



上海交通大学博士学位论文

在 ATLAS 实验上基于矢量玻色子散射和融合
过程的电弱与希格斯玻色子末态检验标准模
型和寻找新物理

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**TEST OF STANDARD MODEL AND SEARCH FOR
NEW PHYSICS WITH VECTOR BOSON
SCATTERING AND FUSION PROCESSES IN
ELECTROWEAK BOSON AND DI-HIGGS FINAL
STATES AT ATLAS**

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摘 要

这篇论文在粒子物理领域的三个方面做出了探索, 分别是标准模型 (SM) 物理的精确检验, 超出标准模型的新物理寻找以及探索在下一代未来轻子对撞机上探索新物理的可能性。本论文的第一部分报告了在 ATLAS 实验上对于电弱产生的 W 玻色子和光子与两个强子喷注过程的寻找。这是 ATLAS 合作组首次观测到了电弱 $W\gamma jj$ 过程。这个物理过程检验了标准模型中电弱规范对称性破缺机制。本分析使用了 ATLAS 收集到的 140fb^{-1} 积分亮度的数据, 观测到的统计显著度超过了 6 倍标准偏差, 非常接近理论预期的结果。微分截面的测量结果也与标准模型预测的非常吻合, 并且对敏感的新物理做出了约束。第二部分是利用 ATLAS 探测器 140fb^{-1} 积分亮度的数据寻找矢量玻色子融合过程产生的希格斯玻色子对过程, 本分析寻找了洛伦兹加速框架下的底夸克对产生过程, 借助了希格斯衰变道中拥有最大分支比的底夸克对末态, 研究结果把耦合系数 κ_{2V} 在 95% 置信度下限制到了 0.55 到 1.49 之间, 以 3.8 倍标准偏差的统计显著度排除了 $\kappa_{2V} = 0$ 的可能性。本项工作还对新的零自旋共振态粒子做出了寻找, 结果显示没有显著的新物理出现。第三部分是在未来轻子对撞机上的研究, 这部分研究探讨了在环形正负电子对撞机 (CEPC) 上对反常希格斯衰变物理的寻找的可能性, 这个过程是由一个轻的标量玻色子引起的强一阶电弱相变过程。这个研究同样寻找了希格斯玻色子衰变到了底夸克对的末态, 假设标量粒子的质量从 15GeV 到 60GeV , 这项研究利用了 CEPC 上产生的模拟数据, 对反常衰变的希格斯物理作用截面做出了寻找, 并且给出了作用截面的理论上限, 其模拟结果显著好于在大型强子对撞机上的实验结果。这些研究从标准模型内的物理出发, 延伸到对标准模型外新物理的寻找, 并且从现有的大型强子对撞机出发延伸到了未来的轻子对撞机。从不同角度, 不同层面对现有的标准模型做出检验同时对新物理做出了寻找以及展望。

关键词: 高能物理, 对撞机, 电弱, 标准模型, 超出标准模型新物理, 机器学习

ABSTRACT

This dissertation explores three pivotal aspects of particle physics, examining electroweak interactions within the Standard Model(SM) theory, search for new physics beyond the SM, and chances for new physics search in future lepton colliders.

First, we report the observation of electroweak production of a W boson and a photon in association with two jets, using pp collision data from the ATLAS experiment at the LHC with a center of mass energy of $\sqrt{s} = 13$ TeV. This is the first observation by the ATLAS experiment. The process tests the electroweak gauge symmetry breaking mechanism of the Standard Model. With an integrated luminosity of 140 fb^{-1} , the observed significance exceeds six standard deviations, closely matching the expected significance. Measurements of fiducial and differential cross sections align well with Standard Model predictions, and constraints on new physics effects are derived.

Second, a search for Higgs boson pair production via vector-boson fusion was conducted in the Lorentz-boosted regime using 140 fb^{-1} of data. Focusing on Higgs decays into bottom quark pairs, the study constrains the quartic coupling κ_{2V} to $0.55 < \kappa_{2V} < 1.49$ at 95% confidence level, excluding $\kappa_{2V} = 0$ with a significance of 3.8 standard deviations. Additionally, limits on new heavy spin-0 resonances mediating Higgs pair production were established, showing no significant deviations from the Standard Model.

Third, this thesis investigates a strong first-order electroweak phase transition driven by a light scalar s with a mass between 15 and 60 GeV. The study involves a search for exotic Higgs decays into a pair of spin-zero particles ($h \rightarrow ss$), with each s -boson decaying into b -quarks. Using simulated data from the CEPC, the analysis sets upper limits on the cross-section times branching ratio for $h \rightarrow ss$, with sensitivity significantly higher than achievable at the LHC.

These studies provide crucial insights into electroweak interactions, search for new physics beyond the SM, and potential new physics with future lepton colliders, offering stringent tests and constraints that advance our understanding of fundamental forces.

Key words: High Energy Physics, Collider, Electroweak, Standard Model, BSM Physics, Machine learning

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Chapter 1 Elementary Particle Physics

1.1 The Standard Model Theory

Physics studies matters in the universe and how they interact with one another through space and time. Particle physics is the subject of study that deals with the nature and interactions of elementary particles. The goal of particle physics is to understand the nature behind the fundamental constituents of matter and to explain how the universe we live in was formed.

In 1897, J. Thomson made the groundbreaking discovery of electrons within the cathode ray^[1]. Subsequently, over the following decades, scientists unveiled additional subatomic particles, including photons and protons. The early 1900s marked the establishment and progressive development of the theories of Relativity and Quantum Mechanics. Furthermore, Quantum Field Theory (QFT) emerged as a potent tool, widely employed to investigate diverse particles and their interactions.

Subsequently, a succession of theories was developed to systematically classify all recognized elementary particles and elucidate three of the four fundamental interactions prevalent in the universe, namely the electromagnetic, weak, and strong interactions, with gravity being the exception. This culmination resulted in the establishment of the Standard Model (SM) in Particle Physics. The formulation of the Standard Model reached its finalized state in the 1970s following experimental validation of the existence of quarks.

The theoretical framework of the Standard Model (SM) classifies elementary particles into two primary categories: fermions and bosons, each playing distinct roles in the cosmos, as illustrated in Figure 1–1.

Fermions, constituting the fundamental building blocks of matter, adhere to the Pauli Exclusion Principle, which dictates that they cannot simultaneously occupy identical quantum states. Characterized by half-integer spins, fermions are further divided into two classes: quarks and leptons.

- **Quarks:** There are six distinct flavors of quarks—up, down, charm, strange, top, and bottom. The up, charm, and top quarks carry a fractional electric charge of $+2/3$, while the down, strange, and bottom quarks carry a fractional charge of $-1/3$. Quarks

exhibit a unique feature in that they interact via all three fundamental non-gravitational forces: strong, weak, and electromagnetic. Additionally, quarks possess an intrinsic property known as 'color charge', which governs their interaction through the strong force. Each quark flavor is associated with three color charges (and their corresponding three opposite charges).

- **Leptons:** Similar to quarks, leptons are also categorized into six types distributed across three generations: electron, muon, tau particles, and their corresponding neutrinos. The electron, muon, and tau each carry a unit negative charge and interact through the weak and electromagnetic forces. Neutrinos, being neutral, participate solely in weak interactions.

In contrast, bosons function as force mediators and possess integer spins, enabling them to occupy the same quantum state. The Standard Model recognizes several bosons, each with specific roles in fundamental interactions:

- **Photon:** Serving as the force carrier for the electromagnetic force, the photon governs interactions between electrically charged particles. It is a massless particle that propagates at the speed of light.
- **W and Z bosons:** These bosons act as mediators for the weak nuclear force, which regulates certain types of nuclear decay, such as beta decay. The W bosons carry a unit positive or negative charge, while the Z boson is electrically neutral. The substantial masses of W and Z bosons contribute to the short-range nature of the weak force.
- **Gluons:** Responsible for mediating the strong nuclear force, gluons play a crucial role in binding quarks within protons, neutrons, and other hadronic particles. Gluons carry a color charge, allowing them to interact among themselves.
- **Higgs boson:** Associated with the Higgs field, the Higgs boson is a key element of the Brout-Englert-Higgs mechanism, providing an explanation for the unique "Yukawa" interaction^[2] through which particles acquire mass.

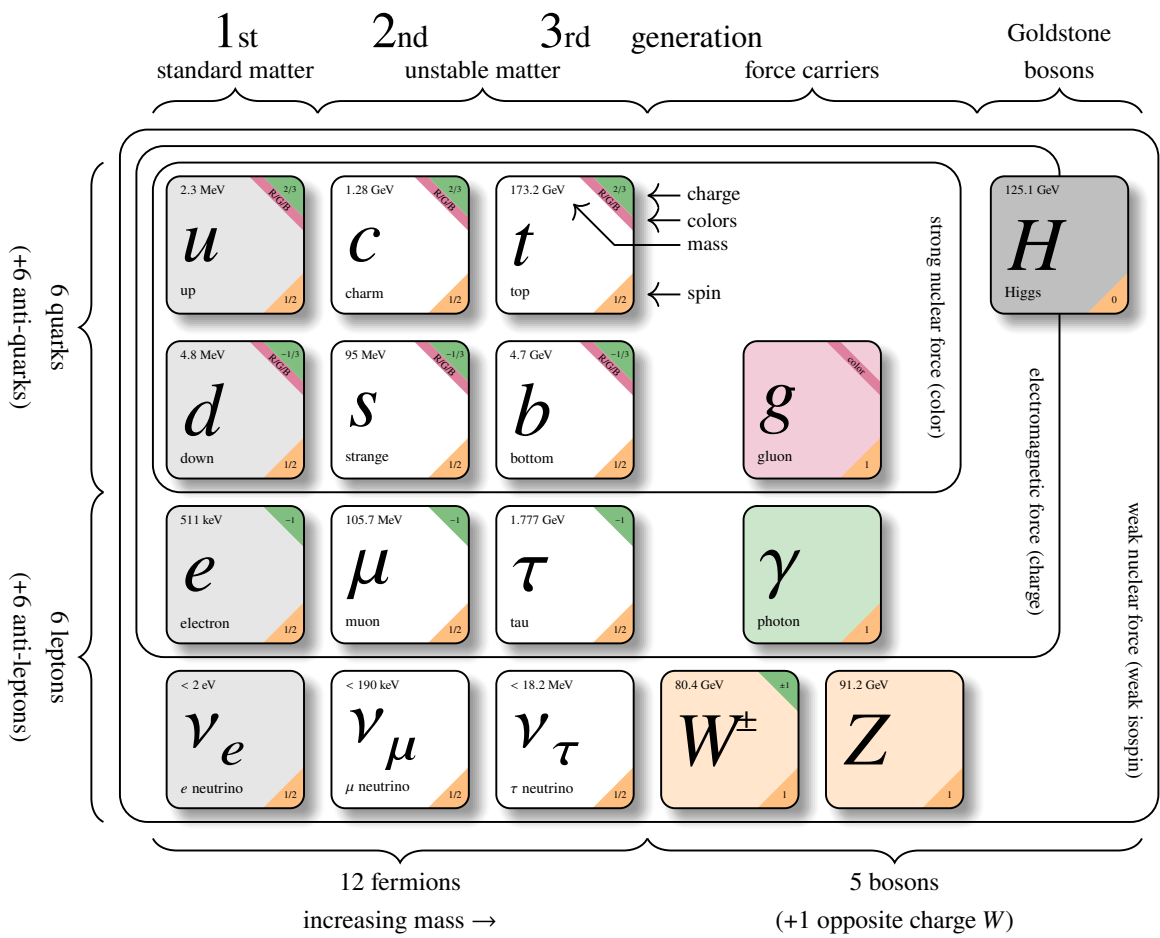


Figure 1–1 The properties of elementary particles in the Standard Model.

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} \quad (1-1)$$

$$+ i\bar{\Psi}\not{D}\Psi + \text{h.c.} \quad (1-2)$$

$$+ \Psi_i y_{ij} \Psi_j \phi + \text{h.c.} \quad (1-3)$$

$$+ |D_\mu \phi|^2 - V(\phi) \quad (1-4)$$

$$(1-5)$$

The mathematical formulation of the Standard Model is complex. Interactions and other information is encoded in the Lagrangian of SM theory, which could be briefly described as Equation 1-1. The first term $-\frac{1}{4}F^{\mu\nu}F_{\mu\nu}$ encodes all interaction particles except the Higgs boson. μ and ν are Lorentz indices representing the spacetime components. The second term $i\bar{\Psi}\not{D}\Psi$ describes the interactions between force carriers and matter particles. The field Ψ stands for fermions like quarks and leptons. This term includes three of the fundamental interactions (electromagnetic, weak and strong) despite the fact that those interactions are different. The third term $\Psi_i y_{ij} \Psi_j \phi$ that includes the Higgs boson field ϕ describes the interactions among matter particles and the Higgs boson. Yukawa matrix y_{ij} shows the coupling parameters to the Higgs field which is responsible for the mass of these particles. The last two terms $|D_\mu \phi|^2 - V(\phi)$ describes how the force carriers interact to the Higgs field and the Higgs potential.

1.2 Electroweak Theory and Spontaneous Symmetry Breaking

1.2.1 Abelian Higgs model

Before the discovery of the Higgs boson in 2012^[3-4], the Standard Model (SM) of particle physics had not been fully realized. Given that the measured masses of the W and Z bosons are substantial and nonzero^[5-6], we focus on a $U(1)$ gauge theory described by its Lagrangian

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} \quad (1-6)$$

$$(1-7)$$

the term of $F_{\mu\nu} = \partial_\nu A_\mu - \partial_\mu A_\nu$ is the strength tensor of the gauge field A_μ . The statement of local $U(1)$ gauge invariance guarantees that the Lagrangian is invariant under the transfor-

mation such as $A_\mu(x) \rightarrow A_\mu(x) - \partial_\mu \eta(x)$ for any η and x .

If one extends the model by adding a single complex scalar field with couples to the photon with charge $-e$. The lagrangian is then written as

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + |D_\mu\phi|^2 - V(\phi) \quad (1-8)$$

$$(1-9)$$

where $D_\mu = \partial_\mu - ieA_\mu$ is the covariant derivative, and $V(\phi) = \mu^2|\phi|^2 + \lambda(|\phi|^2)^2$ is the potential of the scalar field ϕ . The potential $V(\phi)$ is now permissible under the constraints of $U(1)$ gauge invariance and can also be renormalized

This Lagrangian is invariant under both global $U(1)$ rotations and local gauge transformations:

$$\phi \rightarrow e^{i\theta}\phi \quad (1-10)$$

$$A_\mu(x) \rightarrow A_\mu(x) - \partial_\mu \eta(x) \quad (1-11)$$

$$\phi(x) \rightarrow e^{-ie\eta(x)}\phi(x) \quad (1-12)$$

$$(1-13)$$

The first transformation is the global $U(1)$ rotation, and the last two transformations are local gauge transformations.

Now there are two cases for the potential, $\mu^2 > 0$ and $\mu^2 < 0$ as shown in figure1-2. In the first case where $\mu^2 > 0$, the potential shows symmetries of the Lagrangian, the states reaches its lowest energy at the point where $\phi = 0$ which is also named the vacuum state. This model is simply quantum electrodynamics with a massless photon and a charged scalar field ϕ with mass μ .

