mu$ [260], based on a profile-likelihood ratio, is introduced. It is used to quantify the compatibility of data with an assumed signal strength μ and is given by

$$\tilde{q}_\mu = \begin{cases} -2 \ln \frac{L(\mu, \hat{\boldsymbol{\theta}}(\mu))}{L(0, \hat{\boldsymbol{\theta}}(0))} & \text{if } \hat{\mu} < 0, \\ -2 \ln \frac{L(\mu, \hat{\boldsymbol{\theta}}(\mu))}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})} & \text{if } 0 \leq \hat{\mu} \leq \mu, \\ 0 & \text{if } \hat{\mu} > \mu. \end{cases} \quad (9.5)$$

The set $\hat{\boldsymbol{\theta}}$ includes the so-called conditional maximum likelihood estimators of the nuisance parameters $\boldsymbol{\theta}$. That means this set of nuisance parameters maximizes the likelihood function for a specific signal strength μ under test. The values $\hat{\mu}$ and $\hat{\boldsymbol{\theta}}$ are the unconditional maximum likelihood estimators. At those values the likelihood function has its global maximum. The natural logarithm is introduced to the likelihood ratios to have a better analytical and numerical handle to the products in the likelihood function. The factor of -2 is typically introduced to have a positively defined test statistic whose probability density distribution can, under certain conditions, be approximated with a χ^2 function.⁶

The test statistic $\tilde{q}_\mu$ is evaluated as a function of μ . However, which of the three terms in Equation 9.5 is used in the test statistic depends on the unconditional estimator $\hat{\mu}$ that maximizes the likelihood function. These three cases are discussed in the following.

In the case of $0 \leq \hat{\mu} \leq \mu$, the likelihood ratio $L(\mu, \hat{\boldsymbol{\theta}}(\mu)) / L(\hat{\mu}, \hat{\boldsymbol{\theta}})$ is used. If the signal strength μ under test is close to the maximum likelihood estimator $\hat{\mu}$, then the ratio is

⁶ This asymptotic approximation, based on the results from Wilks and Wald [260, 268, 269], drastically reduces the computational requirements for the exclusion limit setting. However, this approximation is not applicable in this thesis where the expected background yield in the signal region is less than two events.

close to one and $\tilde{q}_\mu$ becomes close to zero. The opposite scenario, where μ and $\hat{\mu}$ have very different likelihood results, which also means that there is a large disagreement between the μ hypothesis and the observed data, leads to a small likelihood ratio and a correspondingly large $\tilde{q}_\mu$.

Although the signal strength μ is defined to be not negative, it is still appropriate for the estimator to take negative values, $\hat{\mu} < 0$, e.g., when the observed data fluctuates below the background expectation. In this case the closest agreement between data and a physical value of μ is given by $\mu = 0$. Hence, the denominator in the likelihood ratio is evaluated for $\mu = 0$ and $\hat{\theta}(0)$.

If the maximum likelihood estimator is above the signal strength under test, $\hat{\mu} > \mu$, the test statistic is set to zero. The reason for this is that when setting upper limits, a data observation that leads to a high $\hat{\mu}$, should not contribute to the rejection of a signal with a lower signal strength μ .

9.3.4 Exclusion Limit Calculation

For a given data observation, a $\tilde{q}_\mu^{\text{obs}}$ is determined from Equation 9.5 for every μ hypothesis under test. The disagreement between data and a hypothesized μ can be expressed with the p -value

$$p_\mu = \int_{\tilde{q}_\mu^{\text{obs}}}^{\infty} f(\tilde{q}_\mu | \mu) d\tilde{q}_\mu, \quad (9.6)$$

where $f(\tilde{q}_\mu | \mu)$ is the probability density function of the test statistic, which is to be determined in a subsequent part of this section. This p -value can already be used, if it falls below a certain predefined threshold, to reject a signal plus background hypothesis. However, such an approach has the drawback, in particular in a low-statistics scenario, that a signal may be excluded due to a downward fluctuation of the background in data [270]. To compensate this effect, the so-called CL_s method [271] is employed, which also considers the p -value of the background-only hypothesis

$$p_b = 1 - \int_{\tilde{q}_\mu^{\text{obs}}}^{\infty} f(\tilde{q}_\mu | 0) d\tilde{q}_\mu. \quad (9.7)$$

The CL_s value is then calculated with

$$\text{CL}_s(\mu) = \frac{p_\mu}{1 - p_b}.$$

If this value falls below a certain threshold $\text{CL}_s(\mu) \leq \alpha$, a signal with signal strength μ is considered to be excluded with $(1 - \alpha)$ confidence level (CL). It is common practice in particle physics to use a threshold of $\alpha = 0.05$ for the calculation of upper limits, that means to determine the signal strength that is excluded at 95% CL.

As can be seen in Equations 9.6 and 9.7, the probability density functions of the test statistic for the signal plus background and for the background-only hypotheses are needed to calculate the exclusion limit. Their distributions are determined by generating so-called pseudo experiments. For this purpose, the sets of nuisance parameters $\hat{\theta}^{\text{obs}}(\mu)$

and $\hat{\theta}^{\text{obs}}(0)$ are determined that best describe the data observation, given the signal plus background and background-only hypotheses, respectively. Then, by using Monte Carlo techniques, pseudo experiments are generated by a random sampling of nuisance parameters around the fixed sets of $\hat{\theta}(\mu)$ and $\hat{\theta}(0)$, according to the probability distribution terms in Equation 9.4. Afterwards, the test statistic $\tilde{q}_\mu$ is computed for every pseudo experiment, whereas the maximum likelihood estimators are allowed to be reevaluated freely. An example distribution of the test statistic is shown in Figure 9.6 for the $m_X = 1.8$ TeV signal with a signal strength μ close to the observed exclusion limit.

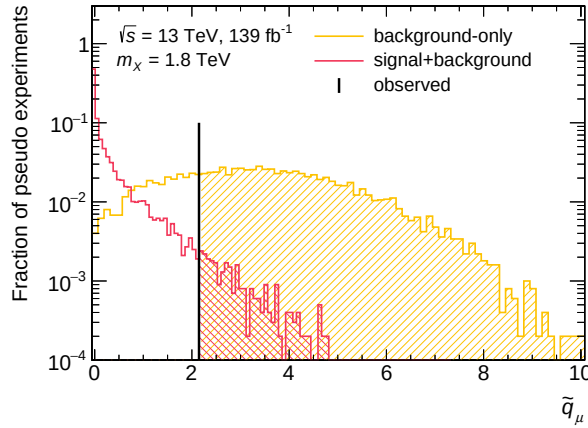


Figure 9.6: Distributions of the test statistic $\tilde{q}_\mu$ for a signal with $m_X = 1.8$ TeV at a signal strength μ close to the observed exclusion limit. The yellow histogram represents the distribution for the background-only pseudo experiments, the red histogram represents the signal plus background pseudo experiments, and the black line shows the test statistic value $\tilde{q}_\mu^{\text{obs}}$ that is observed in data. The shaded areas indicate the integrals p_μ and $1 - p_b$ that are used to compute the CL_s value.

To assess the expected sensitivity of the analysis, an expected exclusion limit is computed from the background-only pseudo experiments. The CL_s values are computed for each background-only pseudo experiment in order to construct a cumulative probability distribution of signal strengths that are excluded at 95% confidence level. The expected limit is given by the median of this cumulative probability distribution. The $\pm 1\sigma$ uncertainty band around the expected limit is given by the points where the cumulative probability crosses the 16% and 84% quantiles. Analogously, the $\pm 2\sigma$ uncertainty band is determined from the 2.5% and 97.5% quantiles.

9.4 Results

Exclusion limits on the resonant Higgs pair production are determined individually for each of the nine signal processes with resonance masses from 1 TeV to 3 TeV. For each signal process, ten thousand signal plus background pseudo experiments and ten thousand background-only pseudo experiments are generated. The distribution of the test statistic for a signal strength μ close to the observed exclusion limit is shown in Figure 9.6 for the 1.8 TeV mass point. The corresponding distributions for other mass points can be found in Appendix B.1.

9.4.1 Nuisance Parameter Impact

The distribution of the test statistic in a simple Poisson counting experiment without any systematic uncertainties is discrete. By introducing systematic uncertainties with nuisance parameters, the test statistic is smeared out to a continuous distribution.⁷ In the following, the impacts of the most important nuisance parameters that are considered in this thesis are discussed. This is illustrated in Figure 9.7 by ranking nuisance parameters based on their impact on the signal strength estimator $\hat{\mu}$. In general, this ranking differs from the systematic uncertainties on the background expectation shown in Table 9.2, as it also considers the uncertainties on the signal under test. For this reason, compared to the preceding table, systematic uncertainties that strongly affect the signal process, such as the di- τ scale factor uncertainties, are ranked higher than those only affecting the background processes.

The ranking is shown for three representative signal masses of 1.2 TeV, 1.8 TeV, and 2.5 TeV, whose results are determined from the three signal subregions. The corresponding figures for all mass points can be found in Appendix B.2. The impact $\Delta\hat{\mu}$ on the signal strength is determined by fixing the value of a nuisance parameter to a value of $\pm 1\sigma$ apart from its nominal value. Then, the signal strength estimator $\hat{\mu}$ as well as all remaining nuisance parameters are reevaluated. It is distinguished between ‘pre-fit’, where the nominal nuisance parameters and their uncertainties are given by the auxiliary measurements, and ‘post-fit’, for which the set of nuisance parameters $\hat{\theta}$ that best describe the observed data is determined. In this thesis, only very small differences between pre- and post-fit values are found. This typically indicates that the experiment is well described by the chosen parametric model of the statistical analysis. On the other hand, a close agreement between pre- and post-fit observables is to be expected in an one-bin counting experiment, as it offers limited scope for the fit to further constrain certain nuisance parameters.

The ranking results in Figures 9.7(a) and 9.7(b) are similar, because they are derived from the m_{hh}^{vis} -inclusive and $m_{hh}^{\text{vis}} > 900$ GeV signal subregions, which have a quite similar

⁷ An analysis with a small background expectation and small systematic uncertainties can show a test statistic distribution with distinct peaks that are smeared but do not overlap. This potentially leads to too optimistic exclusion limits when zero data events are observed, as detailed in Reference [272]. Such an effect was also observed in the development of the analysis in this thesis when the expected limit is calculated with only statistical uncertainties or with a small subset of systematic uncertainties. However, with the full set of systematic uncertainties, the distributions of the test statistics, as shown in Figure 9.6 and Appendix B.1, are found to be continuous and unaffected.