The $\mu^2 < 0$ case potential is usually called a Mexican Hat potential, $\phi = 0$ is not the global minimum anymore, and the field is not stable. The potential of this special occasion could be written as

$$V(\phi) = -|\mu^2||\phi|^2 + \lambda(|\phi|^2)^2, \quad (1-14)$$

and the minimum energy of the state is given when $\langle \phi \rangle = \sqrt{(-\frac{\mu^2}{2\lambda})}$, $\langle \phi \rangle$ stands for the vacuum expectation value (VEV) of ϕ . The direction of the field is arbitrary for people to choose but we conventionally choose the direction of ϕ to be on the real axis. Of course,

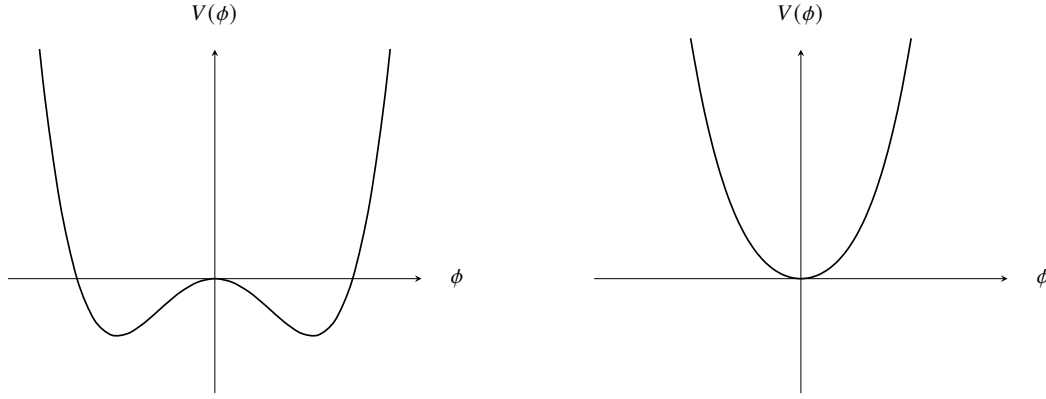


Figure 1-2 The potential of the Higgs field at the cases of $\mu^2 < 0$ (left) and $\mu^2 > 0$ (right).

there is another situation where $\lambda < 0$. However, this case would result in an unstable state of the Higgs field. The negative λ leads to a potential that the physics state would spontaneously move away from the state near the origin. So in this case, the Higgs field would be unstable. ϕ could be rewritten as

$$\phi \equiv \frac{1}{\sqrt{2}} e^{i\frac{\chi}{v}} (\nu + h). \quad (1-15)$$

In this equation 1-15, χ and h are real fields which have no VEVs. We can have another writing format of Lagrangian if we substitute back with this equation. One can have the Lagrangian like the following:

$$\mathcal{L} = -\frac{1}{4} F^{\mu\nu} F_{\mu\nu} - e\nu A_\nu \partial^\mu \chi + \frac{e^2 \nu^2}{2} A_\mu A^\mu \quad (1-16)$$

$$+ \frac{1}{2} (\partial_\mu h \partial^\mu h + 2\mu^2 h^2) + \frac{1}{2} \partial_\mu \chi \partial^\mu \chi \quad (1-17)$$

$$+ (h, \chi \text{ interactions}). \quad (1-18)$$

$$(1-19)$$

Now this equation describes a model with a photon of mass $M_A = e\nu$, a scalar field h with mass-squared $-2\mu^2 > 0$, and a massless scalar field χ . It is not difficult to find out that if one transform the field A_μ as $A'_\mu \equiv A_\mu - \frac{1}{e\nu} \partial_\mu \chi$. The term $-e\nu A_\nu \partial^\mu \chi$ and $\frac{1}{2} \partial_\mu \chi \partial^\mu \chi$ would be absorbed into the term of $\frac{e^2 \nu^2}{2} A_\mu A^\mu$ which ends up giving photon mass. This is what we call as the Higgs mechanism and the χ field is often called Goldstone boson.

The Higgs mechanism can be summarized by saying that the spontaneous breaking of a gauge theory by a non-zero VEV results in the disappearance of a Goldstone boson and its transformation into the longitudinal component of a massive gauge boson.

1.2.2 Weinberg-Salam Model

Accessing the conventional Weinberg-Salam model for electroweak interactions is straightforward^[7-8]. This model is based on the gauge group $SU(2)_L \times U(1)_Y$. It includes three gauge bosons associated with $SU(2)_L$, denoted as W_μ^i (where $i = 1, 2, 3$), and one gauge boson for $U(1)_Y$, represented as B_μ . The kinetic energy terms for these gauge bosons in the Lagrangian are given by:

$$\mathcal{L}_{KE} = -\frac{1}{4}W_{\mu\nu}^i W^{\mu\nu i} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} \quad (1-20)$$

where the field strength tensors are defined as:

For the $SU(2)_L$ gauge bosons:

$$W_{\mu\nu}^i = \partial_\nu W_\mu^i - \partial_\mu W_\nu^i + g\epsilon^{ijk}W_\mu^j W_\nu^k, \quad (1-21)$$

And for the $U(1)_Y$ gauge boson:

$$B_{\mu\nu} = \partial_\nu B_\mu - \partial_\mu B_\nu. \quad (1-22)$$

The model also features a complex scalar $SU(2)$ doublet, Φ , which is crucial for the mechanism of symmetry breaking:

$$\Phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}, \quad (1-23)$$

The dynamics of this scalar doublet are governed by the scalar potential:

$$V(\Phi) = \mu^2 |\Phi^\dagger \Phi| + \lambda \left(|\Phi^\dagger \Phi| \right)^2, \quad (1-24)$$

where $\lambda > 0$. This potential is the most general form that is both renormalizable and invariant under $SU(2)_L$ transformations, which is essential for the model's stability and predictive power.

In the context of the Abelian model discussed in Section 1.2.1, for the case where $\mu^2 < 0$, the state of minimum energy is not found at $\Phi = 0$. Instead, the scalar field develops a vacuum expectation value (VEV), indicating spontaneous symmetry breaking. The direction of the

minimum in the $SU(2)_L$ space is indeterminate because the potential depends only on the combination $\Phi^\dagger \Phi$. To simplify, we arbitrarily choose the VEV of Φ as follows:

$$\langle \Phi \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix}, \quad (1-25)$$

where v signifies the magnitude of the VEV. This selection implies that the scalar doublet Φ has a $U(1)_Y$ charge (hypercharge) $Y_\Phi = 1$. The electromagnetic charge, denoted by Q , is defined as:

$$Q = \frac{(\tau_3 + Y)}{2}, \quad (1-26)$$

where τ_3 represents the third component of the weak isospin, and Y is the hypercharge. Consequently, it follows that:

$$Q \langle \Phi \rangle = 0, \quad (1-27)$$

showing that electromagnetism remains unbroken by the scalar VEV. This choice for the VEV of Φ results in the desired symmetry breaking pattern:

$$SU(2)_L \times U(1)_Y \rightarrow U(1)_{EM}, \quad (1-28)$$

where $U(1)_{EM}$ denotes the unbroken electromagnetic symmetry. This mechanism of symmetry breaking is a cornerstone of the Higgs mechanism in the Weinberg-Salam model, elucidating how particles acquire mass while preserving the gauge symmetry of electromagnetism.

Following the framework established in the Abelian Higgs model, as outlined in Section 1.2.1, we can similarly derive how the Higgs mechanism gives masses to the W and Z gauge bosons. This process is described by the contribution of the scalar doublet to the Lagrangian:

$$\mathcal{L}_s = (D^\mu \Phi)^\dagger (D_\mu \Phi) - V(\Phi), \quad (1-29)$$

where the covariant derivative D_μ is defined as:

$$D_\mu = \partial_\mu + i \frac{g}{2} \tau \cdot W_\mu + i \frac{g'}{2} B_\mu Y. \quad (1-30)$$

In the unitary gauge, Goldstone bosons are absent, leaving only the physical Higgs scalar in the spectrum after spontaneous symmetry breaking has occurred. Hence, the scalar doublet in the unitary gauge can be expressed as:

$$\Phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h \end{pmatrix}, \quad (1-31)$$

This setup leads to the gauge boson mass terms derived from the scalar kinetic energy term:

$$\frac{1}{2} (0, v) \left(\frac{1}{2} g \tau \cdot W_\mu + \frac{1}{2} g' B_\mu \right)^2 \begin{pmatrix} 0 \\ v \end{pmatrix}. \quad (1-32)$$

This framework demonstrates how spontaneous symmetry breaking, facilitated by the Higgs field's vacuum expectation value (VEV), generates masses for the W and Z bosons, analogous to the mechanism for photon mass generation in the Abelian Higgs model.

The physical gauge fields are delineated as two charged fields, $W^\pm$, and two neutral gauge bosons, Z and γ . Their formulations are as follows:

$$\begin{aligned} W_\mu^\pm &= \frac{1}{\sqrt{2}} (W_\mu^1 \mp i W_\mu^2), \\ Z^\mu &= \frac{-g' B_\mu + g W_\mu^3}{\sqrt{g^2 + g'^2}}, \\ A^\mu &= \frac{g B_\mu + g' W_\mu^3}{\sqrt{g^2 + g'^2}}. \end{aligned}$$

From the Higgs mechanism, the gauge bosons acquire masses as follows:

$$\begin{aligned} M_W^2 &= \frac{1}{4} g^2 v^2, \\ M_Z^2 &= \frac{1}{4} (g^2 + g'^2) v^2, \\ M_A &= 0. \end{aligned}$$

The existence of the massless photon, which couples with electromagnetic strength e , allows for the definition of the weak mixing angle θ_W , through the relationships between the coupling constants:

$$e = g \sin \theta_W, \quad (1-33)$$

$$e = g' \cos \theta_W. \quad (1-34)$$

Counting the degrees of freedom before and after spontaneous symmetry breaking is enlightening. Initially, we have:

- A complex scalar $SU(2)_L$ doublet, Φ , with 4 degrees of freedom.
- A massless $SU(2)_L$ gauge field, W_i , with 6 degrees of freedom.
- A massless $U(1)_Y$ gauge field, B , with 2 degrees of freedom.

This totals 12 degrees of freedom. After spontaneous symmetry breaking, the configuration changes to:

- A physical real scalar field, h , with 1 degree of freedom.
- Massive W and Z fields with 9 degrees of freedom (3 each for W^+ , W^- , and Z).
- A massless photon with 2 degrees of freedom.

The transformation involves scalar degrees of freedom being "eaten" to provide longitudinal components to the $W^\pm$ and Z gauge bosons.

In gauges other than the unitary gauge, such as the Feynman gauge, Goldstone bosons ($\hat{\omega} = (\omega^\pm, z)$) appear in the spectrum, related to the masses M_W and M_Z . These play a key role in understanding the dynamics of a heavy Higgs boson in the Standard Model.

Fermions, including the electron and its neutrino, are integrated by considering their projections:

$$\psi_{L,R} = \frac{1}{2}(1 \mp \gamma_5)\psi. \quad (1-35)$$

Given the W -boson's exclusive coupling to left-handed fermions, the $SU(2)_L$ doublet is constructed as:

$$L_L = \begin{pmatrix} \nu_L \\ e_L \end{pmatrix}. \quad (1-36)$$

The assignment of hypercharge (Y) is essential for ensuring gauge invariance and consistency with experimental observations within the Standard Model. The lepton doublet, which includes a neutrino (ν_L) and an electron (e_L), is assigned a hypercharge of $Y_L = -1$. This is based on the observation that neutrinos are massless and exhibit left-handed helicity. Consequently, the right-handed electron, e_R , does not interact with the W boson and is thus considered an $SU(2)_L$ singlet with a hypercharge of $Y_{e_R} = -2$.

The gauge-invariant coupling of leptons to the $SU(2)_L \times U(1)_Y$ gauge fields is represented in the Lagrangian as follows:

$$\mathcal{L}_{\text{lepton}} = i\bar{e}_R\gamma^\mu \left(\partial_\mu + i\frac{g'}{2}Y_e B_\mu \right) e_R + i\bar{L}_L\gamma^\mu \left(\partial_\mu + i\frac{g'}{2}Y_L B_\mu + i\frac{g}{2}\tau \cdot W_\mu \right) L_L \quad (1-37)$$

All known fermions can be accommodated in the Standard Model in a manner similar to the leptons. The $SU(2)_L$ and $U(1)_Y$ charge assignments of the first generation of fermions are summarized in the table below.

Field	$SU(3)$	$SU(2)_L$	$U(1)_Y$
$Q_L = \begin{pmatrix} u_L \\ d_L \end{pmatrix}$	3	2	$\frac{1}{3}$
u_R	3	1	$\frac{4}{3}$
d_R	3	1	$-\frac{2}{3}$
$L_L = \begin{pmatrix} \nu_L \\ e_L \end{pmatrix}$	1	2	-1
e_R	1	1	-2
$\Phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}$	1	2	1

Table 1-1 Fermion Fields of the Standard Model

In the Standard Model, directly generating fermion mass terms through $\bar{\psi}\psi$ is prohibited by gauge invariance, as left-handed and right-handed fermions transform differently under $SU(2)_L$ and $U(1)_Y$. Nonetheless, the Higgs boson enables the creation of fermion masses via Yukawa couplings, which are gauge invariant. The Yukawa coupling for down-type quarks in the Lagrangian is expressed as:

$$\mathcal{L}_d = -\lambda_d \bar{Q}_L \Phi d_R + \text{h.c.}, \quad (1-38)$$

leading to the effective coupling:

$$-\lambda_d \frac{1}{\sqrt{2}} \left(\bar{u}_L, \bar{d}_L \right) \begin{pmatrix} 0 \\ v + h \end{pmatrix} d_R + \text{h.c.}, \quad (1-39)$$

which implies a mass term for the down quark upon making the identification:

$$\lambda_d = \frac{m_d \sqrt{2}}{v}. \quad (1-40)$$

To generate a mass term for the up quark, the conjugate Higgs field $\Phi^c \equiv -i\tau_2 \Phi^*$, an $SU(2)_L$ doublet, is utilized, allowing for the $SU(2)_L$ invariant coupling:

$$\mathcal{L}_u = -\lambda_u \bar{Q}_L \Phi^c u_R + \text{h.c.}, \quad (1-41)$$

thus generating a mass term for the up quark. Similar couplings are used to generate mass terms for the charged leptons. Since the neutrino lacks a right-handed partner, it remains massless within this framework.

For the case involving multiple fermion families, the Yukawa couplings^[9], λ_d and λ_u , evolve into $N_F \times N_F$ matrices (with N_F indicating the number of families). This modification ensures that the Higgs boson's interactions with fermion mass eigenstates are flavor diagonal, preventing the Higgs from flavor-changing interactions.

By analyzing the fermion kinetic energy in relation to the gauge boson mass eigenstates, we can outline the charged and neutral weak current interactions of the fermions. The parameter ν could be measured from the charged current observed in muon decay, $\mu \rightarrow e \bar{\nu}_e \nu_\mu$, as depicted in the Feynman diagram:

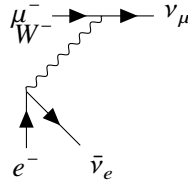


Figure 1–3 Determination of the vacuum expectation value ν from μ decay

The Fermi coupling constant, G_F , is precisely measured as $G_F = 1.16639 \times 10^{-5} \text{ GeV}^{-2}$, facilitating the determination of ν . Considering the negligible momentum carried by the W boson compared to M_W in the context of m_μ , we identify:

$$\frac{G_F}{\sqrt{2}} = \frac{g^2}{8M_W^2} = \frac{1}{2\nu^2}, \quad (1-42)$$

yielding:

$$\nu = (\sqrt{2}G_F)^{-1/2} = 246 \text{ GeV}. \quad (1-43)$$

A pivotal aspect of the Higgs mechanism is the deterministic nature of the Higgs boson's couplings to fermions and gauge bosons, solely based on coupling constants and fermion masses. The scalar potential, originally defined with parameters μ and λ , can be reparam-

terized as:

$$v^2 = -\frac{\mu^2}{\lambda}, \quad (1-44)$$

$$M_h^2 = 2\lambda v^2. \quad (1-45)$$

With no adjustable parameters remaining, Higgs production and decay processes can be unambiguously computed based solely on the Higgs mass.

1.2.3 Vector Boson Fusion and Vector Boson Scattering

Vector boson fusion(VBF) and vector boson scattering(VBS) are important physics categories which have been studied in LHC experiment at CERN. It has two typical high-energetic jets in the forward regions of the detector system. It also have clearly reduced jet activity in the central region. These processes benefit from its high center-of-mass energy during different running periods. The sensitivity of these processes are boosted therefore high precision measurements of these processes are possible. In VBF and VBS, a quark or anti-quark scatters with another one via a space-like exchange of a W, Z or photon. Off this t-channel process, single Higgs or electroweak gauge boson could also be emitted which makes the VBF process in a stricter sense. But basically the emission of two bosons defines the VBS process.

The self-interactions of vector bosons are precisely determined by the $SU(2)_L \times U(1)_Y$ gauge symmetry. Studying the scattering of two vector bosons, $VV \rightarrow VV$ where $V = W, Z, \gamma$, offers a crucial method to explore the electroweak sector of the Standard Model (SM). The process covered in this dissertation $W\gamma jj$ process is sensitive to both the triple and quartic gauge boson couplings, providing potential insights into new physics beyond the SM. Additionally, the scattering of massive vector bosons is vital for understanding the nature of electroweak symmetry breaking.

Among all the $VVjj$ processes where VV decays leptonically, the electroweak production of same-sign WW , $WZjj$, and $ZZjj$ processes have been observed^[10-15]. The VBS topology features two high-energy jets in the backward and forward regions, along with two vector bosons. Both electroweak and QCD processes can produce the same final state, making it challenging to distinguish VBS processes from non-VBS processes. Consequently, measurements are typically conducted in the VBS-enhanced region.

1.3 Physics Beyond the Standard Model

Experiments conducted globally have examined the Standard Model of particle physics at different levels of accuracy. These investigations affirm the model's remarkable capability to describe the phenomena of our universe, yet it remains incomplete. There are still many phenomena that the Standard Model cannot explain.

Dark matter is one of the most puzzling phenomena in particle physics^[16-18], is a type of matter that doesn't interact with light or any form of electromagnetic radiation. We infer its existence from gravitational effects that can't be explained by general relativity unless we assume there's more matter out there than what we can see. Such phenomena include the formation and evolution of galaxies, gravitational lensing, the large-scale structure of the observable universe, the distribution of mass in galactic collisions, galaxy motions within clusters, and anomalies in the cosmic microwave background.

Dark energy, another mysterious entity, influences the cosmos on its grandest scales, primarily manifesting as the force behind the universe's accelerating expansion^[19-21]. Within the framework of the Λ -CDM cosmological model^[22], dark energy constitutes the majority of the universe's energy at 68%, with dark matter and ordinary matter contributing 26% and 5%, respectively. Contributions from neutrinos and photons are virtually negligible.

The Standard Model masterfully accounts for three fundamental forces—electromagnetic, weak nuclear, and strong nuclear—yet excludes gravity. General relativity currently fills this gap, describing gravity's role. However, unifying general relativity with the quantum mechanics principles of the Standard Model, to include a quantum theory of gravity essential for comprehending spacetime and matter at their minutest dimensions, presents a significant unresolved challenge.

Contrary to the Standard Model's assumption of massless neutrinos, the detection of neutrino oscillations reveals they possess mass. This phenomenon is analogous to quark mixing described by the CKM matrix, with the Pontecorvo-Maki-Nakagawa-Sakata matrix explaining neutrino mass eigenstates mixing. Determining neutrino masses, establishing the mass hierarchy, and precise oscillation parameters remain key objectives of current and future experiments.

Moreover, observations indicate a universe predominantly composed of matter, with negligible antimatter, a disparity the Standard Model fails to fully account for. It remains a mys-

tery why the Big Bang did not generate equal amounts of matter and antimatter, which would have led to mutual annihilation.

1.3.1 DiHiggs production

The discovery of the Higgs boson marked a significant milestone in particle physics, but it does not signify the conclusion of research. Presently, the emphasis has shifted towards examining the properties of this particle and comparing the findings with the predictions of the Standard Model (SM). A promising research direction, and the focus of this analysis, is the investigation of Higgs boson pair production.

Studying Higgs boson pair, or di-Higgs (HH), production serves as a probe for both the Standard Model and Beyond the Standard Model (BSM) theories^[23-29]. HH production is directly related to the Higgs self-coupling, the interaction of the Higgs boson with itself. This self-coupling is a crucial element of the Electroweak Symmetry Breaking theory, and constraining this coupling provides a significant test of the Standard Model's validity.

The dominant SM HH production mechanism is gluon-gluon fusion (ggF), with a Standard Model cross-section of $\sigma_{ggF HH}^{\text{SM}} = 31.05 \pm 3\%$ (PDF+ α_s) $^{+6\%}_{-23\%}$ (Scale + m_{top}) fb^[30] at next-next-to-leading order (NNLO) with finite top approximation for a SM Higgs boson mass of 125 GeV. The " m_{top} " represents the uncertainty from the scheme and scale choice of the virtual top mass. The two tree-level Feynman diagrams illustrating this process are shown in Figure 1–4. Figure 1–4a is known as the *box* diagram, which depends on the Higgs to Top quark Yukawa coupling and its modifier, κ_t , expressed as the ratio of the modified coupling to its SM value. The *triangle* diagram, Figure 1–4b, depends on both the Higgs to Top quark Yukawa coupling and the trilinear Higgs self-coupling, which is the interaction among three Higgs bosons. Its modifier, κ_λ , is expressed as the ratio of the modified coupling to its SM value.

These two diagrams (box and triangle) destructively interfere within the SM. The maximal interference occurs at $\kappa_\lambda = 2.4\kappa_t$. The box diagram's m_{HH} peaks near $2m_t$, and when the triangle diagram is included, the m_{HH} becomes softer. The contribution of the triangle diagram increases with higher absolute κ_λ values, generally causing the m_{HH} to peak at lower values. For $\kappa_\lambda = 2.4$ ($\kappa_t = 1$), a local minimum is generated around $2m_t$ ($m_{HH} \sim 350$ GeV), as illustrated in Figure 1–5. However, the amplitude varies with κ_λ , and the cross-section

rapidly increases from the point of maximal interference^[31].

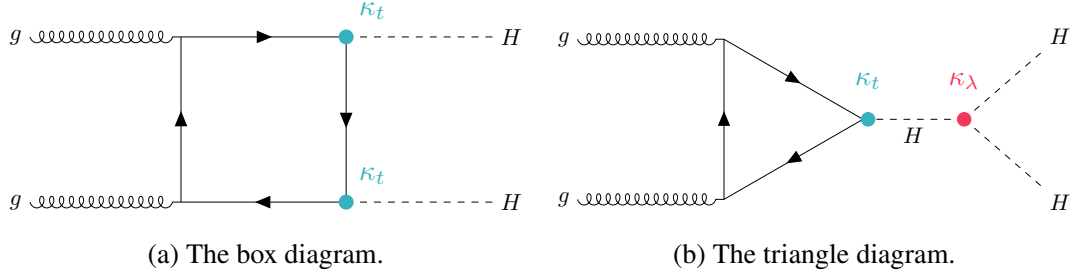


Figure 1-4 The Leading order gluon-gluon fusion di-Higgs production Feynman diagrams.

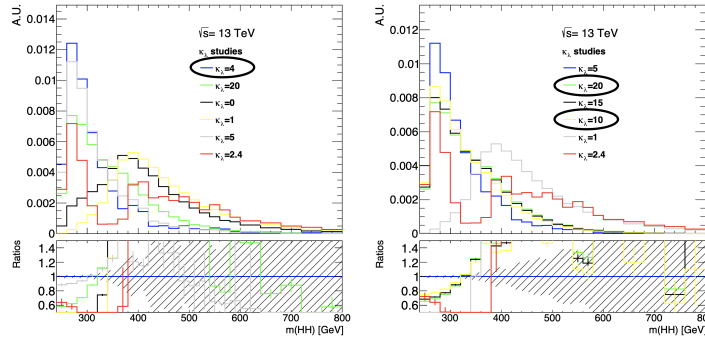


Figure 1-5 m_{HH} distributions for various κ_λ values of the non-resonant ggF production.^[32]

The second-most significant HH production process is vector boson fusion (VBF), with an SM cross-section that is over an order of magnitude smaller than ggF, $\sigma_{VBF}^{SM} = 1.726 \pm 2.1\%$ (PDF+ α_s) $^{+0.03\%}_{-0.04\%}$ (Scale) fb^[33] at next-to-next-to-next-to-leading order (N3LO) for a SM Higgs boson with mass of 125 GeV. VBF is uniquely sensitive to the interaction between two Higgs bosons and two vector bosons. The three tree-level Feynman diagrams representing this process are shown in Figure 1-6. Figures 1-6a and 1-6b illustrate the dependence on κ_λ and the VV interaction vertex modifier, κ_{2V} , respectively.

In the SM, the diagrams in Figures 1-6b and 1-6c are canceled due to destructive interference. However, if κ_{2V} deviates from its SM value of one, the diagram in Figure 1-6b begins to dominate, leading to a significantly increased cross-section^[34] and more pronounced kinematics.

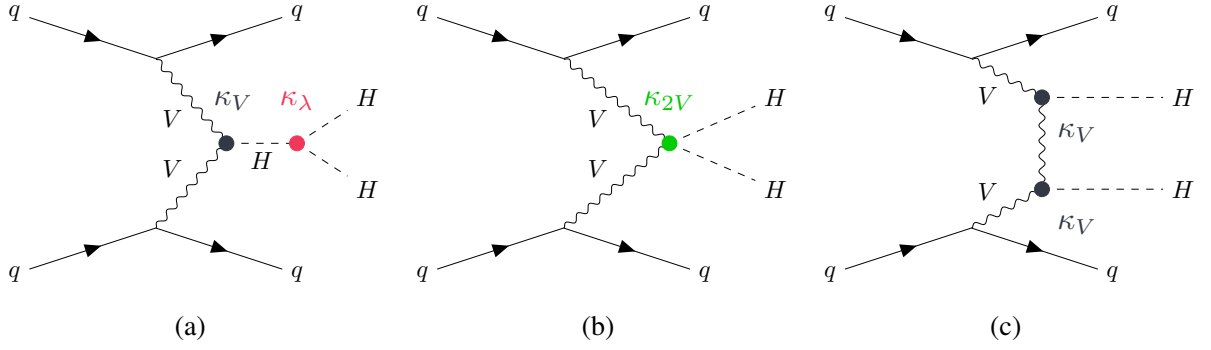


Figure 1-6 The three tree-level vector boson fusion di-Higgs production Feynman diagrams.

1.3.2 Composite Higgs Model

In the standard model, fundamental principles explain chiral fermions from irreducible representations of the Lorentz group, and massless force mediators (gauge bosons) arise from gauge invariance. Massive gauge bosons and fermions arise from spontaneous breaking of gauge symmetry. However, the breaking of gauge symmetry by the Higgs vacuum expectation value (VEV) is parametrically induced, without any dynamic or underlying principle behind it. Most of the free parameters of the standard model are found in the Higgs sector. The stability of these parameters under radiative corrections is also questionable, and leads to the "naturalness" problem. Thus, additional symmetries and/or dynamics are motivated.

One way of phrasing this question is, why is the Higgs boson so light when new physics at a high scale should drive up its mass to large values. One old idea is that the Higgs doublet (4 fields) is a Nambu-Goldstone mode generated from the spontaneous breaking of a larger global symmetry^[35]. In this scenario, the Higgs boson and the W_L, Z_L are all Nambu-Goldstone bosons. The simplest example of the global symmetry is $SO(5)$ which breaks to the $SO(4)$ symmetry of the Higgs sector. Since Nambu-Goldstone bosons are expected to be massless, a small explicit breaking of the global symmetry has to be introduced, causing the Higgs to be not an exact (massless) Nambu-Goldstone mode but a pseudo-Nambu-Goldstone boson (light pNGB). Models such as holographic Higgs and Little Higgs build on these ideas to engineer the Higgs VEV " v " to be small compared to the global symmetry-breaking scale " f " at which new strong dynamics occurs.

To study this new strong dynamics, we can take advantages from the VBS topology. High-energy quarks emit longitudinal vector bosons and those vector bosons have interaction with

this strong dynamics which generates resonances. The lightest resonance will decay to the pseudo-Nambu-Goldstone bosons which are much lighter, i.e. longitudinal gauge bosons and Higgs bosons. It is similar to the $\rho \rightarrow \pi\pi$ decay in QCD. Now the simplified model^[36] could be used in experiments where the lightest resonance is assumed to be a scalar η that decays via the diboson modes $\eta \rightarrow HH, Z_L Z_L, W_L W_L$ exclusively with the branching ratios in the 1:1:2 proportion.

The width of the η resonance in the simplified model is $\Gamma_\eta = \frac{a_\eta^2 m_\eta^3}{8\pi f^2}$ where a_η is a coupling parameter between the η and the pNGBs. For simplicity one can make the assumption that the unitarization of longitudinal vector boson scattering is achieved by the combination of Higgs and η exchange and the heavier resonances in this unitarization is not significant. Unitarity is fully preserved by setting $a_\eta = 1$. The resonance mass m_η and the new symmetry-breaking (compositeness) scale f are free parameters of the model which is equivalent to the mass and width of the resonance.

We have two advantages over effective field theory (EFT) interpretations with this model. High-energy collider such as the LHC is a great opportunity to have direct probing for heavy resonances. And the EFT is appropriate for describing small deviations in values of observables at low mass compared to the collision energy. Second, ad-hoc unitarization is not needed for this model since it preserves unitarity. This eliminates the complications of ad-hoc unitarization for anomalous couplings and higher-dimensional EFT operators when used for describing high-energy scattering.

Chapter 2 Large Hadron Collider and ATLAS

2.1 Introduction to the Large Hadron Collider

The Large Hadron Collider (LHC)^[37], known as the biggest and most potent particle accelerator globally, began operations on September 10, 2008. It is the most recent expansion of CERN's series of particle accelerators. Featuring a 27-kilometer loop filled with superconducting magnets, the LHC also includes various acceleration devices that increase the particles' energy as they move along.

The 27-kilometer ring of the Large Hadron Collider is the stage for four primary experiments: ATLAS^[38-39], CMS^[40], LHCb^[41], and ALICE^[42], each strategically positioned along the ring. ATLAS and CMS serve as comprehensive, general-purpose particle detectors, crafted to detect a broad array of physical events. Their objectives, architecture, and sensitivities are closely matched, affirming the reproducibility of experimental physics findings. LHCb is tailored to scrutinize the phenomena of Flavor Physics and CP-violation. ALICE, on the other hand, is specially designed for probing into the quark-gluon plasma through the medium of heavy-ion collisions. A diagram, as referenced, would provide a visual representation of the LHC's intricate arrangement and the diverse detector systems integrated into it.

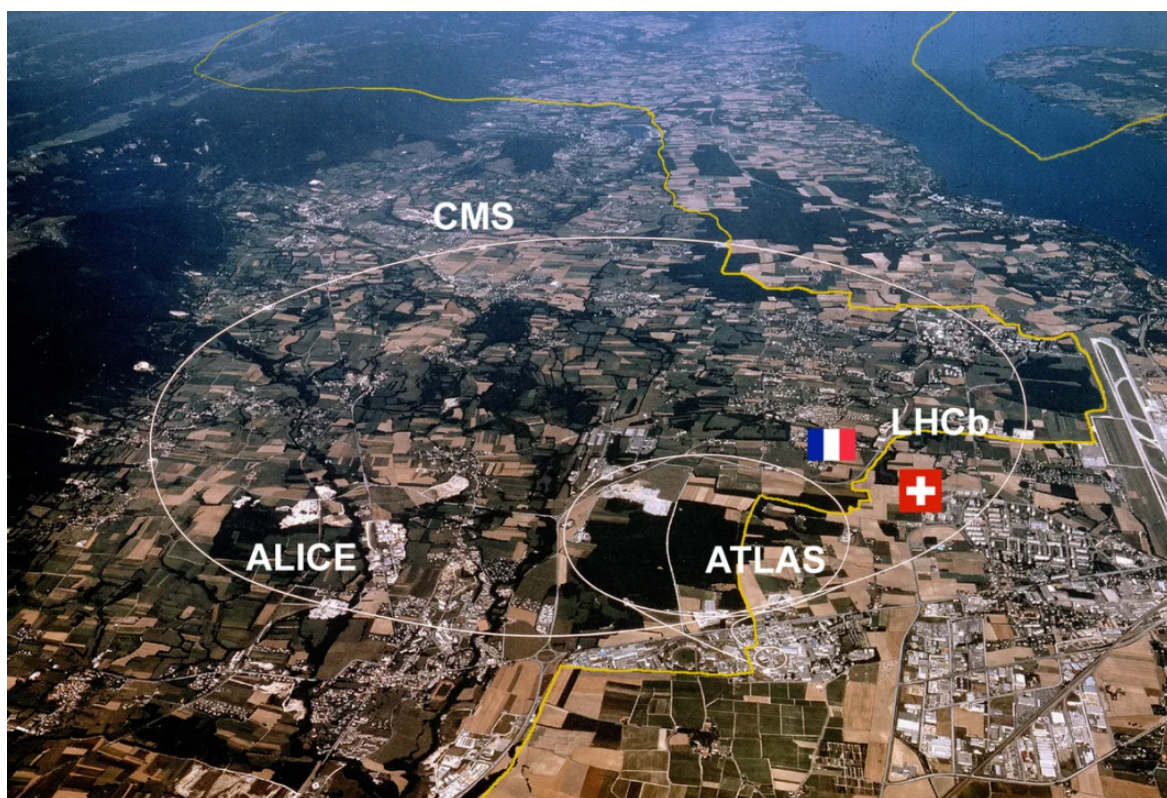


Figure 2–1 Components and Detector Systems of Large Hadron Collider (LHC).

The accelerator complex as illustrated in Figure2–2 at CERN is a marvel of engineering, designed as a series of interconnected machines that incrementally boost the energy levels of particle beams. Each accelerator in the sequence propels the particles to a predetermined energy level before passing them to the subsequent machine, which further increases their velocity. At the culmination of this chain sits the LHC, where particles achieve their peak energies.