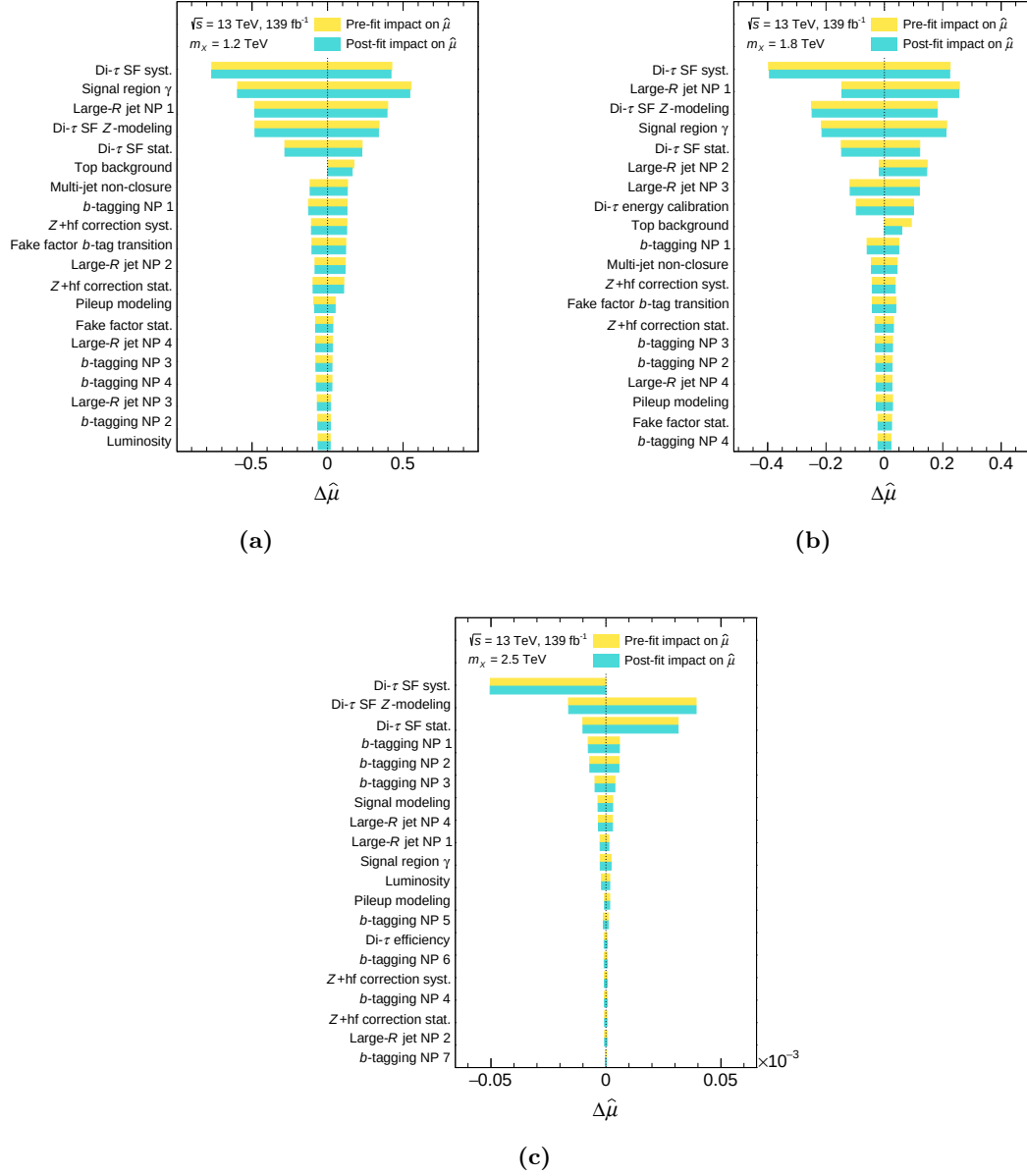


Figure 9.7: Ranking of the nuisance parameters based on their impact $\Delta\hat{\mu}$ on the signal strength estimator for the 1.2 TeV (a), 1.8 TeV (b), and 2.5 TeV signals. The pre-fit and post-fit impacts are represented by the yellow and blue bars, respectively. Only the twenty highest-ranked nuisance parameters are shown.

background expectation and the same number of observed data events. The uncertainties related to the di- τ scale factor have the highest ranking, followed by nuisance parameters related to the large- R jet calibration. The nuisance parameter γ , which parameterizes the statistical uncertainty on the background model in the signal region, is relatively highly ranked, indicating that increased background Monte Carlo statistics might improve the limit results moderately. The $m_{hh}^{\text{vis}} > 1200$ GeV signal subregion has less than one expected background events and no data events observed. In this case, the signal strength estimator $\hat{\mu}$ is close to zero and the impact of the nuisance parameters in terms of $\Delta\hat{\mu}$ is accordingly small, as can be seen in Figure 9.7(c). It is predominantly affected by nuisance parameters related to the signal efficiency, which are the di- τ scale factor and b -tagging uncertainties.

9.4.2 Exclusion Limit Results

The CL_s exclusion limits on the signal strengths are translated into upper limits on the product of the cross section to produce a narrow scalar resonance in proton–proton collisions, $\sigma(pp \rightarrow X)$, and its branching ratio to decay into SM Higgs bosons, $\text{BR}(X \rightarrow hh)$. The 95% CL upper limits on $\sigma(pp \rightarrow X) \times \text{BR}(X \rightarrow hh)$ are shown in Figure 9.8 as a function of resonance masses from 1 TeV to 3 TeV. SM branching ratios are assumed for the decays of the SM Higgs bosons into a pair of b quarks and a pair of hadronically decaying τ leptons. At the mass points of 1.6 TeV and 2.5 TeV, where the m_{hh}^{vis} requirements of the signal subregions change, respectively, from m_{hh}^{vis} -inclusive to a 900 GeV cut and from a 900 GeV cut to a 1200 GeV cut, the exclusion limits are evaluated twice. This is necessary to perform an extrapolation between neighboring mass points without changing the selection requirements within the extrapolation. This can be seen in two discontinuities in the limit curve. At 1.6 TeV only a small difference is seen between imposing no m_{hh}^{vis} requirement and the 900 GeV cut. At 2.5 TeV, however, the limit results are considerably improved by the more stringent $m_{hh}^{\text{vis}} > 1200$ GeV requirement, as it drastically reduces background processes.

The observed limit is within the 1σ uncertainty band of the expected limit, showing that the data are well described by SM processes and that no hints for new physics are found by this analysis. The observed limit is slightly above the expectation for signals derived from the m_{hh}^{vis} -inclusive and $m_{hh}^{\text{vis}} > 900$ GeV signal subregions, since the two observed data events are slightly above the background expectation. The two mass points from the $m_{hh}^{\text{vis}} > 1200$ GeV signal subregion show limits slightly below the expectation because no data events are observed, whereas a small background is expected.

This analysis, with a very low background expectation and signal yields excluded down to a few events, is mostly limited by the available data statistics and by the signal acceptance and efficiency that is achieved in the signal region. This can be seen in a comparison of the limit curve with the signal acceptance times efficiency of Figure 9.1. The highest sensitivity is reached for mass points with the highest signal acceptance times efficiency and vice versa. As discussed in detail in Section 9.1, the most limiting factors for the signal efficiency are the di- τ selection and b -tagging requirements, and specifically for the lowest mass points, the trigger acceptance and large- R jet p_T thresholds.

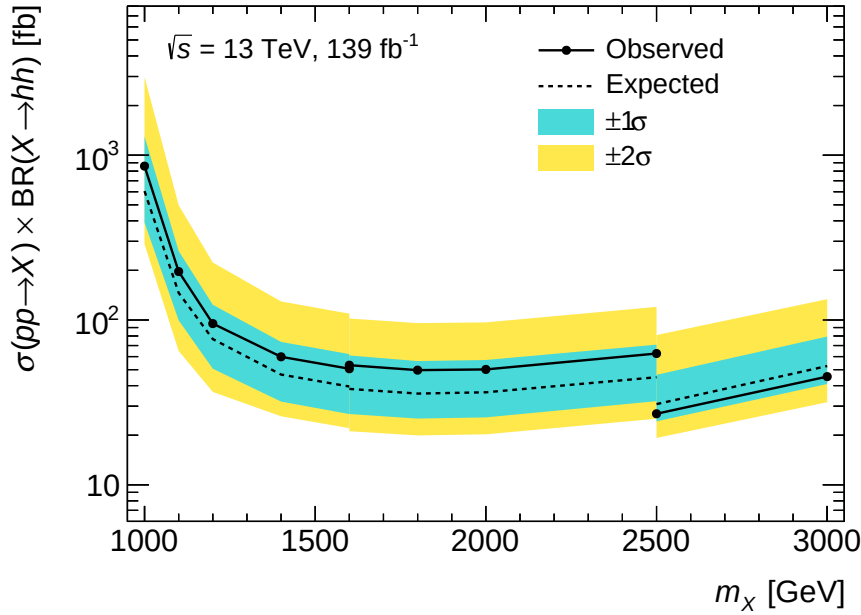


Figure 9.8: Expected and observed 95% CL upper limits on the product of the cross section to produce a narrow scalar resonance, $\sigma(pp \rightarrow X)$, and its branching ratio to decay into SM Higgs bosons, $\text{BR}(X \rightarrow hh)$, as a function of the resonance mass m_X . SM branching ratios are assumed for the decays of the SM Higgs bosons into a pair of b quarks and a pair of hadronically decaying τ leptons. The $\pm 1\sigma$ and $\pm 2\sigma$ uncertainties of the expected limit are represented by the blue and yellow bands, respectively.

The limit results from this thesis are shown in Figure 9.9 in conjunction with previous ATLAS results of a search for resonant Higgs boson pair production in resolved $b\bar{b}\tau^+\tau^-$ final states [5]. The analysis of resolved $b\bar{b}\tau^+\tau^-$ final states used 36 fb^{-1} of proton–proton collision data and considered final states with two hadronically decaying τ leptons, as well as final states with one hadronic and one leptonic τ decay. Resonance masses between 260 GeV and 1 TeV were considered. Subsequent to the analysis of this thesis, the ATLAS collaboration presented preliminary results [13] in the resolved $b\bar{b}\tau^+\tau^-$ final state using the full Run 2 dataset. The sensitivity improved by over a factor four compared to the results with 36 fb^{-1} . Apart from this improvement in sensitivity, it can already be seen in Figure 9.9 that the search for resolved $b\bar{b}\tau^+\tau^-$ final states is more sensitive to the 1 TeV mass point than the search for boosted final states. This is mainly due to the use of the electron, muon, and hadronic τ decay triggers, whose thresholds are much lower than those of the large- R jet triggers employed in this thesis. In the 1 TeV signal, the large majority of τ leptons and b quarks in the final state are still accessible with the standard resolved reconstruction techniques, however, the sensitivity decreases significantly with increasing resonance masses. As a potential future improvement of the search for boosted $b\bar{b}\tau^+\tau^-$ final states, it is worth to consider an alternative trigger strategy, in particular to increase the sensitivity in the mass range from 1.0 TeV to 1.2 TeV, e.g., by employing di-jet, $E_{\text{T}}^{\text{miss}}$, or hadronic τ decay triggers. Also the inclusion of an analysis channel with one τ lepton in the leptonic decay mode is promising, as it would approximately double the number of accessible signal events.