Within the confines of the LHC, particle beams are accelerated to velocities that verge on the speed of light. These beams are sent whirling in opposite directions, each confined to its own ultra-high vacuum tube. Their course around the ring is precisely dictated by a powerful magnetic field, which is generated by superconducting electromagnets. These materials, once cooled below a certain threshold temperature, enter a state of superconductivity, eliminating electrical resistance. The LHC's electromagnets are therefore cooled to a brisk -271.3°C , which is even more frigid than the cosmic backdrop of outer space, to utilize this superconducting property. To sustain such extreme temperatures, the accelerator is in-

egrated with a comprehensive liquid helium cooling system, which not only maintains the superconductivity of the magnets but also caters to other operational necessities.

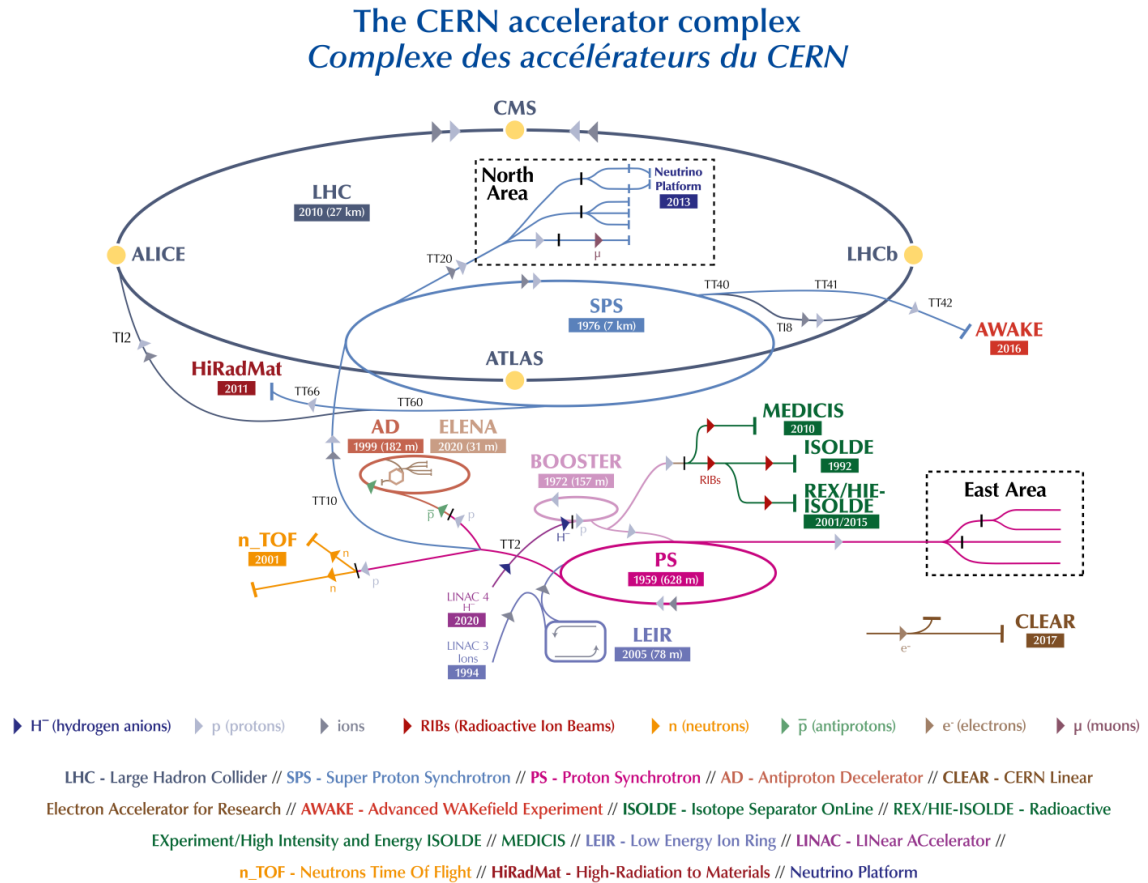


Figure 2–2 CERN accelerator complex^[43]

The accelerator employs thousands of magnets, varying in type and size, to navigate the beams along its course. This array comprises 1,232 dipole magnets, each 15 meters long, which curve the beams' path, and 392 quadrupole magnets, ranging from 5 to 7 meters in length, tasked with focusing the beams. To enhance collision probabilities, a different kind of magnet is utilized just before collision to "squeeze" the particles closer together. Given the minuscule size of these particles, orchestrating their collision is comparable to the challenge of shooting two needles from a distance of 10 kilometers apart and achieving their meeting point precisely in the middle.

As described in Section 1.1, the Standard Model has been exceptionally successful in

predicting various phenomena and explaining nearly all particle physics experiments to date. Yet, there are vital mysteries that the Standard Model does not unravel, questions that the Large Hadron Collider(LHC) seeks to clarify. One of the most fundamental questions is the origin of mass. The Standard Model, as it originally stood, did not provide an explanation for why particles have the masses they do, or why some particles are weighty and others are massless. This conundrum was addressed by theorists Robert Brout, François Englert, and Peter Higgs, who introduced the Brout-Englert-Higgs mechanism. This mechanism proposes that particles acquire mass through their interaction with the ubiquitous Higgs field. The more intense the interaction, the heavier the particle; those with a slight interaction remain light. The Higgs boson, a particle associated with this field, was hypothesized and then, after a long search, confirmed by CERN in July 2012. The discovery was a monumental milestone, yet the exploration continues as scientists delve into the Higgs boson's properties and its uncommon decay patterns.

Supersymmetry is another theoretical framework that the LHC could probe. This theory posits that every standard particle has a heavier supersymmetric partner and could pave the way for a unified theory of all fundamental forces, including gravity, which the Standard Model fails to incorporate.

Furthermore, the LHC could shed light on the cosmic components of dark matter and dark energy. Ordinary matter, which makes up stars and galaxies, constitutes a mere 4% of the universe. In contrast, dark matter and dark energy together make up the remaining 96%, yet they remain enigmatic.

Another profound mystery is the asymmetry between matter and antimatter. Theoretically, the Big Bang should have created equal amounts of both, yet the universe is predominantly matter.

Lastly, the LHC's experiments with lead ion collisions recreate conditions akin to those just after the Big Bang. This allows physicists to study the quark-gluon plasma, a state of matter believed to have given rise to the particles that form the universe. Observing how this plasma cools could provide insight into how matter as we know it came to be.

Each of these queries represents a door to new physics beyond the Standard Model, potentially leading to groundbreaking discoveries about the fundamental nature of reality.

2.2 ATLAS experiment

To evaluate the LHC's operational performance, it's crucial to analyze data collected by its several detectors, since the collider by itself doesn't capture the results of particle collisions. Within this collection of detection tools, the ATLAS detector emerges as a key general-purpose device, adept at capturing a broad range of physics phenomena.

Shaped like a cylinder, the ATLAS detector spans 46 meters in length and 25 meters in width, residing in a deep cavern 100 meters underground. Weighing 7,000 tonnes, it parallels the mass of the Eiffel Tower.

ATLAS is intricately designed to detect some of the smallest and most energetic particles known, thanks to a complex configuration of six different detection subsystems arranged in layers around the site of particle collisions. These subsystems collaborate to accurately track, measure, and categorize particles based on their trajectory, momentum, and energy. A powerful magnet system is also in place to adjust the paths of charged particles, thereby improving the precision of momentum calculations.

At the core of ATLAS, particles accelerated to speeds approaching the speed of light, and with energies up to seven trillion electron-volts, collide. This collision creates a multitude of new particles that scatter in every direction. The detector manages to process over a billion particle interactions per second, a volume of data equivalent to the global population conducting 20 phone conversations simultaneously. Of these interactions, a mere one in a million is selected for in-depth study. ATLAS is instrumental in investigating a variety of physics topics, from the exploration of the Higgs boson and top quark to the search for new dimensions and the components of dark matter.

Considering our connection with the ATLAS collaboration and its extensive data collection across various operational phases, we will leverage ATLAS data to illustrate the LHC's operational trends over time. The ensuing figures and tables provide a comprehensive view of the luminosity levels reached and their corresponding uncertainties during different operational stages.

The graph on the left of Figure 2–3 illustrates the evolution of luminosity delivered to the ATLAS experiment from 2011 through 2018, focusing on stable beams and high-energy proton-proton collisions. The LHC's primary goal is to achieve high luminosity, providing ATLAS and other experiments with a sufficient number of collision events to facilitate

precise measurements and the discovery of new physics. The incremental increase in luminosity over the years reflects continuous advancements in the LHC's operational capabilities and maintenance. Each point on the graph represents a unique operational phase, with the upward trend in luminosity owing to machine upgrades, operational enhancements, and the introduction of more intense particle beams, thereby increasing the availability of collision events for data analysis and potentially leading to significant scientific breakthroughs.

The graph on the right presents data on the average number of interactions per crossing from 2015 to 2018 at a center-of-mass energy of 13 TeV. This period marks the LHC's restart after a prolonged shutdown, operating at an energy level nearly double that of its initial run, which signifies a major step forward in its operational capacity. The graph encompasses all records from ATLAS during stable beam operations in this timeframe, featuring the integrated luminosity and the mean number of interactions per crossing (μ), which aligns with the mean of a Poisson distribution. This distribution is a critical statistical measure for estimating the likelihood of events within a specified interval of time or space.

The formula used to calculate this average, $\mu = \mathcal{L}_{\text{bunch}} \times \sigma_{\text{inel}} / f$, where $\mathcal{L}_{\text{bunch}}$ denotes the instantaneous luminosity for each bunch, indicating the density of particles in a given beam bunch. The inelastic cross-section (σ_{inel}), estimated at 80 mb for 13 TeV collisions, quantifies the probability of interactions between particles. Furthermore, f represents the LHC's revolution frequency, showing how often the particles in the beam complete a full circuit of the accelerator's main ring. In collider physics, the frequency of interactions per crossing is a determinant of event complexity^[44], with higher values indicating more simultaneous interactions. This increase in event density not only raises the potential for significant discoveries but also necessitates advanced techniques for isolating the desired signals from the multitude of interactions.

During Run 2 of the ATLAS experiment at the LHC, operating at a center-of-mass energy of $\sqrt{s} = 13$ TeV, Table 2–1 offers a detailed overview of the integrated luminosities following stringent data-quality evaluations. The data cover the period from 2015 to 2018, showcasing a progressive increase in luminosity: starting at 3.24 fb^{-1} in 2015 and rising to 33.40, 44.63, and 58.79 fb^{-1} in the subsequent years, cumulatively reaching 140 fb^{-1} . This table not only lists the integrated luminosities year by year but also explores the calibration uncertainties unique to each annual dataset. Notably, some sources of uncertainty, indicated

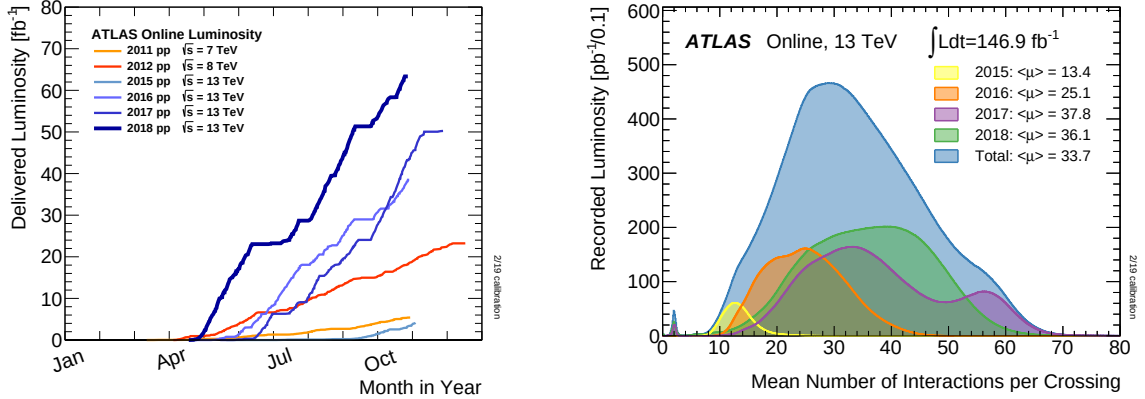


Figure 2-3 Public ATLAS Luminosity Results for Run-2 of the LHC^[45]. Left: **Delivered Luminosity Over Time (2011-2018):** The graph depicts the cumulative luminosity delivered to ATLAS as a function of time during stable beams and for high-energy p-p collisions. Right: **Interactions per Crossing (2015-2018 at 13 TeV):** This illustration showcases the luminosity-weighted distribution of the average interactions per crossing. The data encompasses all records from ATLAS during stable beams between 2015 and 2018. The integrated luminosity and the mean μ value are indicated. The average interactions per crossing align with the Poisson distribution's mean, ascertained for each bunch.

with an asterisk (*), are presumed to be fully correlated over the years, whereas others are considered uncorrelated. This detailed compilation is crucial, offering insight into the extensive dataset collected by ATLAS throughout these years and the level of precision achieved in luminosity measurements. It highlights the factors that affect the vdM calibration's absolute accuracy and the computed overall relative uncertainties, reflecting the comprehensive effort and attention to detail applied in these analyses.

Data sample	2015	2016	2017	2018	Comb
Integrated luminosity [fb^{-1}]	3.24	33.40	44.63	58.79	140.07
Total uncertainty [fb^{-1}]	0.04	0.30	0.50	0.64	1.17
Uncertainty contributions [%]:					
Statistical uncertainty	0.07	0.02	0.02	0.03	0.01
Fit model*	0.14	0.08	0.09	0.17	0.12
Background subtraction*	0.06	0.11	0.19	0.11	0.13
FBCT bunch-by-bunch fractions*	0.07	0.09	0.07	0.07	0.07
Ghost-charge and satellite bunches*	0.04	0.04	0.02	0.09	0.05
DCCT calibration*	0.20	0.20	0.20	0.20	0.20
Orbit-drift correction	0.05	0.02	0.02	0.01	0.01
Beam position jitter	0.20	0.22	0.20	0.23	0.13
Non-factorisation effects*	0.60	0.30	0.10	0.30	0.24
Beam-beam effects*	0.27	0.25	0.26	0.26	0.26
Emittance growth correction*	0.04	0.02	0.09	0.02	0.04
Length scale calibration	0.03	0.06	0.04	0.04	0.03
Inner detector length scale*	0.12	0.12	0.12	0.12	0.12
Magnetic non-linearity	0.37	0.07	0.34	0.60	0.27
Bunch-by-bunch σ_{vis} consistency	0.44	0.28	0.19	0.00	0.09
Scan-to-scan reproducibility	0.09	0.18	0.71	0.30	0.26
Reference specific luminosity	0.13	0.29	0.30	0.31	0.18
Subtotal vdM calibration	0.96	0.70	0.99	0.93	0.65
Calibration transfer*	0.50	0.50	0.50	0.50	0.50
Calibration anchoring	0.22	0.18	0.14	0.26	0.13
Long-term stability	0.23	0.12	0.16	0.12	0.08
Total uncertainty [%]	1.13	0.89	1.13	1.10	0.83

Table 2–1 Integrated luminosities, alongside uncertainties of each yearly data sample from Run 2 pp collision at $\sqrt{s} = 13$ TeV. The table presents not only the integrated luminosities, total uncertainties, but also a detailed split of contributions to the vdM calibration’s absolute accuracy, extra uncertainties related to the physics data sample, and the total relative uncertainty in percentage.

Chapter 3 ATLAS Detector and Object Reconstruction

3.1 Inner Detector

Figure 3–1 illustrates the configuration of the Inner Detector^[46]. It is capable of detecting particles originating from the LHC beam-interaction area within a pseudorapidity range of $|\eta| < 2.5$, offering complete angular coverage in ϕ . Designed to achieve precise measurements, the detector ensures a resolution of transverse momentum, orthogonal to the beam axis, at $\sigma_{p_T}/p_T = 0.05\% p_T \text{ GeV} \oplus 1\%$, alongside a resolution of the transverse impact parameter at $10\mu\text{m}$ for particles with high momentum located in the central region of η . The Inner Detector is composed of three distinct sub-detectors, each fulfilling a unique role: the Pixel Detector, the Semi-Conductor Tracker, and the Transition Radiation Tracker, with their key attributes summarized in the following sections.

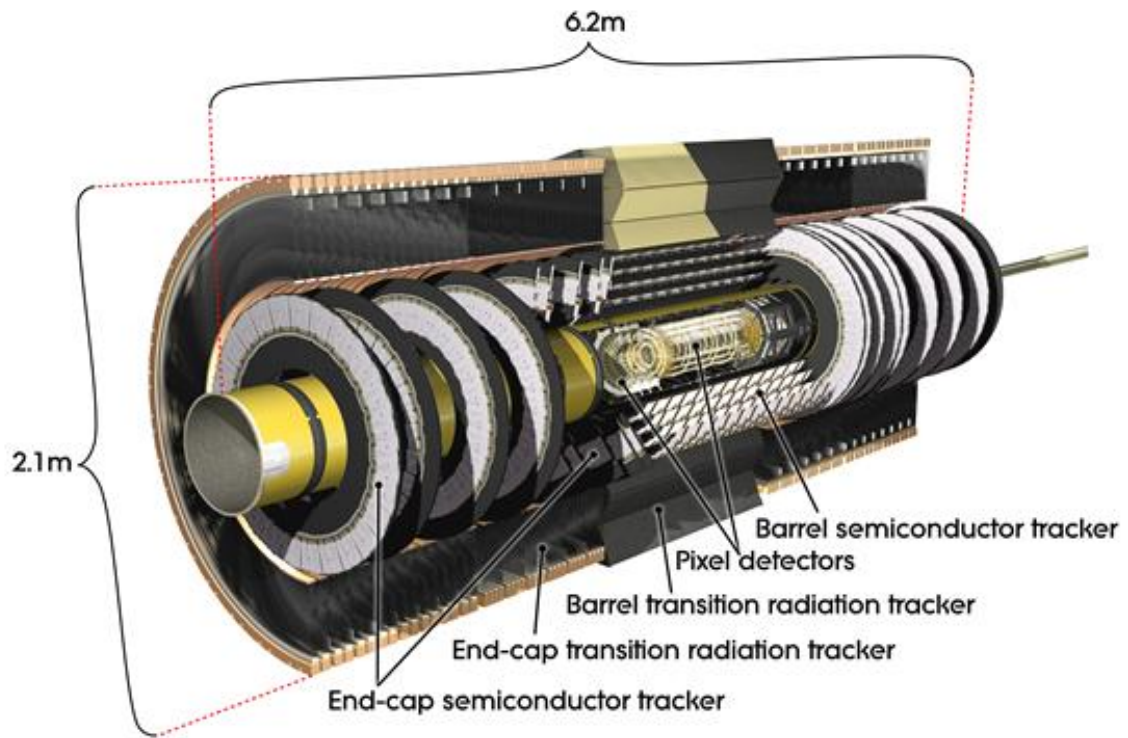


Figure 3–1 Simulated cut-away image of the ATLAS inner detector

3.1.1 The Pixel Detector

The sensitive components of the pixel detector^[47] span radial distances from 50.5 mm to 150 mm. This detector is composed of 1744 silicon pixel modules, which are organized into three concentric barrel layers and two endcaps, each with three disks. For particles generated from the beam-interaction zone, it typically provides three measurement points. Each module encompasses an active area of $16.4\text{mm} \times 60.8\text{mm}$ and holds 47232 pixels, the majority of which measure $50\mu\text{m} \times 400\mu\text{m}$. The local x-coordinate on the module, indicating the direction of high precision position measurement in the $R\phi$ plane, is defined by the orientation of the shorter pitch. Conversely, the longer pitch defines the local y-coordinate, aligning roughly with the z axis in the barrel and with R in the endcaps. Module readout is facilitated by 16 radiation-hard front-end chips, which are bump-bonded to the sensor, encompassing approximately 80.4 million readout channels in total. A pixel's hits are captured if its signal surpasses a set threshold, with the pulse height determined through the Time-over-Threshold (ToT) technique. Figure 3–2 displays an image of the pixel detector.

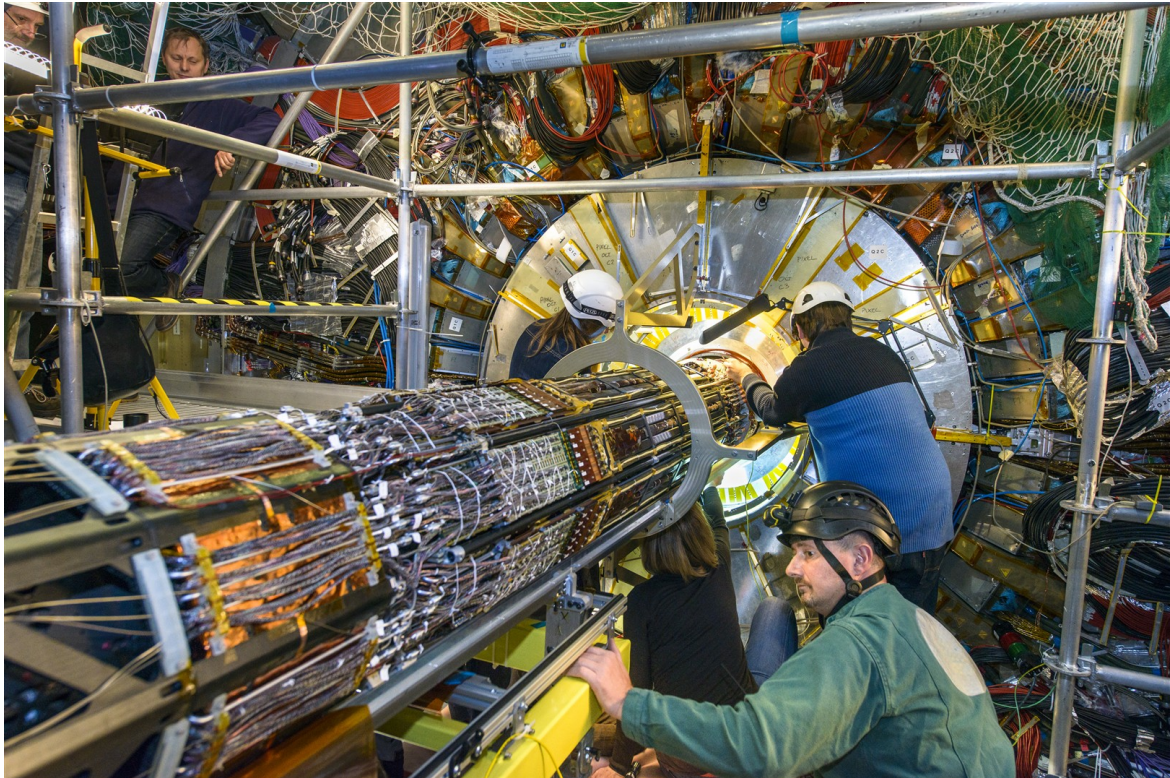


Figure 3–2 Picture of the pixel detector which is the first point of detection in the ATLAS experiment.

3.1.2 The SemiConductor Tracker(SCT)

The SCT^[48] features sensitive elements extending radially from 299 mm to 560 mm. Comprising 4088 modules of silicon-strip detectors, the SCT is structured into four concentric barrels and two endcaps, each with nine disks. Typically, it provides eight strip measurements, equivalent to four space-points, for particles that originate from the beam-interaction zone. Within the barrels, the strips run approximately parallel to both the solenoid field and the beam axis and maintain a constant pitch of $80\ \mu\text{m}$. In contrast, the strips in the endcaps are oriented radially with a variable pitch. Most modules are assembled from four silicon-strip sensors; on each side, two sensors are interconnected in a daisy-chain configuration, resulting in 768 strips around 12 cm long. To facilitate space point measurement, a second pair of identical sensors is attached back-to-back to the first pair at a stereo angle of 40 mrad. Strip data is collected through radiation-hard front-end readout chips, with each chip handling 128 channels, culminating in a total of approximately 6.3 million readout channels. An interior view of the SCT is depicted in Fig 3–3. The system registers a hit based on binary hit information, activated when the pulse height in a channel surpasses a predefined threshold, typically set to correspond to a charge of 1 fC.

The methodology for measurements in silicon detectors often includes a criterion based on the incident angle of a track on a module. The angle α is defined as the angle between a track and the perpendicular to a sensor's plane, while ϕ_{local} describes the angle between a track and this perpendicular within the plane formed by the perpendicular to the sensor and the local x -axis.

3.1.3 The Transition Radiation Tracker(TRT)

The TRT^[49] spans radial distances from 563 mm to 1066 mm. It is composed of 298,304 proportional drift tubes, known as straws, each with a diameter of 4 mm, and these are interconnected through 350,848 electronic channels for data readout. In the barrel region, the straws are organized into three cylindrical layers and divided into $32\ \phi$ sectors, featuring split anodes for dual-sided readout. Conversely, the endcap regions house the straws in a radial orientation, assembled into 80 wheel-like modular structures. The layout of the TRT straws ensures that charged particles, possessing a transverse momentum $p_T > 0.5\text{GeV}$ and within a pseudorapidity range of $|\eta| < 2.0$, typically traverse over 30 straws. Illustrated in

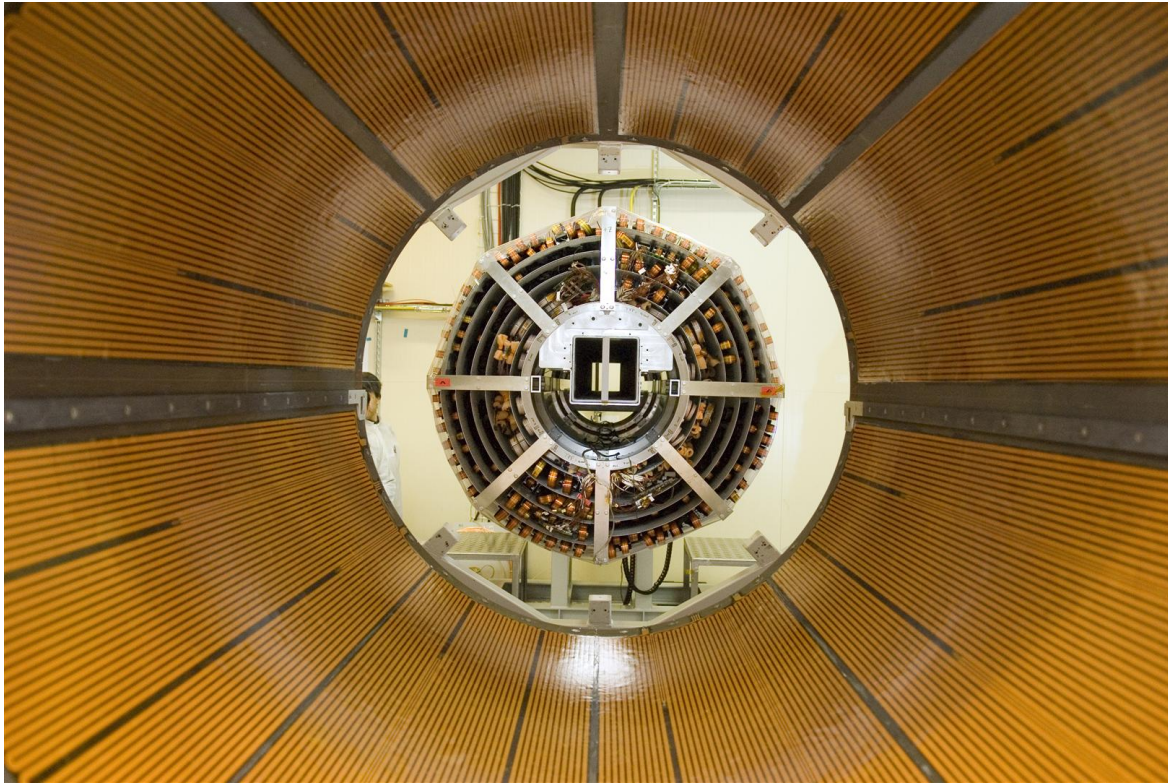


Figure 3-3 Insight of the semiconductor tracker of ATLAS experiment which measures particle tracks with a precision of up to $25\ \mu\text{m}$

Fig 3-4, the TRT facilitates electron identification by capturing transition radiation emitted from polypropylene fibers in the barrel or foils in the endcaps, placed amongst the straws. This transition radiation, significantly more energetic at approximately 6 keV than the few hundred eV from ionizing particles in the gas mixture of Xe, CO_2 , O_2 , is detected using a secondary, high-threshold discriminator within the radiation-hard front-end electronics.

3.1.4 The Beam Conditions Monitor(BCM)

The BCM is specifically designed for monitoring the flux of background particles and safeguarding the silicon trackers from immediate, intense radiation doses resulting from incidents with the LHC beam. The BCM is composed of two stations, termed forward and backward, with each station housing four modules. These modules are strategically positioned at a radius of 5.5 cm and are located $\pm 1.84\text{m}$ away from the central interaction point. Within each module, two pCVD (polycrystalline Chemical Vapor Deposition) diamond sensors are employed, each offering a surface area of $1 \times 1\text{cm}^2$ and a thickness of $500\mu\text{m}$, and

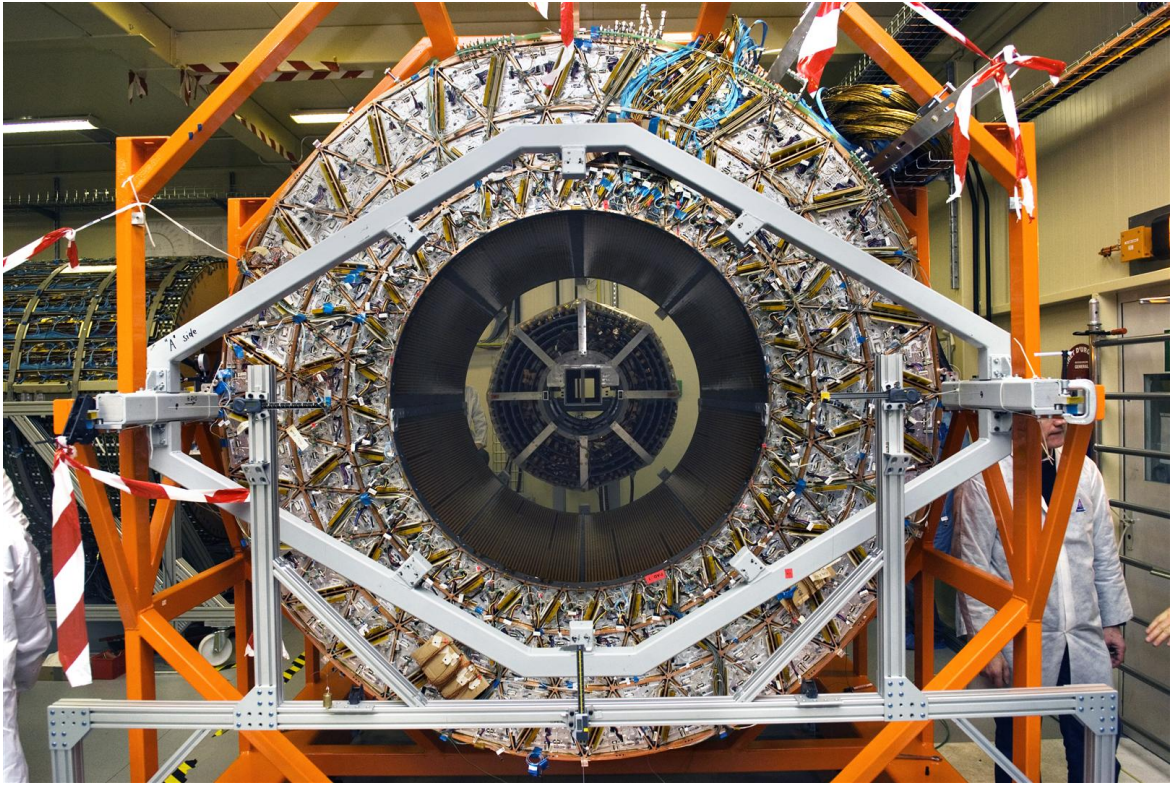


Figure 3–4 Photo of the ATLAS TRT which provides information on the particle type that flew through the detector.

are mounted back-to-back. The quick signal rise-time of 1 ns is a crucial feature, enabling the differentiation between particle hits from collisions (referred to as in-time) and those from background sources (termed out-of-time). The signals generated by the BCM are utilized for two primary purposes: they contribute to trigger information and provide an immediate hit-rate that serves as a critical input for generating a beam-abort signal, thus playing a key role in the protective measures for the silicon trackers.

3.1.5 Readout systems

The readout systems of the Pixel and SCT detectors employ optical transmission for both the dispatch of data from modules and the receipt of timing, trigger, and control data. This transmission relies on Vertical-Cavity Surface-Emitting Lasers (VCSELs) that operate at a wavelength of 850 nm , alongside radiation-hardened fibers. Specifically, for each SCT module, dual optical links are utilized, each with a transmission rate of 40 Mbits/s for data readout. A redundancy feature is built into the system to relieve the impact of losing a single optical

link, thereby preserving the integrity of data transmission. During sessions dedicated to capturing cosmic-ray data, the Pixel Detector's links were also set to function at 40 Mbits/s. In contrast, the TRT employs shielded twisted-pair lines for data transfer to a patch panel located within the muon spectrometer. Here, up to 31 lines can be combined into a single optical link capable of transmitting at a speed of 1.6 Gbits/s.