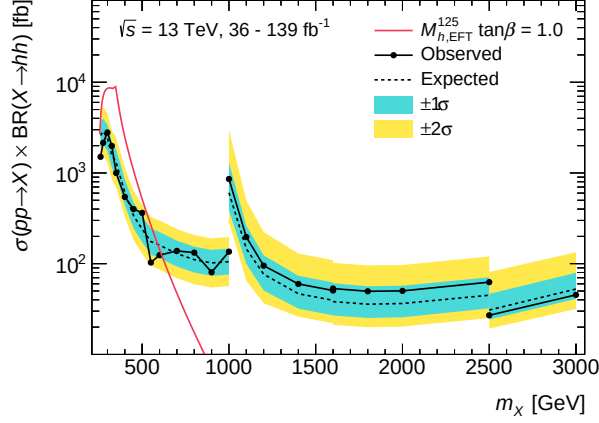


Figure 9.9: Expected and observed 95% CL upper limits on $\sigma(pp \rightarrow X) \times \text{BR}(X \rightarrow hh)$, using a search for resolved $b\bar{b}\tau^+\tau^-$ final states in 36 fb^{-1} of ATLAS data in the mass range from 260 GeV to 1 TeV [5] and using a search for boosted $b\bar{b}\tau^+\tau^-$ final states as presented in this thesis in the range from 1 TeV to 3 TeV. SM branching ratios are assumed for the decays of the SM Higgs bosons. The red line represents the prediction of the $M_{h,\text{EFT}}^{125}$ [77] benchmark scenario for a CP-even Higgs boson decaying into two SM Higgs bosons assuming a $\tan\beta = 1.0$.

Figure 9.9 also shows the cross section prediction for a CP-even heavy Higgs boson decaying into two SM Higgs bosons in the $M_{h,\text{EFT}}^{125}$ [77] benchmark scenario with an assumed $\tan\beta$ parameter of 1.0. The predictions of the cross sections and branching ratios are provided by the LHC Higgs Cross Section Working Group [49]. The Higgs masses and mixing are computed in the FeynHiggs [78–85] program. The branching ratios are obtained from the most precise results of the FeynHiggs, HDECAY [86–89], and PROPHECY4f [90–92] programs. The inclusive gluon–gluon fusion Higgs production cross sections are calculated with the SusHi [273, 274] program, with NLO QCD corrections [275], as well as with NNLO QCD corrections for top quark contributions [276–280] and electroweak contributions of light quarks [281, 282]. In addition, N3LO top quark corrections are considered for the SM-like Higgs boson [283–285].

From this benchmark scenario, heavy CP-even Higgs bosons with masses of up to about 600 GeV can be excluded at 95% confidence level, when assuming a $\tan\beta = 1.0$. At higher $\tan\beta$ values, the branching ratio for the decay into SM Higgs bosons decreases, which also leads to a reduced range of excluded masses. In the mass range above 1 TeV, which is the main target of the analysis presented in this thesis, no exclusions in the parameter space of this model can be set. This is mainly because the branching ratio is strongly reduced at high masses, once the decay into $t\bar{t}$ becomes kinematically allowed. This can be seen in the rapid decrease of the predicted $\sigma(pp \rightarrow X) \times \text{BR}(X \rightarrow hh)$ in Figure 9.9.

An interpretation of this analysis with signal signatures like $X \rightarrow hh_S \rightarrow b\bar{b}\tau^+\tau^-$, as they are predicted in models like the NMSSM,⁸ are worth to consider for future iterations of this analysis. Depending on the mixing, a coupling of the additional Higgs boson h_S to SM particles can be strongly suppressed, in which case typical searches for a direct production

⁸ Here, h_S is an additional Higgs boson with a mass different from the SM Higgs boson, as described in the NMSSM overview in Section 2.2.2.

would not be sensitive. The new physics would then show up predominantly in cascade decays of Higgs bosons with decreasing masses. A search inspired by such a scenario was recently published by the CMS collaboration [286]. In particular, if the additional Higgs boson h_S is lighter than the SM Higgs boson, a search for boosted topologies becomes important. A re-interpretation of the analysis of this thesis, would require the production of signal samples with varying resonance masses m_X and m_{h_S} and small adjustments to the large- R jet mass and m_{hh}^{vis} requirements, whereas the main analysis strategy can be kept unchanged.

Chapter 10

Summary

In this thesis, novel techniques for the reconstruction and identification of a boosted pair of hadronically decaying τ leptons in the ATLAS experiment are presented. A calibration and validation of the di- τ algorithms is performed using data of 139 fb^{-1} of proton–proton collisions at a center-of-mass energy of 13 TeV. A data set enriched with SM processes that include a boosted pair of τ leptons, mainly $Z/\gamma^* \rightarrow \tau^+\tau^- + \text{jets}$, is used for this purpose. Finally, a search for a heavy scalar resonance decaying via $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ is performed for resonance masses from 1 TeV to 3 TeV. The results were first presented at the 8th Conference of Large Hadron Collider Physics [287] and were later published in the Journal of High Energy Physics [11].

The di- τ techniques involve the reconstruction of a boosted τ pair as a large- R jet, followed by a detection of smaller subjets that contain the τ decay products. The di- τ identification uses boosted decision trees and a set of identification variables to distinguish genuine boosted τ pairs from quark- or gluon-initiated jets. The performance of the di- τ algorithms is investigated in the BSM processes $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ and $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$. The di- τ reconstruction is found to have an efficiency of more than 80% when the angular distance between the τ leptons is $\Delta R = 0.4$. At this distance, the standard τ reconstruction becomes inefficient because it can no longer resolve the τ pair. At the chosen operating point of the di- τ identification, the identification efficiency is found to be higher than 60%, whereas the probability to misidentify a quark- or gluon-initiated jet as signal is less than 0.01%. A first proof of concept for the di- τ algorithms was shown in a master thesis [288]. Since then, the di- τ algorithms have been significantly improved and are now implemented in the ATLAS experiment’s event reconstruction software, Athena [160, 289]. In this thesis, only hadronically decaying τ leptons are considered. However, there are first proofs of concept for the reconstruction and identification of boosted τ pairs with one of the τ leptons decaying into an electron or muon [290, 291].

Before the di- τ algorithms are used in a search for new physics, a data-based calibration of the di- τ efficiency is performed using data of well-known SM processes. The boosted τ pairs arise mainly from events of Z +jets and from small contributions of di-boson, Vh , and $t\bar{t}$ events. A normalization scale factor of 0.84 ± 0.09 (stat) $^{+0.14}_{-0.13}$ (Z -modelling) $^{+0.19}_{-0.20}$ (syst) is derived. A good agreement between data and simulations is found for the di- τ energy scale.

In the $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ signal region, no significant deviations between data and the expected SM backgrounds are observed. A statistical analysis is performed based on profile-likelihood ratios and the CL_s method. Upper limits are derived on the cross section for the production of a narrow scalar resonance times its branching ratio to decay into a Higgs boson pair, $\sigma(pp \rightarrow X) \times \text{BR}(X \rightarrow hh)$. Exclusion limits from 858 fb to 27 fb are observed at 95% CL. The most stringent exclusion limit is found for the 2.5 TeV signal hypothesis. For the lowest considered masses the limit results are less sensitive, which is mainly related to the trigger acceptance and the large- R jet p_T thresholds. Expected and observed exclusion limits agree within the 1σ uncertainty band over the entire mass range.

In this thesis, X is motivated by a scalar Higgs boson in a 2HDM scenario as implemented in the MSSM. The presented analysis can also be used for a search for heavy resonances in the RS model such as a radion or a graviton. However, such interpretations would potentially require dedicated signal simulations. The radion is a scalar boson, as is the simulated X in this thesis. Exclusion limits for the production of a radion are expected to be similar to those presented as long as the width of the radion is small compared to the experimental resolution. The graviton is a spin-2 particle, which implies certain differences in the decay kinematics compared to a scalar resonance. Depending on $k/\bar{M}_{\text{Pl}}$, the width of the graviton signal can become considerably large. In this case, dedicated signal samples are needed to model the width and their effect on the decay kinematics appropriately.

In comparison to other searches for resonant production of Higgs boson pairs, the latest searches in the $b\bar{b}b\bar{b}$ final state [14, 23] provided the most stringent exclusion limits to date in the very high-mass regime. This is explained mainly by the higher branching ratio of the $h \rightarrow b\bar{b}$ decay. This compensates the larger multi-jet and $t\bar{t}$ backgrounds that are observed in this final state. The analysis of this thesis will certainly benefit from larger data sets to be taken in the future, especially to fully exploit the advantage of the good background separation that can be achieved with τ leptons. The di- τ identification criterion can be tightened and di- τ mass cuts can be introduced to reduce the multi-jet and $Z \rightarrow \tau^+\tau^-$ backgrounds, respectively. It can be expected that when more data are taken, the background can be kept very low, while maintaining almost the same signal efficiency.

The use of the di- τ reconstruction and identification is not limited to a search for $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$. One of the design principles in the development of the di- τ algorithms was to be as independent as possible of the initial resonance and of event signatures other than the τ pair. This is illustrated, for example, by the fact that the performance studies utilized simulations of spin-0 and spin-2 resonances decaying into a Higgs boson pair, whereas the data-based calibration showed that the same algorithms are also applicable to $Z \rightarrow \tau^+\tau^-$ decays. In the following, a non-exhaustive compilation of analyses is given, in which the di- τ algorithms might be beneficial. The exact gain would, of course, have to be examined in detail in separate studies, which is beyond the scope of this thesis.

An application for the di- τ algorithms can be found in the ATLAS measurements of the SM Higgs boson production cross sections in the $h \rightarrow \tau^+\tau^-$ [292] decay channel. In the measurement of the gluon-gluon fusion cross section, the Higgs boson must have a certain momentum to achieve a sufficient signal sensitivity. However, in this analysis there

is a requirement that hadronic τ decays are separated by $\Delta R > 0.6$ to reject events with merging τ pairs. This is sufficient for the majority of events but the exclusion of highly boosted Higgs bosons limits the signal acceptance. In particular the highly boosted regime is sensitive to BSM contributions, e.g., from the superpartner of the top quark, leading to an increase in the gluon–gluon fusion production of high- p_T Higgs bosons [49]. In the associated production with a vector boson, Vh , the Higgs boson has an inherent boost as it recoils against the vector boson. Similar to gluon–gluon fusion, the associated production is particularly sensitive to BSM effects in the high- p_T regime.

Another potential application for the di- τ algorithms is in the search for heavy vector bosons V' , which are predicted by various BSM scenarios [293]. A search for such heavy resonances decaying into a weak vector boson and a Higgs boson was recently published by the ATLAS collaboration [294]. Here, resonance masses from 1.5 TeV to 5 TeV and the decay channels $Z' \rightarrow Zh \rightarrow q\bar{q}b\bar{b}$ and $W' \rightarrow Wh \rightarrow q\bar{q}'b\bar{b}$ are considered. Due to the high resonance masses, dedicated techniques are necessary for the reconstruction of the boosted final state particles. Since both the Z and Higgs bosons can decay into a pair of τ leptons, an inclusion of the τ final states can provide a sizable increase in signal acceptance. The CMS collaboration conducted such a search in the $q\bar{q}\tau^+\tau^-$ final state with an early Run 2 data set [295].

Finally, searches for light resonances can also benefit from a reconstruction of boosted pairs of τ lepton. The main focus of this thesis are high-mass resonances, but this is not the only source of highly boosted τ pairs in a final state. For example, in exotic decays of the Higgs boson [296], such as $h \rightarrow aa \rightarrow b\bar{b}\tau^+\tau^-$ and $h \rightarrow aa \rightarrow \tau^+\tau^-\tau^+\tau^-$, the τ leptons are very collimated if the intermediate resonance a is substantially lighter than the Higgs boson. Here, the light resonance a is a pseudo-scalar boson that arises, for example, in the NMSSM. Another example is the production of a light resonance in association with a top quark pair, $t\bar{t}X$, in the decay channel $X \rightarrow \tau^+\tau^-$. In the gluon–gluon fusion production, the τ leptons may be too low-energetic to be accepted by a trigger. In this case, the associated production and a leptonic decay of a top quark can be utilized for online event selection. The resonance X recoils against the $t\bar{t}$ system and provides the τ pair with a substantial Lorentz boost. In a search for a light resonance, the τ leptons have significantly lower momenta than the final states considered in this thesis. In this case, certain modifications to the di- τ algorithms become necessary. This is primarily a lowering of the p_T threshold in the di- τ reconstruction and an inclusion of low- p_T di- τ candidates in the training of the di- τ identification. However, the main concepts presented in this thesis are expected to be applicable to low- p_T pairs of τ leptons.

The reconstruction of boosted di- τ final states offers novel opportunities for the search for new physics with the ATLAS experiment. A first application is shown in the search for $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ and there are many more signatures to be investigated with current and future data sets provided by the LHC. A total integrated luminosity of up to 350 fb^{-1} is expected for the end of LHC Run 3 and at least 3000 fb^{-1} will be accumulated by the High-Luminosity LHC [146]. This will enable unprecedented sensitivities to rare signatures such as highly boosted final states in searches for new physics phenomena.

Appendix A

Implementation Details

This Appendix provides a summary of the technical details and software releases used for the physics analysis in this thesis. The sample production and event reconstruction is performed in ATLAS with the Athena [160, 289] framework, which is based on the Gaudi [297] software architecture.

For the data analysis, the Good Run Lists shown in Table A.1 are used. They contain the run numbers and luminosity blocks that are approved by the ATLAS collaboration for use in physics analyses. The data samples of 2015 and 2016 are processed in Athena release 21.0.20. The 2017 and 2018 data samples are produced in different releases from 21.0.53 to 21.0.83 [298]. The data sets as well as the Good Run Lists are centrally provided by the ATLAS collaboration.

The MC samples used in this thesis are listed in Tables A.2 to A.9. The simulation samples are produced in three campaigns: MC16a, MC16d, and MC16e, to represent the 2015–2016, 2017, and 2018 data takings, respectively. Information about the sample production is collected in the ATLAS metadata interface (AMI) [299]. Each sample has a set of AMI tags, as can be seen in the following tables. An AMI tag consists of a letter followed by a four-digit number that encodes the software release and configuration used for sample production. There are *e*-tags, which correspond to the event generation, *s*-tags describing the detector simulation, and *r*-tags corresponding to the event reconstruction. At this point the samples are provided in the so-called xAOD format, i.e., the common data format in ATLAS that can be read in both Athena and ROOT. Samples with a *p*-tag are further processed into derivations, which is done here for all data and MC samples used in the search for resonant Higgs boson pair production. Derivations have basically the same format as the xAOD samples, but are smaller due to an event preselection and a reduced amount of information per event. The derivation type **HIGG4D6** [300] is specifically developed for the analysis in this thesis. It makes sure that the remaining selected events have at least one reconstructed di- τ candidate, at least two large- R jets with $p_T > 300$ GeV, and that a large- R jet trigger has fired. The derivations are produced in the **AthDerivation** project of the Athena framework in release 21.2.52 or in a compatible version with the same derivation definition.

The derivations are further processed in the CxAOD framework [301]. Here, the event selection, the calibrations and systematic uncertainties are applied to create the histograms

for the subsequent statistical analysis. The CxAOD framework and the analysis software is compiled in the **AnalysisBase** project of the the Athena framework in release 21.2.78. The statistical analysis is performed with the HistFitter [262] framework in version 0.61.0 [302].

Table A.1: Good Run Lists per year of data taking with their integrated luminosities. The Good Run Lists are centrally provided by the ATLAS collaboration and ensure that the data is recorded under good detector conditions [162].

Year	Good Run List	Int. luminosity
2015	data15_13TeV.periodAllYear_DetStatus-v89-pro21-02_Unknown_PHYS_StandardGRL_All_Good_25ns.xml	3.2 fb ⁻¹
2016	data16_13TeV.periodAllYear_DetStatus-v89-pro21-01_DQDefects-00-02-04_PHYS_StandardGRL_All_Good_25ns.xml	33.0 fb ⁻¹
2017	data17_13TeV.periodAllYear_DetStatus-v99-pro22-01_Unknown_PHYS_StandardGRL_All_Good_25ns_TriggerNo17e33prim.xml	44.3 fb ⁻¹
2018	data18_13TeV.periodAllYear_DetStatus-v102-pro22-04_Unknown_PHYS_StandardGRL_All_Good_25ns_TriggerNo17e33prim.xml	58.5 fb ⁻¹

Table A.2: List of MC samples used to simulate the signal process of $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ with their cross section σ , k factor and efficiency of the generator filter $\varepsilon_{\text{filter}}$. The production tags correspond to sample productions in the MC16a, MC16d and MC16e campaigns, respectively. The cross section of the samples are set to a value so that $\sigma(pp \rightarrow X) \times \text{BR}(X \rightarrow hh) = 1 \text{ pb}$ when assuming SM branching ratios for the decays of the SM Higgs bosons into a pair of τ leptons and a pair of b quarks.

$X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$	$\sigma \text{ [pb]}$	k	$\varepsilon_{\text{filter}}$
mc16_13TeV.450160.MadGraphHerwig7EvtGen_PDF23LO_X1000tohh_bbtatau_hadhad Production tags: e7319_s3126_r9364_p3759, e7319_s3126_r10201_p3759, e7319_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.370
mc16_13TeV.450173.MadGraphHerwig7EvtGen_PDF23LO_X1100tohh_bbtatau_hadhad Production tags: e7969_s3126_r9364_p3759, e7969_s3126_r10201_p3759, e7969_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.374
mc16_13TeV.450174.MadGraphHerwig7EvtGen_PDF23LO_X1200tohh_bbtatau_hadhad Production tags: e7319_s3126_r9364_p3759, e7319_s3126_r10201_p3759, e7319_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.378
mc16_13TeV.450176.MadGraphHerwig7EvtGen_PDF23LO_X1400tohh_bbtatau_hadhad Production tags: e7319_s3126_r9364_p3759, e7319_s3126_r10201_p3759, e7319_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.384
mc16_13TeV.450178.MadGraphHerwig7EvtGen_PDF23LO_X1600tohh_bbtatau_hadhad Production tags: e7319_s3126_r9364_p3759, e7319_s3126_r10201_p3759, e7319_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.389
mc16_13TeV.450179.MadGraphHerwig7EvtGen_PDF23LO_X1800tohh_bbtatau_hadhad Production tags: e7319_s3126_r9364_p3759, e7319_s3126_r10201_p3759, e7319_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.392
mc16_13TeV.450180.MadGraphHerwig7EvtGen_PDF23LO_X2000tohh_bbtatau_hadhad Production tags: e7319_s3126_r9364_p3759, e7319_s3126_r10201_p3759, e7319_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.395
mc16_13TeV.450182.MadGraphHerwig7EvtGen_PDF23LO_X2500tohh_bbtatau_hadhad Production tags: e7319_s3126_r9364_p3759, e7319_s3126_r10201_p3759, e7319_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.398
mc16_13TeV.450184.MadGraphHerwig7EvtGen_PDF23LO_X3000tohh_bbtatau_hadhad Production tags: e7319_s3126_r9364_p3759, e7319_s3126_r10201_p3759, e7319_s3126_r10724_p3759	7.31×10^{-2}	1.00	0.404

Table A.3: List of MC samples used to simulate the process of $G \rightarrow hh \rightarrow \tau^+ \tau^- \tau^+ \tau^-$ with their cross section σ , k factor and efficiency of the generator filter $\varepsilon_{\text{filter}}$. The production tags correspond to the sample productions in the MC16a, MC16d and MC16e campaigns, as well as to variations of the ATLAS detector model, as detailed in Section 5.6. The cross section of the samples are set to a value so that $\sigma(pp \rightarrow G) \times \text{BR}(G \rightarrow hh) = 1 \text{ pb}$ when assuming SM branching ratios for the decays of the SM Higgs bosons into pairs of τ leptons.

$G \rightarrow hh \rightarrow \tau^+ \tau^- \tau^+ \tau^-$	$\sigma [\text{pb}]$	k	$\varepsilon_{\text{filter}}$
mc16_13TeV.425100.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M1500 Production tags: e5485_s3126_r9364, e5485_s3155_r9476, e5485_s3156_r9477, e5485_s3157_r9478, e5485_s3169_r9552, e5485_s3126_r10201, e5485_s3126_r10724	3.93×10^{-3}	1.00	1.00
mc16_13TeV.425101.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M1750 Production tags: e5485_s3126_r9364, e5485_s3155_r9476, e5485_s3156_r9477, e5485_s3157_r9478, e5485_s3169_r9552, e5485_s3126_r10201, e5485_s3126_r10724	3.93×10^{-3}	1.00	1.00
mc16_13TeV.425102.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M2000 Production tags: e5485_s3126_r9364, e5485_s3155_r9476, e5485_s3156_r9477, e5485_s3157_r9478, e5485_s3169_r9552, e5485_s3126_r10201, e5485_s3126_r10724, e5485_s3430_r11333, e5485_s3431_r11333	3.93×10^{-3}	1.00	1.00
mc16_13TeV.425103.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M2250 Production tags: e5485_s3126_r9364, e5485_s3155_r9476, e5485_s3156_r9477, e5485_s3157_r9478, e5485_s3169_r9552, e5485_s3126_r10201, e5485_s3126_r10724	3.93×10^{-3}	1.00	1.00
mc16_13TeV.425104.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M2500 Production tags: e5485_s3126_r9364, e5485_s3155_r9476, e5485_s3156_r9477, e5485_s3157_r9478, e5485_s3169_r9552, e5485_s3126_r10201, e5485_s3126_r10724	3.93×10^{-3}	1.00	1.00
mc16_13TeV.425105.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M3000 Production tags: e6072_s3126_r9364, e6072_s3155_r9476, e6072_s3156_r9477, e6072_s3157_r9478, e6072_s3169_r9552, e6072_s3126_r10201, e6072_s3126_r10724	3.93×10^{-3}	1.00	1.00
mc16_13TeV.425106.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M4000 Production tags: e6072_s3126_r9364, e6072_s3155_r9476, e6072_s3156_r9477, e6072_s3157_r9478, e6072_s3169_r9552, e6072_s3126_r10201, e6072_s3126_r10724	3.93×10^{-3}	1.00	1.00
mc16_13TeV.425107.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M5000 Production tags: e6072_s3126_r9364, e6072_s3155_r9476, e6072_s3156_r9477, e6072_s3157_r9478, e6072_s3169_r9552, e6072_s3126_r10201, e6072_s3126_r10724	3.93×10^{-3}	1.00	1.00
mc16_13TeV.425108.MadGraphPythia8EvtGen_A14NNPDF23LO_RS_G_hh_4tau_c10_M1000 Production tags: e6072_s3126_r9364, e6072_s3155_r9476, e6072_s3156_r9477, e6072_s3157_r9478, e6072_s3169_r9552, e6072_s3126_r10201, e6072_s3126_r10724	3.93×10^{-3}	1.00	1.00

Table A.4: List of MC samples used to simulate the process of $Z/\gamma^* \rightarrow \tau^+\tau^- + \text{jets}$ with their cross section σ , k factor and efficiency of the generator filter $\varepsilon_{\text{filter}}$. The production tags correspond to sample productions in the MC16a, MC16d and MC16e campaigns, respectively.