Off-detector readout electronics are constructed around custom-made Read-Out Driver (ROD) modules. These RODs compile data associated with a particular trigger event into a unified packet, which is then sent to the ATLAS readout system via optical links operating at 1.6 Gbits/s. Beyond data transmission, the RODs are tasked with conducting monitoring and calibration operations, ensuring the overall system's efficiency and accuracy.

3.1.6 Cooling

The cooling system for the silicon detectors employs a bi-phase evaporative method, specifically designed to circulate C_3F_8 fluid at a temperature of -25°C within the detector's low-mass cooling structures. This approach aims to maintain the silicon sensors at optimal temperatures to counteract the effects of radiation damage: the Pixel Detector at 0°C and the SCT at -7°C . During the 2008 commissioning phase, both detectors regulated the coolant's temperature to -10°C within the circuits that cool their sensors, leading to sensor temperatures ranging between -7°C and $+5^\circ\text{C}$, varying by layer and module type. In 2009, a decision to lower the coolant temperature further resulted in sensor temperatures spanning from -17°C to -7°C for the Pixel Detector, and from -7°C to -2°C for the SCT.

In contrast, the TRT is designed to operate at room temperature, distinguishing it from the silicon detectors. Its electronics are cooled using a separate monophase-liquid cooling loop, distinct from the bi-phase system utilized by the Pixel and SCT detectors.

3.2 Calorimeter System^[50]

3.2.1 Liquid Argon Calorimeter

Figure 3–5 shows the LAr (Liquid Argon) calorimeters housed within three sizable aluminum cryostats. Encasing these cryostats is the barrel hadronic calorimeter, constructed from iron absorbers and utilizing scintillating tiles as the active component, known as Tile-Cal.

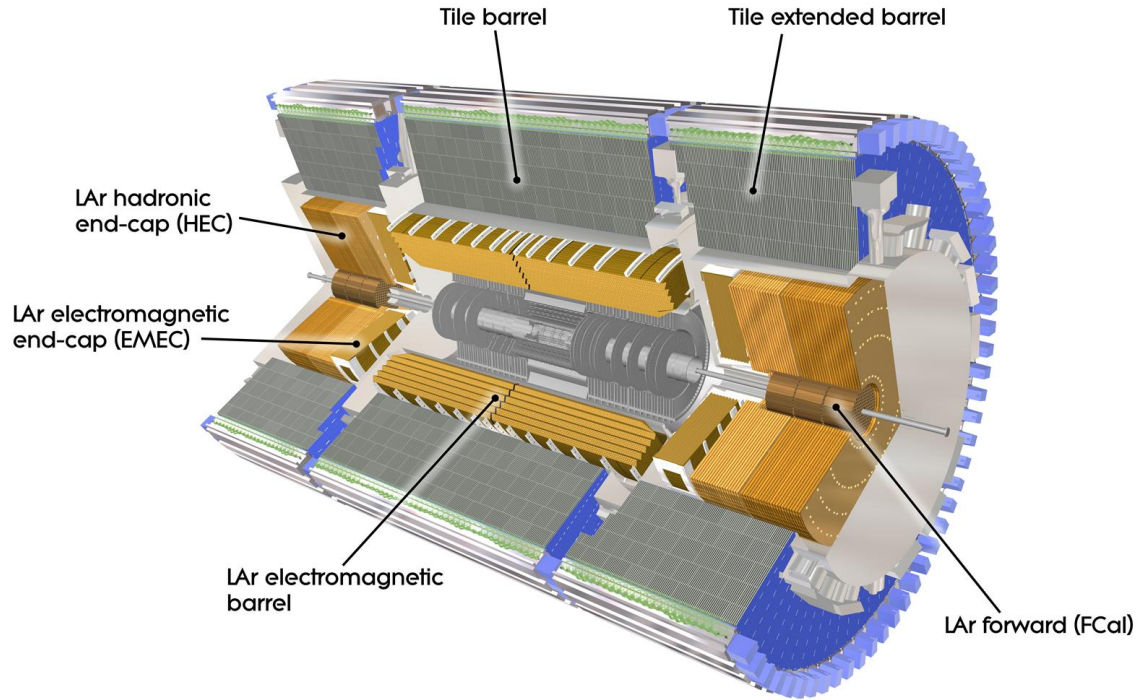


Figure 3–5 Diagram of the ATLAS Liquid Argon (LAr) calorimeter setup. Central to the structure is the barrel cryostat, containing two electromagnetic wheels. On either side, the end cap cryostats accommodate two electromagnetic wheels arranged concentrically, alongside two hadronic wheels and three forward calorimeter wheels.

3.2.1.1 EM Calorimeter

The Barrel Electromagnetic (EM) calorimeter^[51] is composed of two wheels, each featuring 1024 steel-clad lead absorbers. These absorbers are alternated with an equal number of electrodes, which are secured by a honeycomb structure standing 2.1 mm tall that sets the gap size. The electrodes themselves are crafted from copper etchings on polyimide, with two outer conductive layers that distribute high voltage across the electrode's external surfaces. Meanwhile, a central layer sandwiched between two insulating foils captures signals via capacitive coupling. Applying a nominal voltage difference of 2000V between the electrodes and absorbers causes ionisation-induced charges in the argon to drift towards the electrodes within 450 ns. This barrel calorimeter reaches up to a pseudo-rapidity of 1.475, achieving a total thickness of 22 radiation lengths (X_0). The readout electrodes feature etched pads that define three separate depth sections, with signals from neighboring electrodes aggregated to

form the layout.

The EM endcap detector broadens the coverage in pseudo-rapidity, ranging from 1.375 to 3.2. It mirrors the barrel's construction with accordion-shaped absorbers and electrodes assembled into two concentric wheels for each endcap cryostat. These are composed of 256 absorbers for the inner wheel and 768 for the outer wheel. Presampling detectors, which consist of a narrow argon gap in front of the precision detectors, are similarly constructed but feature a different electrode layout in the barrel compared to the endcap.

3.2.1.2 Hadronic End cap calorimeters(HEC)^[52]

The hadronic section's wheels are constructed from 32 modules, each featuring an alternating sequence of copper absorbers—with a thickness of 25 mm in the first wheel and 50 mm in the second—and signal collection gaps. Each gap is further divided into four sub-gaps, each measuring 1.8 mm, separated by three electrodes identical in composition to those used in the EM sections. Two adjacent sub-gaps function together as an electrostatic amplifier, enabling operation at a lower voltage compared to using a single gap. Signals are gathered from the central electrode. The entire hadronic section reaches a cumulative depth of 10 absorption lengths.

3.2.1.3 Forward calorimeters(FCAL)

The forward calorimeter wheels are designed with an initial layer of copper followed by two layers of tungsten matrices, penetrated by cylindrical holes. These holes accommodate the gaps and electrodes, which are constructed from tubes dedicated to signal collection. Inside these tubes, a copper (for the first wheel) or tungsten (for the subsequent wheels) rod is placed. To maintain the position of the tube and the rod, a fiber is wound around them. The diameter of this fiber sets the gap size, with dimensions of 0.25 mm, 0.375 mm, and 0.5 mm for the three respective wheels.

3.2.2 Tile Hadronic Calorimeter

Encasing the Liquid Argon (LAr) calorimeter, the Tile Calorimeter is designed to measure the energy of hadronic particles that do not fully expend their energy within the LAr Calorimeter. It consists of alternating layers of steel and plastic scintillating tiles. When hadronic particles collide with the steel layers, they initiate a cascade of secondary particles.

These secondary particles, in turn, stimulate the plastic scintillators to emit photons. These photons are then transformed into an electrical current, the magnitude of which directly correlates with the energy of the original hadronic particle.

The Tile Calorimeter, TileCal, comprises a stationary central barrel (LB) and two adjustable extended barrels (EB), each formed of 64 modules that cover an azimuthal ϕ angle of $2\pi/64 = 0.1$. Its structure includes layers of iron plates alternated with scintillating tiles. These tiles, positioned perpendicular to the beam path, are arranged in a staggered pattern radially to enhance depth coverage, as depicted in Fig 3–6. The detection process within TileCal utilizes wavelength-shifting (WLS) fibers to channel light from the scintillating tiles to photomultipliers (PMTs), which are situated within the calorimeter’s outer iron frame that also accommodates the front-end electronics. Each calorimeter cell is connected to two PMTs for signal readout.

TileCal’s design, featuring tiles aligned parallel to incoming particles at $\eta = 0$, permits the WLS fibers to extend directly outward, enhancing the calorimeter’s hermeticity and simplifying the tile-fiber coupling. The 3 mm thick tiles, produced through injection molding, contribute to a calorimeter that is both compact and efficient, with an iron-to-scintillator ratio of 4.7 to 1, achieving a sampling frequency conducive to accurate measurements and an effective nuclear interaction length of 20.7 cm.

Internally, TileCal is segmented into three longitudinal layers(A,BC,D), varying in depth across the central and extended barrels, thus providing comprehensive coverage and depth. This segmentation facilitates detailed energy measurement of particles, with a total calorimeter depth reaching 7.4λ at $\eta = 0$, and 9.7λ when including the electromagnetic calorimeter, ensuring thorough particle interaction analysis. The calorimeter’s cells are divided into segments, enhancing resolution and detection capabilities.

Special gap/crack scintillators enhance TileCal’s performance around areas dense with service and electronic components, bridging the extended barrel and LAr electromagnetic end cap calorimeters. With around 5000 cells and 10000 readout channels, TileCal’s electronic system processes PMT signals through amplification and shaping, employing a dual-gain approach and digital sampling at 40 MHz for precise energy and timing reconstruction. This system also contributes to the level-1 trigger signal by aggregating cell outputs within the same projective tower.

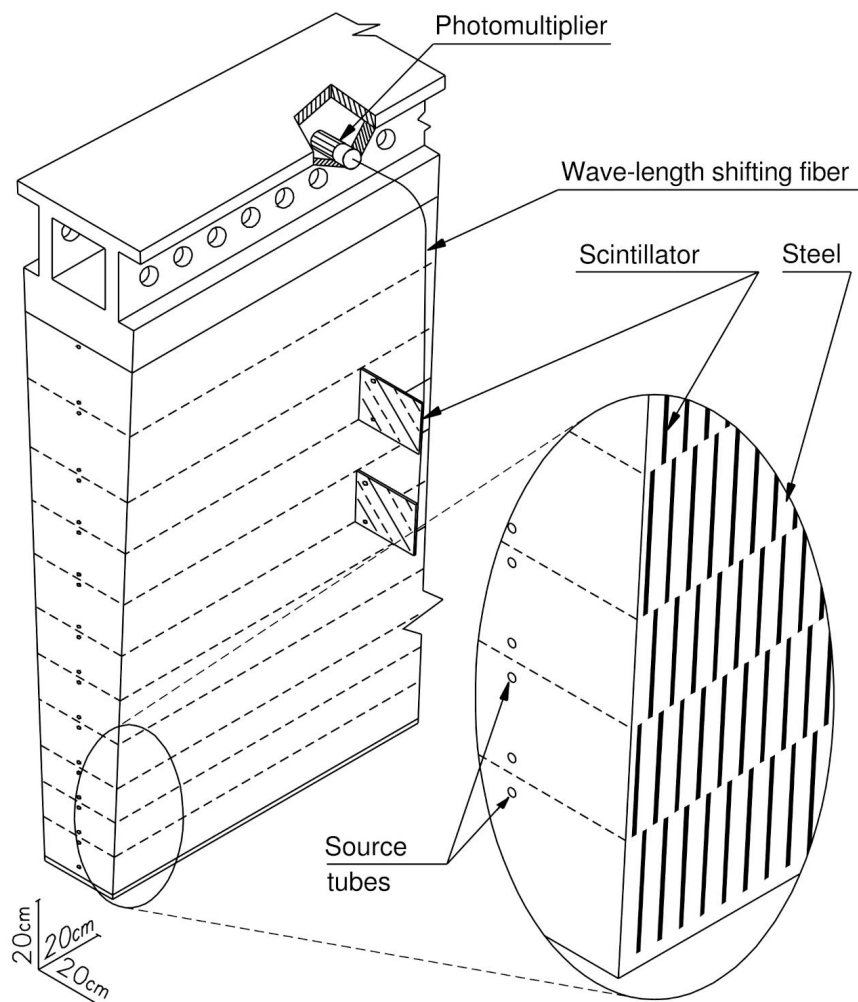


Figure 3–6 Diagram illustrating the configuration of a tile calorimeter module, highlighting the incorporation of optical readout within the interleaved active and passive strata. The depicted source tubes serve the calibration system that utilizes a radioactive source.

TileCal’s development involved extensive *R&D*, prototyping, and optimization, informed by test beam data and simulations from 1993 to 1995, culminating in the Technical Design Report in 1995. The construction phase spanned 1996 to 2004, with installation in the exper-

imental cavern from 2004 to 2006 and commissioning between 2007 and 2009 using cosmic muons, ensuring readiness and high performance for the proton-proton collisions from 2009 to 2012. Upcoming sections will delve into significant findings and future enhancements planned for TileCal.

3.3 Muon Spectrometer

Muons, which are closely related to electrons, are generated from the decay of other particles that result from proton collisions within the ATLAS detector's core. By examining the muons' trails, researchers can deduce the nature of the particles produced from the proton collisions.

The instrument utilized for this purpose is the muon spectrometer^[53], situated as the outermost layer of the ATLAS detector. It is tasked with determining the muons' paths and energies with remarkable precision. This is accomplished by diverting the particles through an intense magnetic field, produced by enormous superconducting magnets. By meticulously analyzing the pathways of muons, combined with other data, physicists successfully identified the elusive Higgs boson.

The muon spectrometer is compartmentalized into three sections as depicted in Figure 3–7: the central Barrel region, covering the rapidity region $|\eta| < 1.2$, and two End-Caps that span the rapidity ranges $1 < |\eta| < 2.7$. Within the Barrel, the toroidal magnetic field is generated by eight superconducting coils arranged in an open geometry, yielding a field integral that fluctuates between 2 and 5 Tesla-meters, varying significantly with the azimuthal angle. The muons' momentum is gauged by measuring the sagitta, the displacement of the muon trajectory under the influence of the magnetic field. The trajectory is mapped at three high-precision measuring stations located within the toroid and equipped with Monitored Drift Tubes (MDT)^[54], set in cylindrical layers around the beam axis. These stations can pinpoint muon positions with an accuracy of around 50 micrometers and provide angular data on track segments to refine full muon track reconstruction. Additionally, specialized trigger detectors known as Resistive Plate Chambers (RPCs) are installed in the Barrel's two outer stations to aid in identifying muon events.

For the End-Cap sections, two air core toroids, identical and coaxial with the barrel toroid, are utilized. Muon momentum in these regions is measured by three stations of chambers

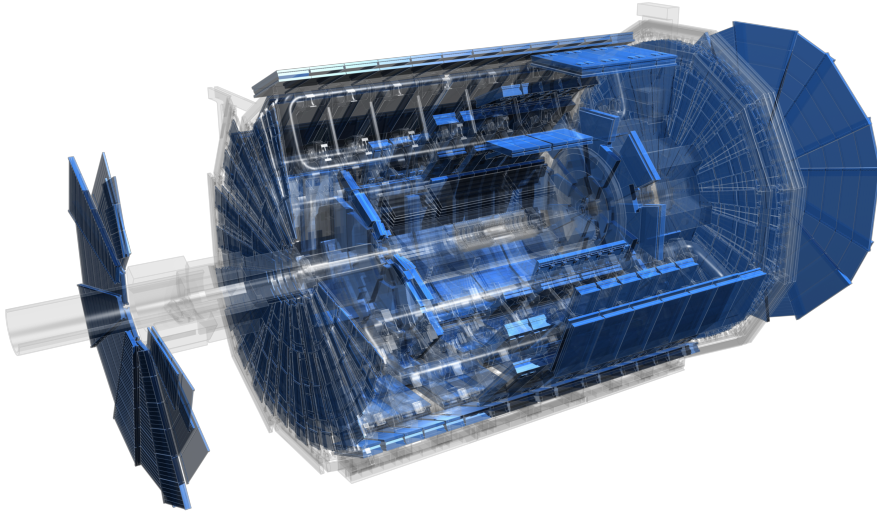


Figure 3–7 Areas of the ATLAS Experiment covered by the Muon Spectrometer

arranged into large disks, or wheels, which are perpendicular to the beam direction. These measure the angular shift of the muon track in the magnetic field. The volume inside the toroids in the End-Caps is not instrumented, making direct sagitta measurements impractical; hence, a point-angle approach is used instead. MDT chambers ensure precision tracking across the full angular range, except for the inner station in the region $2 < |\eta| < 2.7$, where Cathode Strip Chambers (CSCs)^[55] are employed due to their lower occupancy and similar spatial resolution.