$Z/\gamma^* \rightarrow \tau^+\tau^- + \text{jets}$	σ [pb]	k	$\varepsilon_{\text{filter}}$
mc16_13TeV.364128.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV0_70_CVetoBVeto Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	1.98×10^3	0.975	0.821
mc16_13TeV.364129.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV0_70_CFilterBVeto Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	1.98×10^3	0.975	0.113
mc16_13TeV.364130.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV0_70_BFilter Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	1.98×10^3	0.975	0.0645
mc16_13TeV.364131.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV70_140_CVetoBVeto Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	1.10×10^2	0.975	0.689
mc16_13TeV.364132.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV70_140_CFilterBVeto Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	1.11×10^2	0.975	0.183
mc16_13TeV.364133.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV70_140_BFilter Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	1.11×10^2	0.975	0.119
mc16_13TeV.364134.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV140_280_CVetoBVeto Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	4.08×10^1	0.975	0.608
mc16_13TeV.364135.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV140_280_CFilterBVeto Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	4.07×10^1	0.975	0.229
mc16_13TeV.364136.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV140_280_BFilter Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	4.08×10^1	0.975	0.134
mc16_13TeV.364137.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV280_500_CVetoBVeto Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	8.55×10^0	0.975	0.560
mc16_13TeV.364138.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV280_500_CFilterBVeto Production tags: e5313_s3126_r9364_p3759, e5313_s3126_r1020I_p3759, e5313_s3126_r10724_p3703	8.67×10^0	0.975	0.263
mc16_13TeV.364139.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV280_500_BFilter Production tags: e5313_s3126_r9364_p3759, e5313_s3126_r1020I_p3759, e5313_s3126_r10724_p3703	8.68×10^0	0.975	0.173
mc16_13TeV.364140.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV500_1000 Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	1.81×10^0	0.975	1.00
mc16_13TeV.364141.Sherpa_221_NNPDF30NNLO_Ztautau_MAXHTPTV1000_E_CMS Production tags: e5307_s3126_r9364_p3759, e5307_s3126_r1020I_p3759, e5307_s3126_r10724_p3703	1.48×10^{-1}	0.975	1.00

Table A.5: List of MC samples used to simulate the process of $Z/\gamma^* \rightarrow e^+e^- + \text{jets}$ with their cross section σ , k factor and efficiency of the generator filter $\varepsilon_{\text{filter}}$. The production tags correspond to sample productions in the MC16a, MC16d and MC16e campaigns, respectively.

$Z/\gamma^* \rightarrow e^+e^- + \text{jets}$	σ [pb]	k	$\varepsilon_{\text{filter}}$
mc16_13TeV.364114.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV0_70_CVetoBVeto Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	1.98×10^3	0.975	0.821
mc16_13TeV.364115.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV0_70_CFilterBVeto Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	1.98×10^3	0.975	0.113
mc16_13TeV.364116.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV0_70_BFilter Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	1.98×10^3	0.975	0.0638
mc16_13TeV.364117.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV70_140_CVetoBVeto Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	1.10×10^2	0.975	0.690
mc16_13TeV.364118.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV70_140_CFilterBVeto Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	1.11×10^2	0.975	0.184
mc16_13TeV.364119.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV70_140_BFilter Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	1.10×10^2	0.975	0.114
mc16_13TeV.364120.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV140_280_CVetoBVeto Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	4.07×10^1	0.975	0.615
mc16_13TeV.364121.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV140_280_CFilterBVeto Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	4.07×10^1	0.975	0.230
mc16_13TeV.364122.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV140_280_BFilter Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	4.07×10^1	0.975	0.149
mc16_13TeV.364123.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV280_500_CVetoBVeto Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	8.67×10^0	0.975	0.561
mc16_13TeV.364124.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV280_500_CFilterBVeto Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	8.67×10^0	0.975	0.263
mc16_13TeV.364125.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV280_500_BFilter Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	8.68×10^0	0.975	0.172
mc16_13TeV.364126.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV500_1000 Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	1.81×10^0	0.975	1.00
mc16_13TeV.364127.Sherpa_221_NNPDF30NNLO_Zee_MAXHTPTV1000_E CMS Production tags: e5299_s3126_r9364_p3759, e5299_s3126_r10201_p3759, e5299_s3126_r10724_p3703	1.49×10^{-1}	0.975	1.00

Table A.6: List of MC samples used to simulate the process of $W \rightarrow \tau \nu_\tau + \text{jets}$ with their cross section σ , k factor and efficiency of the generator filter $\varepsilon_{\text{filter}}$. The production tags correspond to sample productions in the MC16a, MC16d and MC16e campaigns, respectively.

$W \rightarrow \tau \nu_\tau + \text{jets}$	σ [pb]	k	$\varepsilon_{\text{filter}}$
mc16_13TeV.364184.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV0_70_CVetoBVeto Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	1.92×10^4	0.970	0.825
mc16_13TeV.364185.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV0_70_CFilterBVeto Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	1.92×10^4	0.970	0.129
mc16_13TeV.364186.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV0_70_BFilter Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	1.92×10^4	0.970	0.0446
mc16_13TeV.364187.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV70_140_CVetoBVeto Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	9.48×10^2	0.970	0.674
mc16_13TeV.364188.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV70_140_CFilterBVeto Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	9.47×10^2	0.970	0.222
mc16_13TeV.364189.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV70_140_BFilter Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	9.43×10^2	0.970	0.0839
mc16_13TeV.364190.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV140_280_CVetoBVeto Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	3.39×10^2	0.970	0.596
mc16_13TeV.364191.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV140_280_CFilterBVeto Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	3.40×10^2	0.970	0.290
mc16_13TeV.364192.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV140_280_BFilter Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	3.40×10^2	0.970	0.111
mc16_13TeV.364193.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV280_500_CVetoBVeto Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	7.21×10^1	0.970	0.546
mc16_13TeV.364194.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV280_500_CFilterBVeto Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	7.20×10^1	0.970	0.317
mc16_13TeV.364195.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV280_500_BFilter Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	7.20×10^1	0.970	0.134
mc16_13TeV.364196.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV500_1000 Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	1.50×10^1	0.970	1.00
mc16_13TeV.364197.Sherpa_221_NNP30NNLO_Wtaunu_MAXHTPTV1000_E_CMS Production tags: e5340_s3126_r9364_p3759, e5340_s3126_r1020I_p3759, e5340_s3126_r10724_p3703	1.23×10^0	0.970	1.00

Table A.7: List of MC samples used to simulate the di-boson production with their cross section σ , k factor and efficiency of the generator filter $\varepsilon_{\text{filter}}$. The production tags correspond to sample productions in the MC16a, MC16d and MC16e campaigns, respectively.

$ZZ/ZW/WW + \text{jets}$	σ [pb]	k	$\varepsilon_{\text{filter}}$
mc16_13TeV.361600.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_WWlvlv Production tags: e4616_s3126_r9364_p3759, e4616_s3126_r10201_p3759, e4616_s3126_r10724_p3703	1.06×10^1	1.00	1.00
mc16_13TeV.361601.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_WZlvll_mll4 Production tags: e4475_s3126_r9364_p3759, e4475_s3126_r10201_p3759, e4475_s3126_r10724_p3703	4.50×10^0	1.00	1.00
mc16_13TeV.361602.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_WZlvvv_mll4 Production tags: e4054_s3126_r9364_p3759, e4054_s3126_r10201_p3759, e4054_s3126_r10724_p3703	2.78×10^0	1.00	1.00
mc16_13TeV.361603.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_ZZllll_mll4 Production tags: e4475_s3126_r9364_p3759, e4475_s3126_r10201_p3759	1.27×10^0	1.00	1.00
mc16_13TeV.361604.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_ZZvvll_mll4 Production tags: e4475_s3126_r9364_p3759, e4475_s3126_r10201_p3759, e4475_s3126_r10724_p3703	9.18×10^{-1}	1.00	1.00
mc16_13TeV.361605.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_ZZvvvv_mll4 Production tags: e4054_s3126_r9364_p3759, e4054_s3126_r10201_p3759, e4054_s3126_r10724_p3703	5.49×10^{-1}	1.00	1.00
mc16_13TeV.361606.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_WWlvqq Production tags: e4711_s3126_r9364_p3759, e4711_s3126_r10201_p3759	4.42×10^1	1.00	1.00
mc16_13TeV.361607.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_WZqqll_mll20 Production tags: e4711_s3126_r9364_p3759, e4711_s3126_r10201_p3759, e4711_s3126_r10724_p3703	3.28×10^0	1.00	1.00
mc16_13TeV.361608.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_WZqqvv Production tags: e4711_s3126_r9364_p3759, e4711_s3126_r10201_p3759	5.77×10^0	1.00	1.00
mc16_13TeV.361609.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_WZlvqq_mqq20 Production tags: e4711_s3126_r9364_p3759, e4711_s3126_r10201_p3759	1.01×10^1	1.00	1.00
mc16_13TeV.361610.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_ZZqqll_mqq20mll20 Production tags: e4711_s3126_r9364_p3759, e4711_s3126_r10201_p3759, e4711_s3126_r10724_p3703	2.27×10^0	1.00	1.00
mc16_13TeV.361611.PowhegPy8EG_CT10nloME_AZNLOCTEQ6L1_ZZvvqq_mqq20 Production tags: e4711_s3126_r9364_p3759, e4711_s3126_r10201_p3759	3.94×10^0	1.00	1.00

Table A.8: List of MC samples used to simulate the production of a vector boson in association with a SM Higgs boson with their cross section σ , k factor and efficiency of the generator filter $\varepsilon_{\text{filter}}$. The production tags correspond to sample productions in the MC16a, MC16d and MC16e campaigns, respectively.

$Zh/Wh + \text{jets}$	σ [pb]	k	$\varepsilon_{\text{filter}}$
mc16_13TeV.345053.PowhegPythia8EvtGen_NNP3 NNPDF3_AZNLO_WmH125J_MINLO_lvbb_VpT Production tags: e5706_s3126_r9364_p3759, e5706_s3126_r10201_p3759, e5706_s3126_r10724_p3759	1.79×10^{-1}	0.582	1.00
mc16_13TeV.345054.PowhegPythia8EvtGen_NNP3 NNPDF3_AZNLO_WpH125J_MINLO_lvbb_VpT Production tags: e5706_s3126_r9364_p3759, e5706_s3126_r10201_p3759, e5706_s3126_r10724_p3759	2.83×10^{-1}	0.582	1.00
mc16_13TeV.345055.PowhegPythia8EvtGen_NNP3 NNPDF3_AZNLO_ZH125J_MINLO_llbb_VpT Production tags: e5706_s3126_r9364_p3759, e5706_s3126_r10201_p3759, e5706_s3126_r10724_p3759	7.70×10^{-2}	0.582	1.00
mc16_13TeV.345056.PowhegPythia8EvtGen_NNP3 NNPDF3_AZNLO_ZH125J_MINLO_vvbb_VpT Production tags: e5706_s3126_r9364_p3759, e5706_s3126_r10201_p3759, e5706_s3126_r10724_p3759	1.53×10^{-1}	0.582	1.00
mc16_13TeV.345057.PowhegPythia8EvtGen_NNP3 NNPDF3_AZNLO_ggZH125_llbb Production tags: e5706_s3126_r9364_p3759, e5706_s3126_r10201_p3759, e5706_s3126_r10724_p3759	1.24×10^{-2}	0.582	1.00
mc16_13TeV.345058.PowhegPythia8EvtGen_NNP3 NNPDF3_AZNLO_ggZH125_vvbb Production tags: e6004_s3126_r9364_p3759, e6004_s3126_r10201_p3759, e6004_s3126_r10724_p3759	2.46×10^{-2}	0.582	1.00
mc16_13TeV.345211.PowhegPy8EG_NNP3 NNPDF30_AZNLO_WmH125J_Winc_MINLO_tautau Production tags: e5808_s3126_r9364_p3759, e5808_s3126_r10201_p3759, e5808_s3126_r10724_p3759	3.34×10^{-2}	1.00	1.00
mc16_13TeV.345212.PowhegPy8EG_NNP3 NNPDF30_AZNLO_WpH125J_Winc_MINLO_tautau Production tags: e5808_s3126_r9364_p3759, e5808_s3126_r10201_p3759, e5808_s3126_r10724_p3759	5.27×10^{-2}	1.00	1.00
mc16_13TeV.345217.PowhegPy8EG_NNP3 NNPDF30_AZNLO_ZH125J_Zinc_MINLO_tautau Production tags: e5808_s3126_r9364_p3759, e5808_s3126_r10201_p3759, e5808_s3126_r10724_p3759	5.54×10^{-2}	1.00	1.00

Table A.9: List of MC samples used to simulate the production of top quarks with their cross section σ , k factor and efficiency of the generator filter $\varepsilon_{\text{filter}}$. The production tags correspond to sample productions in the MC16a, MC16d and MC16e campaigns, respectively.

Top quark production	σ [pb]	k	$\varepsilon_{\text{filter}}$
mc16_13TeV.410470.PyPy8EG_A14_ttbar_hdamp258p75_nonallhad Production tags: e6337_s3126_r9364_p3759, e6337_s3126_r10201_p3759, e6337_s3126_r10724_p3703	8.32×10^2	1.00	0.543
mc16_13TeV.410471.PyPy8EG_A14_ttbar_hdamp258p75_allhad Production tags: e6337_s3126_r9364_p3759, e6337_s3126_r10201_p3759, e6337_s3126_r10724_p3703	8.32×10^2	1.00	0.456
mc16_13TeV.410644.PowhegPythia8EvtGen_A14_singletop_schan_lept_top Production tags: e6527_s3126_r9364_p3759, e6527_s3126_r10201_p3759, e6527_s3126_r10724_p3703	2.03×10^0	1.02	1.00
mc16_13TeV.410645.PowhegPythia8EvtGen_A14_singletop_schan_lept_antitop Production tags: e6527_s3126_r9364_p3759, e6527_s3126_r10201_p3759, e6527_s3126_r10724_p3703	1.27×10^0	1.02	1.00
mc16_13TeV.410646.PowhegPythia8EvtGen_A14_Wt_DR_inclusive_top Production tags: e6552_s3126_r9364_p3759, e6552_s3126_r10201_p3759, e6552_s3126_r10724_p3703	3.79×10^1	0.945	1.00
mc16_13TeV.410647.PowhegPythia8EvtGen_A14_Wt_DR_inclusive_antitop Production tags: e6552_s3126_r9364_p3759, e6552_s3126_r10201_p3759, e6552_s3126_r10724_p3703	3.79×10^1	0.946	1.00
mc16_13TeV.410658.PyPy8EG_A14_tchan_BW50_lept_top Production tags: e6671_s3126_r9364_p3759, e6671_s3126_r10201_p3759, e6671_s3126_r10724_p3703	3.70×10^1	1.19	1.00
mc16_13TeV.410659.PyPy8EG_A14_tchan_BW50_lept_antitop Production tags: e6671_s3126_r9364_p3759, e6671_s3126_r10201_p3759, e6671_s3126_r10724_p3703	2.22×10^1	1.18	1.00

Appendix B

Statistical Analysis

This appendix provides additional details on the statistical analysis presented in Chapter 9. In Section B.1, the distributions of the test statistic $\tilde{q}_\mu$ are shown for each of the nine signal hypotheses with resonance masses from 1 TeV to 3 TeV. A ranking of the nuisance parameters based on their impact on the signal strength estimator $\hat{\mu}$ is shown in Section B.2. In Section B.3, the exclusion limits are listed, i.e., the 95% CL upper limits on the product of the cross section to produce a narrow scalar resonance, $\sigma(pp \rightarrow X)$, and its branching ratio to decay into SM Higgs bosons, $\text{BR}(X \rightarrow hh)$.

B.1 Test Statistic Distributions

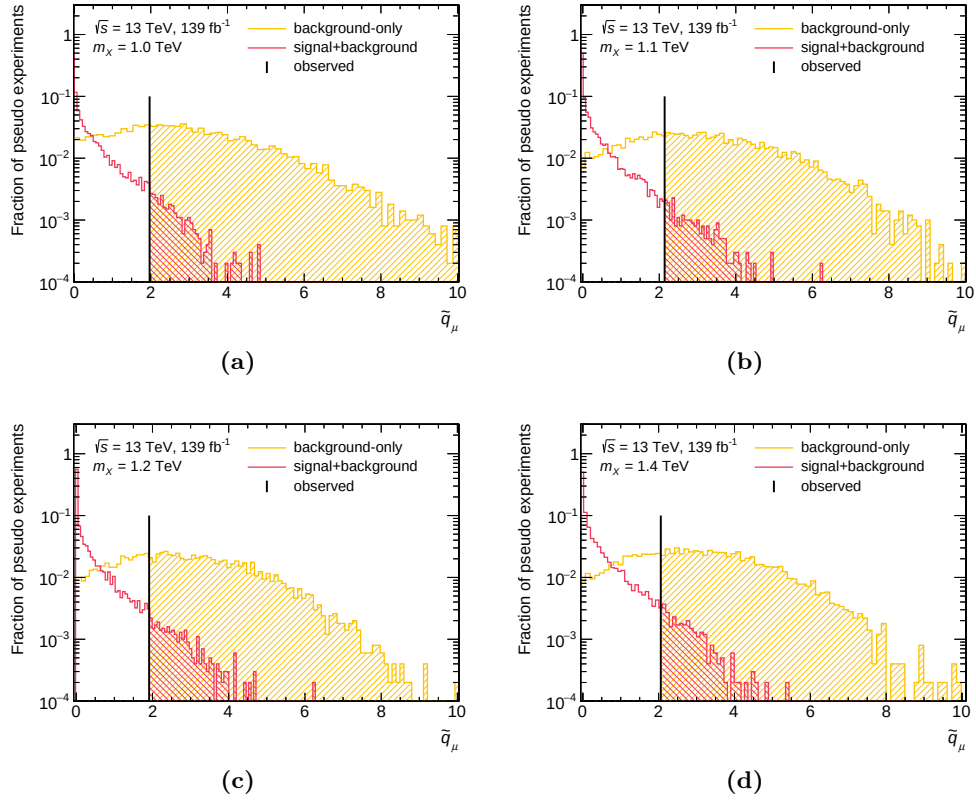


Figure B.1: Distributions of the test statistic $\tilde{q}_\mu$ for signals derived from the m_{hh}^{vis} -inclusive signal subregion. Resonance masses m_X of 1.0 TeV (a), 1.1 TeV (b), 1.2 TeV (c), and 1.4 TeV (d) are shown. A signal strength μ close to the observed exclusion limit is chosen. The yellow histogram represents the distribution for the background-only pseudo experiments, the red histogram represents the signal plus background pseudo experiments, and the black line shows the test statistic value $\tilde{q}_\mu^{\text{obs}}$ which is observed in data. The shaded areas indicate the integrals p_μ and $1 - p_b$ that are used to compute the CL_s value.

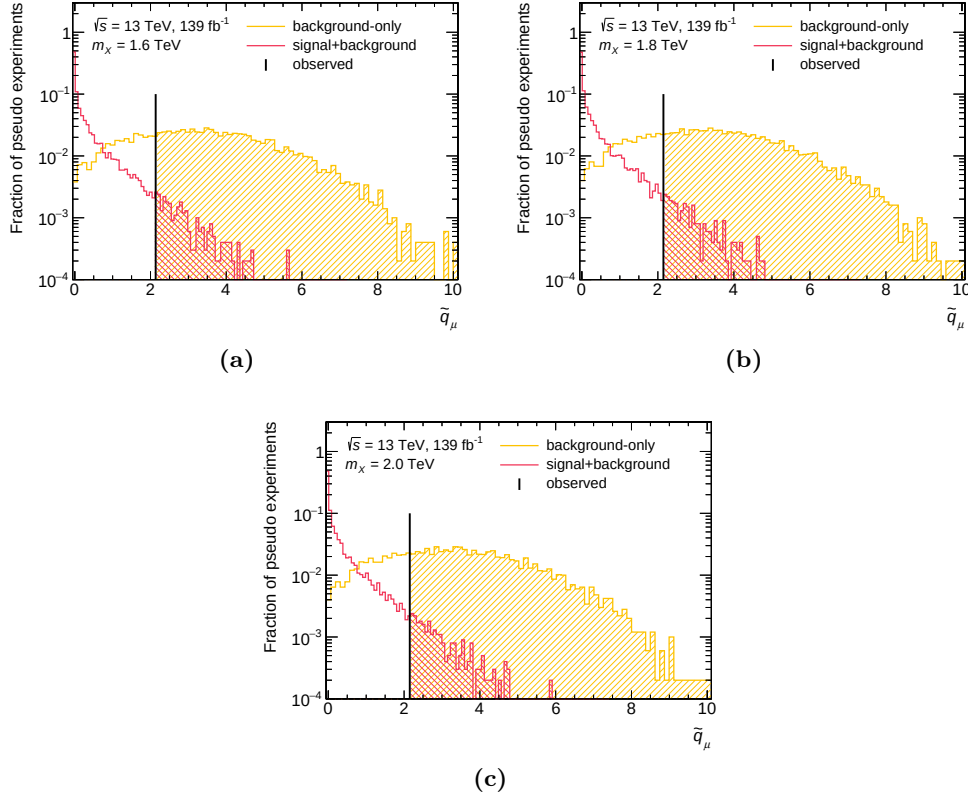


Figure B.2: Distributions of the test statistic $\tilde{q}_\mu$ for signals derived from the $m_{hh}^{\text{vis}} > 900$ GeV signal subregion. Resonance masses m_X of 1.6 TeV (a), 1.8 TeV (b), and 2.0 TeV (c) are shown. A signal strength μ close to the observed exclusion limit is chosen. The yellow histogram represents the distribution for the background-only pseudo experiments, the red histogram represents the signal plus background pseudo experiments, and the black line shows the test statistic value $\tilde{q}_\mu^{\text{obs}}$ which is observed in data. The shaded areas indicate the integrals p_μ and $1 - p_b$ that are used to compute the CL_s value.