The End-Cap’s trigger system, operational up to $|\eta| < 2.4$, utilizes Thin Gap Chambers (TGCs) arranged in two layers for low momentum (pt) triggering and three layers for high pt triggering, integrated with the previous triggering layers. TGCs also measure the second coordinate, with a layer included in the first tracking wheel for this purpose.

The Muon Spectrometer’s design has been finely tuned for high standalone resolution and reliable muon identification, key factors in discerning particle interactions and characteristics within the ATLAS detector.

3.4 Object Reconstruction

The ATLAS experiment employs a variety of techniques to identify and reconstruct particle candidates. Although numerous entities are reconstructed using diverse algorithms, this dissertation concentrates on the fundamental objects essential for the analyses that constitute

the entirety of this academic work.

3.4.1 Electron and photon reconstruction

The algorithm commences by selecting topo-clusters to form electrons and photons, refining tracks for bremsstrahlung and linking them with these clusters. Conversion vertices, derived from the tracks, are then paired with the clusters. This stage leads to separate, simultaneous supercluster algorithms for electrons and photons, which after initial adjustments, couple superclusters with tracks or vertices accordingly. Electrons are identified by their associated tracks, converted photons by their vertices, and unconverted photons lack both.

To resolve instances where an object may qualify as both an electron and a photon, the algorithm applies a selective overlap removal, yet retains sufficient overlap to ensure robust reconstruction. After calibration, the final particle candidates are prepared for the extraction of variables critical for quality and ambiguity assessments, as depicted in Figure 3–8.

3.4.1.1 Topo-cluster reconstruction

Topo-clusters are engineered to reflect the spatial significance patterns characteristic of particle showers. Central to their formation and expansion is the cell significance, ξ_{cell}^{EM} , given by:

$$\xi_{\text{cell}}^{EM} = \frac{|E_{\text{cell}}^{EM}|}{\sigma_{\text{noise,cell}}^{EM}}, \quad (3-1)$$

where E_{cell}^{EM} is the EM scale energy and $\sigma_{\text{noise,cell}}^{EM}$ the predicted noise, incorporating electronic and pile-up components estimated for Run 2's luminosity. Cells from initial detector layers are excluded to avoid noise cluster formation. The process then aggregates cells exceeding a significance threshold of $|\xi_{\text{cell}}^{EM}| \geq 2$, unifying proto-clusters with common cells and engaging adjacent cells without bias towards their energy levels. The absolute significance is used to counteract any noise-induced negative energy and preserve energy measurement integrity, as per the "4-2-0" protocol. Distinctly, cells with pronounced local maxima are identified, with a local maximum being a cell with an energy surplus of 500 MeV, a minimum of four neighboring cells, and unmatched by the signal in adjacent cells.

The reconstruction of electrons and photons derives from these topo-clusters, harnessing EM calorimeter energies, aside from a defined eta region where additional detector readings are factored in. The EM fraction, f_{EM} , indicative of the EM energy's share of the total

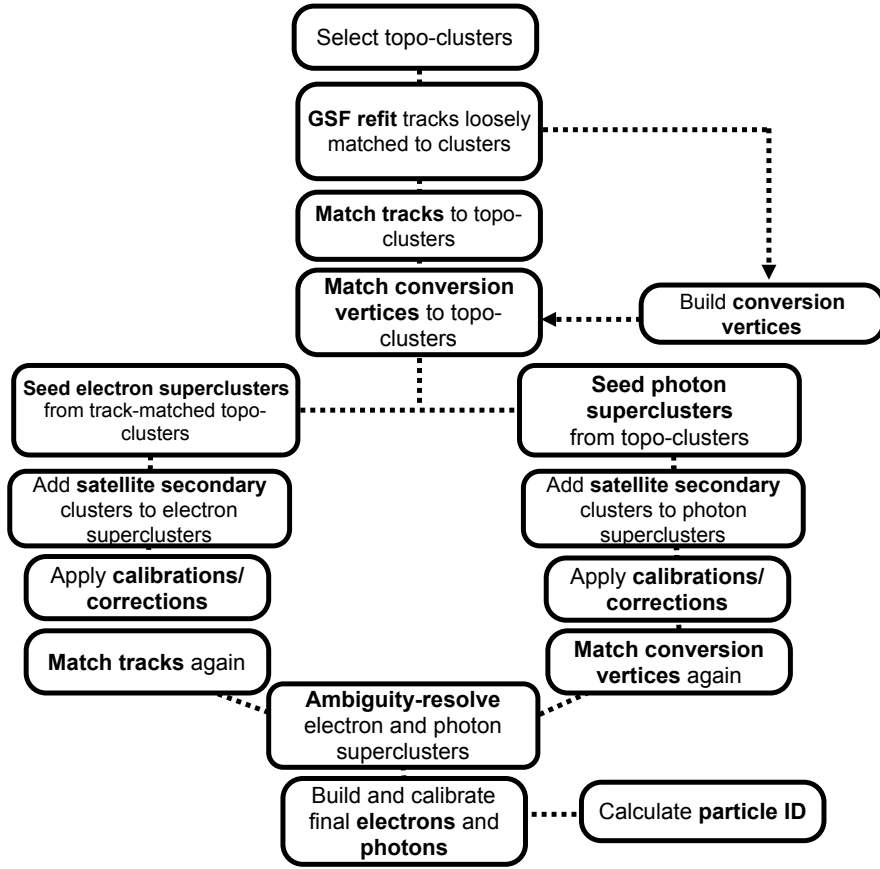


Figure 3–8 Diagram illustrating the new algorithm flow for the electron and photon reconstruction.

cluster energy, is pivotal for cluster selection. Only clusters surpassing the 400 MeV EM energy threshold are considered, with an ideal f_{EM} cutoff of 0.5 to filter out around 60% of the pile-up, thus ensuring a reliable electron cluster selection. Visual representations of f_{EM} 's distribution and electron reconstruction efficiency are provided in subsequent figures.

3.4.1.2 Track reconstruction, track-cluster matching, and photon conversion reconstruction

Electron track reconstruction maintains the established methodology as detailed in Ref^[56-57]. For photon track reconstruction, notable updates include utilizing fixed-size calorimeter clusters to define regions-of-interest (ROIs). These are essential for capturing EM shower profiles, as outlined in Ref^[58]. When standard pattern recognition is insufficient, particularly for silicon track seeds within ROIs, a refined approach that incorporates a Kalman filter-based algorithm comes into play, accommodating up to 30% energy loss at material intersections

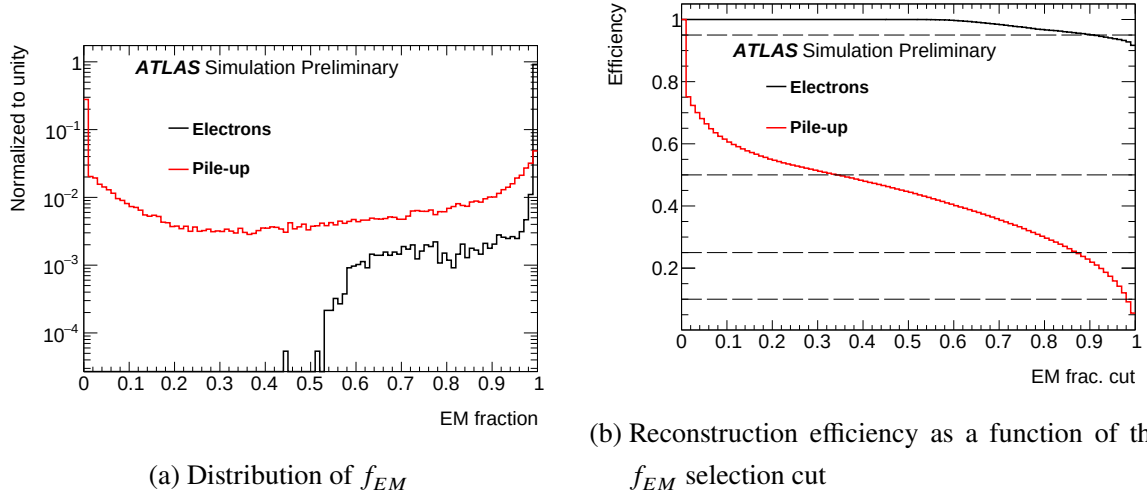


Figure 3–9 (a) Distribution of f_{EM} and (b) reconstruction efficiency as a function of the f_{EM} selection cut for simulated true electron (black) and pile-up (red) clusters.

as mentioned in Ref^[59]. This is further refined by a global χ^2 fitting technique, allowing for additional energy adjustments where the primary fit is inadequate, as per Ref^[60]. Moreover, tracks aligned with silicon hits but not fitting standard clusters undergo a re-fit using a Gaussian sum filter (GSF) technique, enhancing track parameter estimates through a non-linear extension of the Kalman filter^[61].

Subsequently, these adjusted tracks are aligned with EM topo-clusters. The process involves extrapolating the track from its closest point to the primary interaction point up to the second layer of the calorimeter. This step may involve rescaling the track's momentum to correspond with the cluster energy, optimizing the match for electron candidates that have experienced significant energy loss from bremsstrahlung within the tracker. A track's compatibility is determined by comparing its momentum and the reconstructed charge q against the cluster's properties, with criteria allowing for minor discrepancies due to potential energy lost to radiated photons.

The hierarchy of track matching gives precedence to tracks with hits in the pixel detector, followed by those detected in the SCT but absent in the pixel detector. Within these categories, the preference is given to tracks that more closely align with the cluster in the calorimeter's second layer, provided their ΔR —a measure of spatial separation in the detector —remains minimally different. Preference is given to tracks with additional hits in the innermost layer, capitalizing on their precision. The top-ranked track thus defines the

electron's reconstructed attributes.

Photon conversion reconstruction largely mirrors the existing method described in Ref^[56]. Inputs for reconstructing conversion vertices include tracks loosely associated with fixed-size clusters, with specific emphasis on tracks with silicon hits, known as Si tracks, and those exclusively identified in the TRT. The conversion vertices are constructed from pairs of opposite-charge tracks forming vertices consistent with massless particles, or from single-track vertices lacking innermost layer hits. The fidelity of converted-photon reconstruction is augmented by favoring tracks that the TRT likely identifies as electrons, with varied stringency depending on the type of conversion vertex being constructed^[62].

Enhancements to the reconstruction software aim to bolster the efficiency of double-track Si conversions and to diminish the misidentification rate of unconverted photons as single- or double-track TRT conversions. By refining the ambiguity resolution process, especially in discerning which track seeds to retain, a 2%4% increase in efficiency for double-track Si conversions has been achieved, with significant gains for photons with larger conversion radii. This also involves recalibrating the strategy for single-track Si conversions, leading to an approximate 1% overall increase in conversion reconstruction efficacy.

Stringent criteria have been applied to TRT tracks to lower the proportion of unconverted photons inaccurately cataloged as converted. This includes mandating a higher fraction of precision hits and elevating the probability threshold for a track's electron correspondence. Such adjustments have halved the rate of misclassified unconverted photons in events characterized by lower levels of interaction ($\langle\mu\rangle < 60$), as compared to the prior algorithm^[63].

Lastly, EM topo-clusters are matched with conversion vertices, with a bias towards double-track conversions involving two silicon tracks, followed by those with single-track conversions. The selected vertex, within each category, is the one with the smallest conversion radius.

3.4.1.3 Supercluster reconstruction

Electron and photon superclusters are constructed in a sequential two-step process. Initially, EM topo-clusters are evaluated for their potential as seeds for superclusters. Following this, adjacent EM topo-clusters are considered for their role as satellite clusters, which could result from either bremsstrahlung radiation effects or the division of clusters. These satellite clusters are then integrated with the seeds to complete the supercluster formation, contingent

upon meeting set criteria.

The construction of superclusters begins by organizing EM topo-clusters in order of their transverse energy (E_T) from highest to lowest, based on their EM energy measurements. Each cluster is individually assessed for its suitability as a seed. Electron supercluster seeds need an E_T of at least 1 GeV and a corresponding track with a minimum of four silicon detector hits. For photons, the seed clusters must possess an E_T over 1.5 GeV, with no specific demands regarding track or conversion vertex associations. Clusters previously allocated as satellites are excluded from being seeds.

Should a cluster fulfill the criteria for a seed, the algorithm then searches for suitable satellite clusters as depicted in Figure 3–10. A cluster is deemed a satellite based on its proximity to the seed cluster, defined by a $\Delta\eta \times \Delta\phi$ parameter. For electron superclusters, this includes clusters within a 0.125 by 0.300 $\Delta\eta \times \Delta\phi$ vicinity of the seed and sharing the same 'best-matched' track. In the case of photon superclusters, clusters whose best-matched tracks are involved in a silicon hit-based conversion vertex with the seed are also classified as satellites. This method utilizes track information to effectively differentiate between significant photon or electron events and background noises or irrelevant clusters.

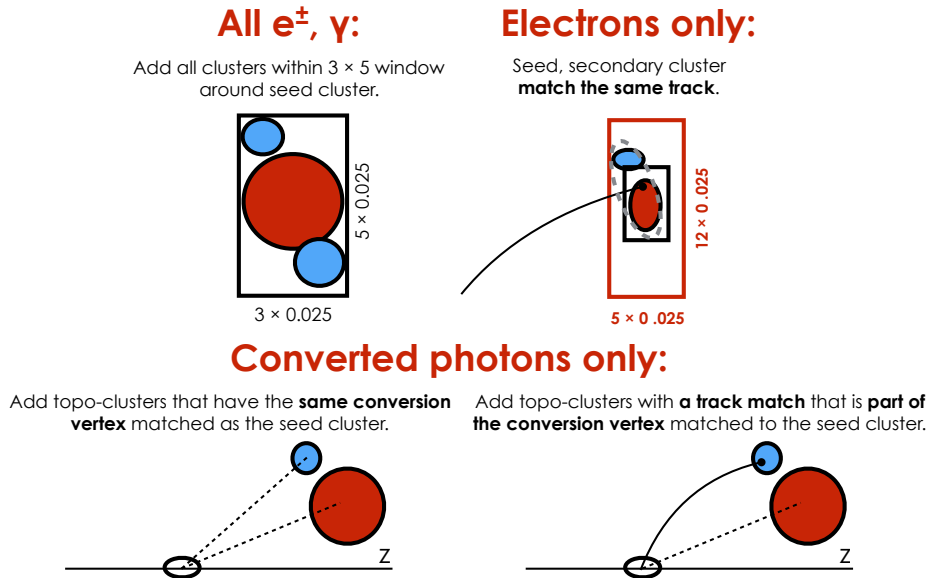


Figure 3–10 Diagram of the superclustering algorithm for electrons and photons. Seed clusters are shown in red, satellite clusters in blue

Superclusters result from the aggregation of seed clusters and their satellite counterparts.

In the final phase of constructing superclusters, specific calorimeter cells are allocated to each supercluster. Selection includes cells from the presampler and the initial LAr calorimeter layers, except within the transition area ($1.4 < |\eta| < 1.6$), where scintillator energy between calorimeter cryostats is also considered. To reduce superclusters' susceptibility to pile-up noise, the extent of each involved topo-cluster is capped at an η width of 0.075 in the barrel and 0.125 in the endcaps. The ID's magnetic field alignment allows for EM shower expansion primarily in the ϕ direction, meaning the η width limitation captures the electron or photon's energy without a ϕ direction constraint.

3.4.1.4 Creation of electrons and photons for analysis

Upon the establishment of electron and photon superclusters, they undergo a primary calibration for energy and adjustments in position, with subsequent matching of tracks to electron superclusters and conversion vertices to photon superclusters. This matching employs a methodology analogous to that utilized for EM topo-clusters, albeit adapted for superclusters. This initiates the derivation of analysis-ready electrons and photons. Owing to the distinct assembly processes for electron and photon superclusters, it is plausible for a single seed cluster to engender both an electron and a photon. The protocol ensures that if an entity distinctly manifests as a photon (lacking an associated track) or as an electron (coupled with a track but devoid of a suitable photon conversion vertex), it is then exclusively categorized for analytical evaluation; ambiguous instances are distinctly flagged to allow precise classification as per the analytical exigencies.

The recalibration of energy for electrons and photons is necessitated by their dependency on the pairing of tracks and conversion vertices, this recalibration occurs subsequent to the initial supercluster calibration as explicated in Ref.^[64]. Post recalibration, determinants such as shower shape alongside other differential variables are evaluated for the identification of electrons and photons^[56-57]. Notably, the analysis of lateral shower shapes, which is pivotal for identification, is predicated on the location of the most energetically potent cell, ensuring its uniform applicability across various clustering methodologies, contingent on the incorporation of the said cell.