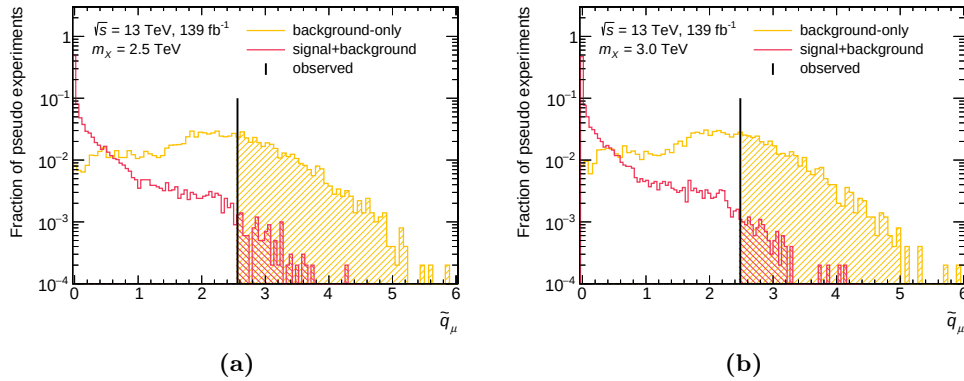


Figure B.3: Distributions of the test statistic $\tilde{q}_\mu$ for signals derived from the $m_{hh}^{\text{vis}} > 1200$ GeV signal subregion. Resonance masses m_X of 2.5 TeV (a) and 3.0 TeV (b) are shown. A signal strength μ close to the observed exclusion limit is chosen. The yellow histogram represents the distribution for the background-only pseudo experiments, the red histogram represents the signal plus background pseudo experiments, and the black line shows the test statistic value $\tilde{q}_\mu^{\text{obs}}$ which is observed in data. The shaded areas indicate the integrals p_μ and $1 - p_b$ that are used to compute the CL_s value.

B.2 Nuisance Parameter Ranking

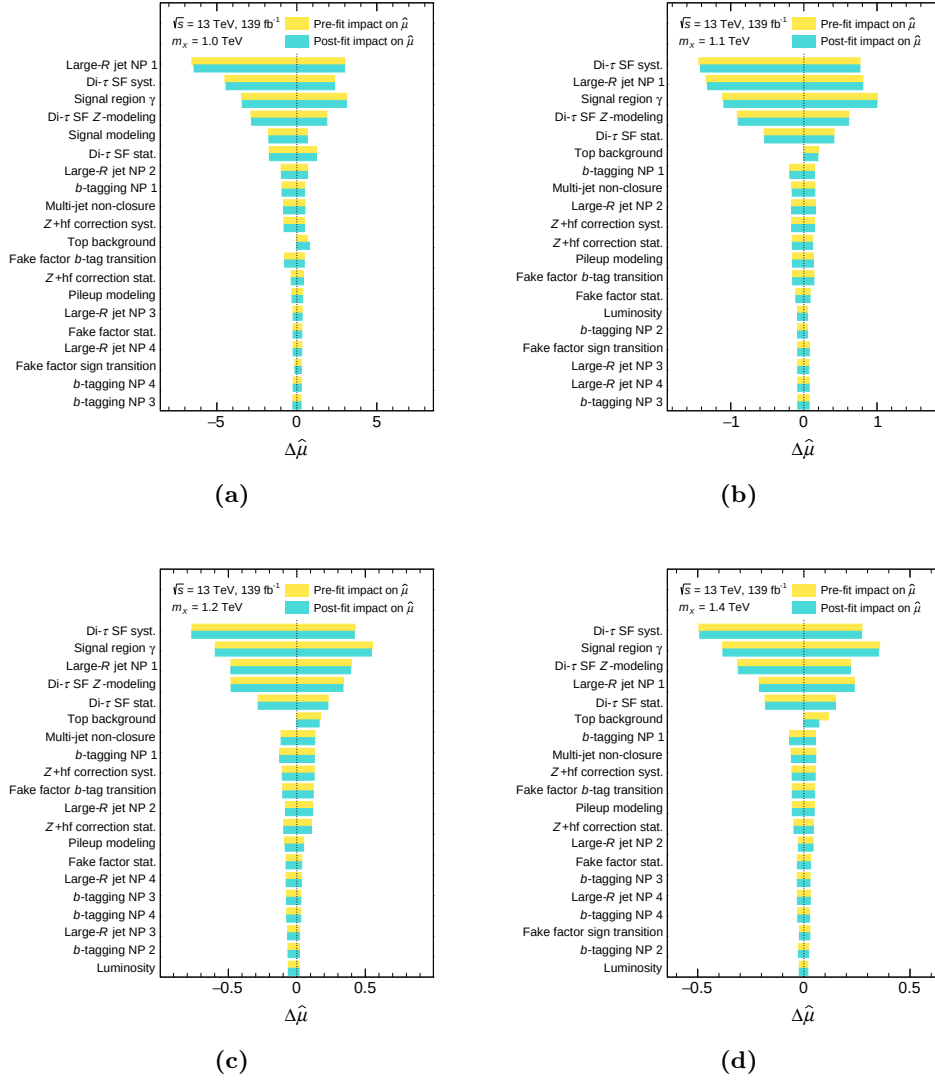


Figure B.4: Ranking of the nuisance parameters based on their impact $\Delta\hat{\mu}$ on the signal strength estimator for signals derived from the m_{hh}^{vis} -inclusive signal subregion. Resonance masses m_X of 1.0 TeV (a), 1.1 TeV (b), 1.2 TeV (c), and 1.4 TeV (d) are shown. The pre-fit and post-fit impacts are represented by the yellow and blue bars, respectively. Only the twenty highest-ranked nuisance parameters are shown.

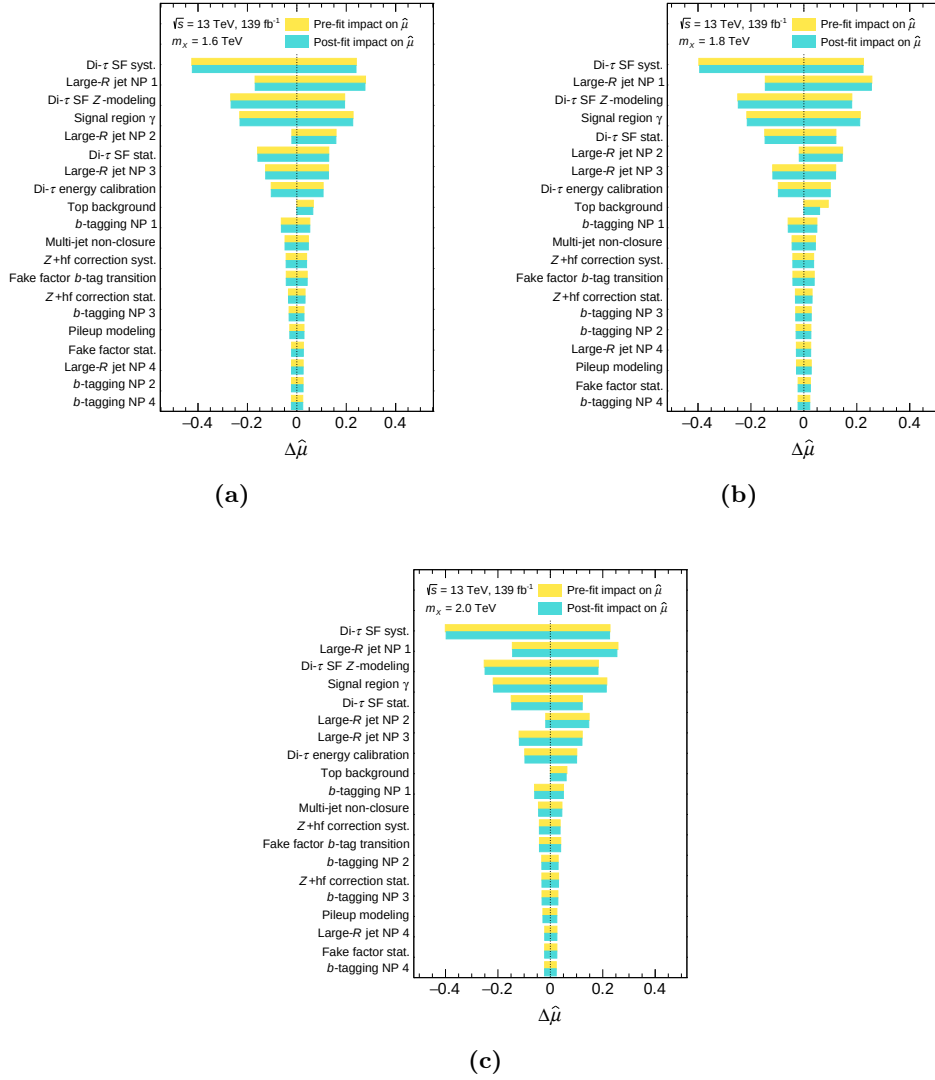


Figure B.5: Ranking of the nuisance parameters based on their impact $\Delta\hat{\mu}$ on the signal strength estimator for signals derived from the m_{hh}^{vis} -inclusive signal subregion. Resonance masses m_X of 1.6 TeV (a), 1.8 TeV (b), and 2.0 TeV (c) are shown. The pre-fit and post-fit impacts are represented by the yellow and blue bars, respectively. Only the twenty highest-ranked nuisance parameters are shown.

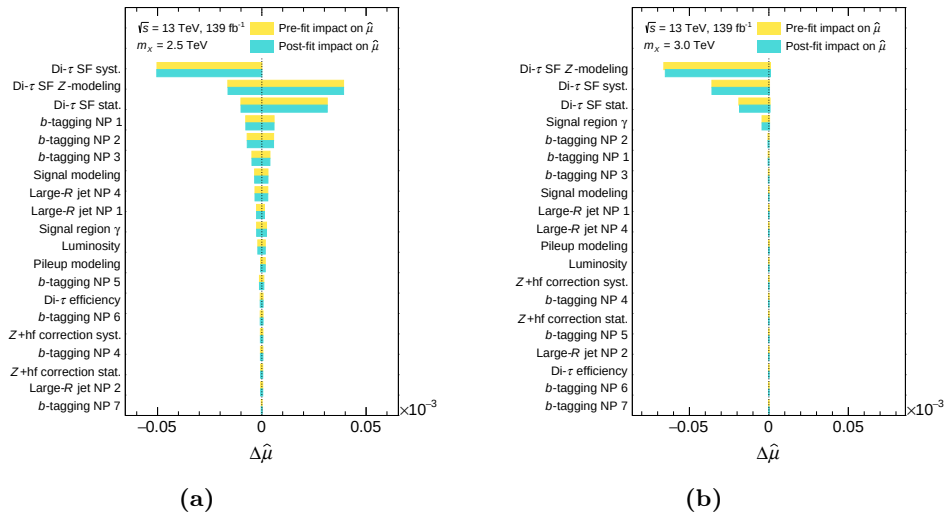


Figure B.6: Ranking of the nuisance parameters based on their impact $\Delta\hat{\mu}$ on the signal strength estimator for signals derived from the m_{hh}^{vis} -inclusive signal subregion. Resonance masses m_X of 2.5 TeV (a) and 3.0 TeV (b) are shown. The pre-fit and post-fit impacts are represented by the yellow and blue bars, respectively. Only the twenty highest-ranked nuisance parameters are shown.

B.3 Exclusion Limit Table

Table B.1: Expected and observed 95% CL upper limits on the product of the cross section to produce a narrow scalar resonance, $\sigma(pp \rightarrow X)$, and its branching ratio to decay into SM Higgs bosons, $\text{BR}(X \rightarrow hh)$, for each resonance mass m_X . SM branching ratios are assumed for the decays of the SM Higgs bosons into a pair of b quarks and a pair of hadronically decaying τ leptons. The $\pm 1\sigma$ and $\pm 2\sigma$ variations of the expected limit are given.

m_X [TeV]	Observed [fb]	Expected [fb]	-2σ [fb]	-1σ [fb]	$+1\sigma$ [fb]	$+2\sigma$ [fb]
1.0	858	606	289	390	1299	2978
1.1	197	146	65	100	262	497
1.2	95	77	37	51	124	223
1.4	60	47	26	32	74	130
1.6	53	38	21	27	61	102
1.8	50	36	20	25	56	96
2.0	50	36	20	26	57	97
2.5	27	31	19	24	46	81
3.0	45	53	32	41	79	134

List of Figures

2.1	Elementary particles in the Standard Model	4
2.2	Feynman diagrams for the production of two Higgs bosons	8
2.3	Branching ratios of H in the $M_{h,\text{EFT}}^{125}$ benchmark scenario	16
2.4	Branching ratios of h in the $M_{h,\text{EFT}}^{125}$ benchmark scenario	17
2.5	Parameter space of the hMSSM approximation	18
2.6	Parameter space of the $M_{h,\text{EFT}}^{125}$ benchmark scenario	18
2.7	Feynman diagrams for the two BSM signal processes	23
3.1	Schematic illustration of the CERN accelerator complex.	26
3.2	Schematic representation of the ATLAS Detector and its subsystems	28
3.3	Schematic representation of the barrel region of the ATLAS inner detector .	29
3.4	Schematic representation of the ATLAS calorimeter system	31
3.5	Schematic representation of the ATLAS muon spectrometer	33
3.6	Integrated luminosity versus time of data taking	35
3.7	Distribution of the mean number of interactions per bunch crossing	36
4.1	Illustration of the anti- k_t algorithm	39
5.1	$\Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}})$ distribution for resonance masses from 1 TeV to 3 TeV . . .	47
5.2	Schematic representation of a reconstructed di- τ object.	48
5.3	Reconstruction efficiency as a function of $\Delta R(\tau_{1,\text{vis}}, \tau_{2,\text{vis}})$	50
5.4	Reconstruction efficiency as a function of $p_{T,\text{vis}}$ and μ	51
5.5	Energy accuracy as a function of $p_{T,\text{vis}}$ and η_{vis}	52
5.6	Energy resolution as a function of $p_{T,\text{vis}}$ and η_{vis}	53
5.7	Distribution of the reconstructed di- τ p_T in signal and background	55
5.8	Identification variables $E_{\Delta R < 0.1}^{\text{sj}_1}/E_{\Delta R < 0.2}^{\text{sj}_1}$ and $E_{\Delta R < 0.1}^{\text{sj}_2}/E_{\Delta R < 0.2}^{\text{sj}_2}$	55
5.9	Identification variables $(p_T^{\text{sj}_1} + p_T^{\text{sj}_2})/p_T^{\text{seed}}$ and $p_T^{\text{sj}_2}/p_T^{\text{seed}}$	57
5.10	Identification variables $n_{\text{tracks}}^{\text{subjects}}$ and $n_{\text{tracks}}^{\text{sj}_1}$	57
5.11	Identification variables $m_{\Delta R < 0.1}^{\text{tracks, sj}_1}$ and $m_{\Delta R < 0.1}^{\text{tracks, sj}_2}$	58
5.12	Identification variables $m_{\Delta R < 0.2}^{\text{tracks, sj}_1}$ and $m_{\Delta R < 0.2}^{\text{tracks, sj}_2}$	58
5.13	Identification variables $\Delta R_{\text{max}}(\text{track, sj}_1)$ and $\Delta R_{\text{max}}(\text{track, sj}_2)$	59
5.14	Identification variable $\sum(p_T^{\text{track}} \Delta R(\text{track, sj}_2))/\sum p_T^{\text{track}}$	59
5.15	Identification variable $\sum(p_T^{\text{iso-track}} \Delta R(\text{iso-track, sj}))/\sum p_T^{\text{iso-track}}$	60
5.16	Identification variable $\sum p_T^{\text{iso-tracks}}/p_T^{\text{seed}}$	60

5.17	Identification variables $d_{0,\text{lead-track}}^{\text{sj1}}$ and $d_{0,\text{lead-track}}^{\text{sj2}}$	61
5.18	BDT discriminant score for signal and background	62
5.19	Inverse background efficiency as a function of signal identification efficiency.	63
5.20	Di- τ identification efficiency as a function of $p_{\text{T,vis}}$ and μ	63
5.21	Di- τ identification efficiency in background as a function of $p_{\text{T,vis}}$ and μ	64
5.22	Efficiency of tight track-multiplicity cut as a function of $p_{\text{T,vis}}$ and μ	65
7.1	BDT discriminant score for quark- and gluon-initiated jet background	80
7.2	Fake factors in ‘FF SS 0- b -tag’ region as a function of di- τ p_{T}	80
7.3	Fake factors used to estimate sign- and b -tag-transition uncertainties	81
7.4	Event distributions in ‘MJ 0- b -tag’ and ‘MJ 1- b -tag’ validation regions	83
7.5	$p_{\text{T},\ell\ell}$ distributions in ‘ $Z + \text{hf}$ ’ control region	84
8.1	Di- τ p_{T} and mass distributions in ‘ Z 0- b -tag’ region	88
8.2	Event distributions in ‘ Z 0- b -tag’ and ‘ Z 1- b -tag’ regions	90
9.1	Signal acceptance times efficiency as a function of m_X	94
9.2	Distributions of m_{J} and m_{hh}^{vis} in the signal region	95
9.3	Event distribution of m_{hh}^{vis} in the signal region.	96
9.4	Event displays of two observed events in the signal region	97
9.5	Polynomial interpolation and exponential extrapolation scheme	103
9.6	Distributions of the test statistic for the $m_X = 1.8$ TeV signal	105
9.7	Ranking of nuisance parameters for 1.2 TeV, 1.8 TeV, and 2.5 TeV signals	107
9.8	Expected and observed 95% CL upper limits	109
9.9	95% CL upper limits in conjunction with resolved final state analysis	110
B.1	Distributions of the test statistic in the m_{hh}^{vis} -inclusive signal subregion	128
B.2	Distributions of the test statistic in the $m_{hh}^{\text{vis}} > 900$ GeV signal subregion	129
B.3	Distributions of the test statistic in the $m_{hh}^{\text{vis}} > 1200$ GeV signal subregion	129
B.4	Ranking of nuisance parameters in the m_{hh}^{vis} -inclusive signal subregion	130
B.5	Ranking of nuisance parameters in the $m_{hh}^{\text{vis}} > 900$ GeV signal subregion	131
B.6	Ranking of nuisance parameters in the $m_{hh}^{\text{vis}} > 1200$ GeV signal subregion	132

List of Tables

2.1	Branching ratios of the decay of a pair of Higgs bosons	9
5.1	Formulas and descriptions of the variables used in the di- τ identification.	56
5.2	Selection uncertainties from simulation variations	67
5.3	Energy response uncertainties from simulation variations	68
6.1	Overlap removal criteria	70
6.2	Trigger requirements and their contributions to total event count	71
6.3	Event selection regions and their respective usages	73
7.1	Event yields in the ‘ $Z + \text{hf}$ ’ control region	84
8.1	Event yields in the ‘ Z 0- b -tag’ control region	89
8.2	Z -modeling uncertainties of the di- τ normalization correction	91
8.3	Systematic uncertainties of the di- τ normalization correction	92
9.1	Event yields in the signal region	96
9.2	Systematic uncertainties on the expected background in the signal region	97
9.3	Uncertainties of the signal acceptance times efficiency	99
A.1	Good Run Lists and integrated luminosities	118
A.2	List of $X \rightarrow hh \rightarrow b\bar{b}\tau^+\tau^-$ MC samples	119
A.3	List of $G \rightarrow hh \rightarrow \tau^+\tau^-\tau^+\tau^-$ MC samples	120
A.4	List of $Z/\gamma^* \rightarrow \tau^+\tau^- + \text{jets}$ MC samples	121
A.5	List of $Z/\gamma^* \rightarrow e^+e^- + \text{jets}$ MC samples	122
A.6	List of $W \rightarrow \tau\nu_\tau + \text{jets}$ MC samples	123
A.7	List of di-boson MC samples	124
A.8	List of Zh and Wh MC samples	125
A.9	List of top quark MC samples	126
B.1	Expected and observed 95% CL upper limits	133

List of Abbreviations

2HDM		Two-Higgs-doublet model
ADD		Arkani-Hamed, Dimopoulos, and Dvali
ATLAS		A Toroidal LHC Apparatus
BDT		Boosted decision trees
CERN		European Organization for Nuclear Research
CL		Confidence level
CMS		Compact Muon Solenoid
BEH		Brout–Englert–Higgs mechanism
FF		Fake factor
hf		Heavy flavor
HLT		High-Level Trigger
IBL		Insertable B-Layer
KK		Kaluza and Klein
L1		Level-1 trigger
lf		Light flavor
LHC		Large Hadron Collider
LO		Leading order
LUCID2		Luminosity Cherenkov Integrating Detector
MC		Monte Carlo
MJ		Multi-jet background
MSSM		Minimal Supersymmetric Standard Model
NLO		Next-to-leading order
NMSSM		Next-to-Minimal Supersymmetric Standard Model
NNLO		Next-to-next-to-leading order
NN		Neural network
OS		Opposite sign

PDF		Parton distribution function
QCD		Quantum chromodynamics
QED		Quantum electrodynamics
QFD		Quantum flavordynamics
RNN		Recurrent neural network
RS		Randall and Sundrum
SCT		Semiconductor tracker
SF		Scale factor
SM		Standard Model of particle physics
SS		Same sign
SUSY		Supersymmetry
TMVA		Toolkit for Multivariate Data Analysis
TRT		Transition radiation tracker

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