3.4.2 Muon reconstruction

In ATLAS, muon identification primarily relies on detecting the hallmarks of a minimum-ionizing particle, which include a track in the Muon Spectrometer (MS) and specific energy deposits in the calorimeters. This identification leverages data chiefly from the Inner Detector (ID) and MS tracking detectors. Additionally, calorimeter data play a role in refining track parameters and accommodating large energy losses in the calorimeters, as well as facilitating MS-independent identification of ID tracks as muons. Detailed accounts of charged particle reconstruction in the ID, MS track reconstruction, and various muon identification algorithms that utilize full detector data are elaborated in Refs.^[65-66]. For a comprehensive understanding, Ref.^[53] provides further information.

3.4.2.1 Muon spectrometer stand-alone track reconstruction

Track reconstruction within the Muon Spectrometer (MS) begins by identifying short straight-line segments from hits in each MS station, employing a Hough transform^[67]. These segments, identified within individual stations, are integrated into preliminary track candidates. The integration uses a loose pointing constraint from the interaction point (IP) and a parabolic path that approximates the muon's trajectory through the magnetic field. This first-order approximation is enhanced with precision measurements in the bending plane, paired with data from the second coordinate in the trigger detectors, to form three-dimensional track candidates. A comprehensive global χ^2 fit of the muon's trajectory is then conducted, accounting for potential interactions with detector material and possible misalignments among the various detector chambers.

The muon's trajectory, as refined by the global χ^2 fit, undergoes further refinement; outlier hits are discarded, and new hits corresponding to the trajectory but not initially assigned to the track candidate are included. This updated fit is processed, resolving ambiguities by excluding tracks with significant hit-quality fractions unless they lack hits in one of three stations—this ensures the selection of high-quality tracks, especially important for the efficient detection of boosted low-mass dimuon systems. Finally, the selected tracks are fitted again, this time with a relaxed IP constraint and incorporating considerations for energy loss in the calorimeters. The tracks are then back-extrapolated to the beamline, with the transverse momentum (p_T) of the extrapolated track expressed at the IP.

3.4.2.2 Muon reconstruction based on complete detector information

Global muon reconstruction utilizes data from both the Inner Detector (ID) and the Muon Spectrometer (MS), as well as calorimetric information. This process unfolds through several main reconstruction strategies, resulting in various muon types: Combined (CB), inside-out combined (IO), MS-extended (ME), segment-tagged (ST), and calorimeter-tagged (CT).

CB muons are reconstructed by aligning MS track data with ID tracks and integrating a consolidated track fit that includes both ID and MS data, accounting for calorimetric energy loss. If the muon spectrometer track linked with the track from the combined fit deviates, a subsequent fit is executed. For high- p_T muons, additional fits may involve ST tracks or tracks extending to the Silicon-Associated Forward (SiF) muons.

A complementary inside-out algorithm is employed for IO muons, extending ID tracks to the MS and identifying at least three suitably aligned MS hits. Here, the ID track, energy dissipated in the calorimeters, and MS hits culminate in a unified track fit. This method does not rely on a standalone MS track reconstruction, enhancing efficiency in areas with sparse MS coverage or low- p_T muons not reaching the middle MS.

When ME muons cannot be linked to an ID track, their parameters are extrapolated back to the beamline to classify an ME muon. Such muons are crucial for extending the acceptance beyond the ID, thus fully leveraging the entire MS coverage up to $|\eta| = 2.7$.

ST muons require an ID track extended to the MS with satisfactory angular matching to at least one MS segment. A successfully matched track is considered a muon candidate, and these parameters are taken directly from the ID track.

CT muons are generated by extrapolating ID tracks through the calorimeters, searching for congruent energy deposits within a muon-identifying profile. Subsequent energy deposits guide the track back to the ID for parameter extraction.

Further refinements include the usage of a parabolic trajectory in the pattern recognition for enhanced matching. The ID track's transverse impact is calculated with increased precision, and nuisance parameters are now included in the muon fit, addressing the transnational and rotational effects. The calorimeter-tagging algorithm has been updated for high- p_T muons, focusing on managing high MS coverage by incorporating an additional sector to the pattern recognition logic.

The above summarizes improvements and strategies in muon reconstruction compared to

those previously reported in Ref.^[68].

3.4.2.3 Identification criteria

In the post-reconstruction phase, muon candidates poised for physics analyses are chosen according to a comprehensive set of criteria. These criteria encompass the number of hits across various ID subdetectors and MS stations, properties related to the track fit, and variables assessing measurement compatibility within the detector systems. Selection criteria specific to each muon category, as defined previously, establish the 'working points' (WPs). Tailored to accommodate the diverse requirements of analyses that include muons, these WPs vary, focusing on the precision of prompt muon identification, momentum measurement resolution, and the suppression of background from non-prompt muon sources. A fine-grained distinction is drawn between non-prompt muons arising from semi-leptonic decays of light hadrons in transit and those from heavy-flavour hadrons. WPs are particularly devised to filter out light hadrons, typically linked with lower-quality muon tracks due to mid-flight decay-induced trajectory deviations. In contrast, decays of bottom and charm quarks tend to yield higher-quality muon tracks, which are discernible from those associated with non-prompt events. These superior tracks are generally more closely linked with the primary interaction point and exhibit greater isolation within the Inner Detector and calorimeters.

To cater to the diverse requirements prevalent in physics analyses, three standard working points (WPs) have been established, denoted as Loose, Medium, and Tight. These WPs are stratified by a trade-off between increasing purity and decreasing efficiency. Muons that meet the criteria of the Medium WP also satisfy the Loose WP by default, and similarly, those meeting the Tight WP also comply with the Medium WP. The Medium WP is tailored for a broad spectrum of analyses, striking a balance between efficiency and purity while maintaining minimal systematic uncertainties for both prompt-muon efficiency and background suppression. Conversely, the Loose WP is particularly calibrated for analyses like the reconstruction of Higgs boson decay in four-muon final states, where a greater muon count and a significant signal-to-background ratio permit an increase in efficiency despite a slight rise in purity trade-off and systematic uncertainties. At the opposite end, the Tight WP is designed for the utmost purity, markedly enhancing background rejection at a minimal efficiency reduction for prompt muons when compared to the Medium WP. This most stringent WP is particularly advantageous for analyses that necessitate stringent control over back-

ground from non-prompt muons. Figure 3–11 showcases the efficacy of the Loose, Medium, and Tight selection working points (WPs) for simulated tracks with transverse momentum (p_T) exceeding 10 GeV.

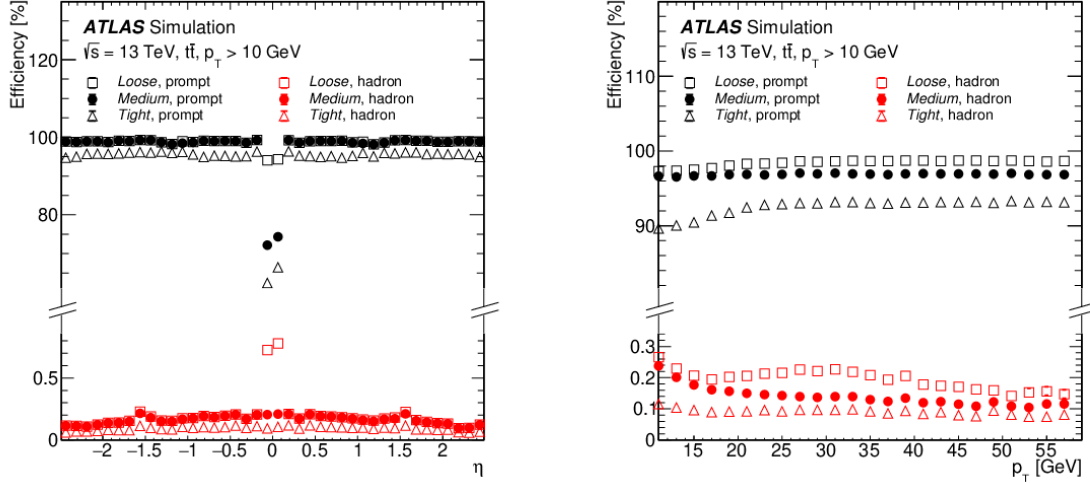


Figure 3–11 Efficiency as a function of pseudorapidity (η) on the left and transverse momentum (p_T) on the right for Loose, Medium, and Tight working point (WP) requirements in simulated $t\bar{t}$ events. This is depicted separately for prompt muons and those from light hadron decays. Efficiency is gauged by the ratio of Inner Detector (ID) tracks corresponding with a reconstructed muon that fulfills the stipulated WP criteria to the total number of generator-level prompt muons or light hadrons.

3.4.3 Jet^[69]

Jet reconstruction can be divided into three primary stages: first the input four-vectors are defined, then the jet algorithm and parameters are defined, and finally the jet is groomed (for large-R jets).

3.4.3.1 Reconstruction

The ATLAS experiment primarily relies on topo-clusters for jet reconstruction. Topo-clusters are clusters of calorimeter cells that are grouped together based on their topology and ability to suppress noise. These clusters start from seed cells that exhibit energy exceeding 4σ , where σ represents the combined expected electronic and pile-up noise, with the latter predominating in the current conditions of data collection^[70]. The formation process

includes adjoining cells in all three dimensions that maintain at least 2σ of energy, and continues until no further adjoining cells meet this criterion. The process completes with the inclusion of all adjacent calorimeter cells, regardless of their energy levels.

Topo-clusters are calibrated either at the raw electromagnetic (EM) scale, summing the energies of all individual cell components, or at the local cell weighting (LCW) scale. The LCW scale compensates for the discrepancies between electromagnetic and hadronic interactions within the ATLAS calorimeters, thus aligning the average topo-cluster energy with the hadronic scale.

The inherent formation method of topo-clusters lends them a natural resistance to pile-up. This suppression is optimized for the average topo-cluster under typical data collection conditions. However, leveraging event-specific measurements of pile-up levels and other local observables allows for further minimization of pile-up dependency. Various techniques have been explored to enhance resolution of low- p_T jets, where pile-up substantially affects jet energy resolution. These improvements are minimal under current conditions but are projected to reach a reduction of up to 30% for jets around $p_T \approx 30\text{GeV}$ as the average number of collisions per bunch crossing increases to 200^[71].

Standard topo-clusters are commonly utilized within ATLAS, employing EM topo-clusters for small- R jets and LCW topo-clusters for large- R jets. The anti- k_t algorithm, as implemented by the FastJet software library^[72-73], is predominantly used for jet reconstruction. This involves different distance parameters R , where $R = 0.4$ is used for small- R jets representing quarks and gluons, and $R = 1.0$ is used for large- R jets indicative of hadronically decaying massive particles.

The larger R value is crucial for capturing all decay products within a single jet, as the angular separation ΔR between decay constituents from a massive particle χ follows $\Delta R \approx 2m_\chi/p_{T,\chi}$, illustrated in Figure 3–12. For more complex decay scenarios, such as $t \rightarrow bW \rightarrow bq\bar{q}$, the decay products are more spread out, necessitating larger R values.

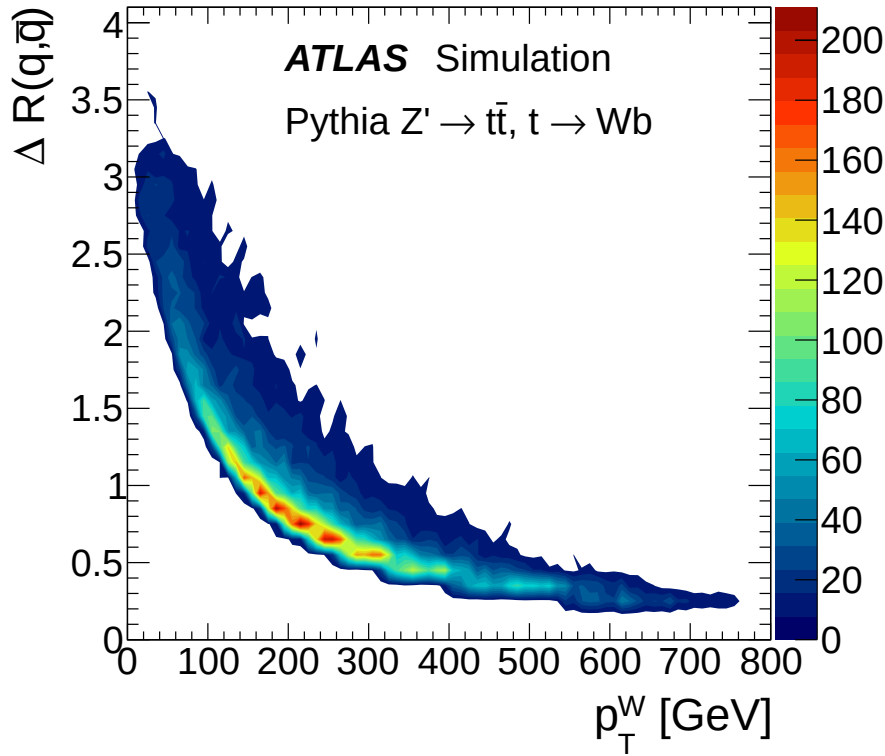


Figure 3–12 The separation ΔR between the pair of quarks from a hadronically decaying W boson, demonstrating the two-body decay behaviour of $\Delta R \gtrsim 2m'/p_T'$.^[74]

Large- R jets are necessary to encompass the entirety of hadronic decays of massive particles, but this also increases their susceptibility to pile-up effects due to the extensive calorimeter volume they encompass. Pile-up, typically of low energy, may not significantly alter overall jet kinematics but can obscure the crucial angular structure within the jet necessary for identifying decays of massive particles.

To address these issues, large- R jets are often groomed using techniques that discard certain jet constituents based on predefined criteria, thus reconstructing the jet from the remaining constituents. A common method employed by ATLAS is the trimming procedure, where the original anti- k_t jet is re-clustered using the k_t algorithm with a sub-jet radius $R_{\text{sub}} = 0.2$, discarding any sub-jet where its p_T falls below 5% of the large- R jet's p_T ^[75–76]. This technique has been shown to maintain a stable jet mass distribution from conditions in 2012 up through scenarios involving 200 collisions per bunch crossing.

3.4.3.2 Jet calibration

Post-construction, jets undergo a calibration process to mitigate various effects. This process, depicted in Figure 3–13, entails three main stages: initial suppression of pile-up contributions at the jet level for small- R jets, calibration of the jet to the Monte Carlo (MC) truth scale, and subsequent adjustments to reconcile differences between MC simulations and actual data.

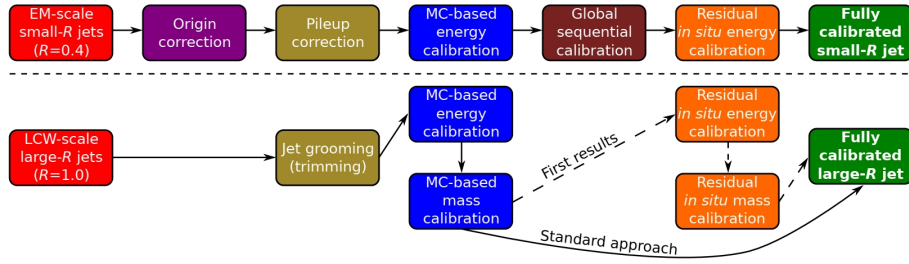


Figure 3–13 Depiction of the calibration chain for both small- R and large- R jets. The dashed line for large- R jets indicates preliminary results not yet utilized in physics analyses, while the solid line denotes the standard process.

The initial step involves the subtraction of pile-up contributions using multiplicative scale factors. For large- R jets, this subtraction is achieved through grooming techniques that remove pile-up topo-clusters from the jets. Small- R jets, however, employ a different multi-step approach:

The jet axis is first adjusted to align with the primary hard-scatter vertex, termed the origin correction. Next, the energy density ρ is calculated within $|\eta| < 2.0$ ^[77], providing an assessment of the global pile-up energy in an event. This value, combined with the jet’s area A_{jet} —determined for each jet in every event—helps compute the local pile-up energy, which is then subtracted from the jet’s original four-vector. While effective within the calculated ρ region, this method requires additional adjustments in areas where $|\eta| > 2.0$, using average correction factors dependent on the number of reconstructed primary vertices N_{PV} and the average number of interactions per bunch crossing μ . The final corrected transverse momentum is given by:

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

where α and β are the derived correction factors. The impact of these steps is illustrated in Figure 3–14.

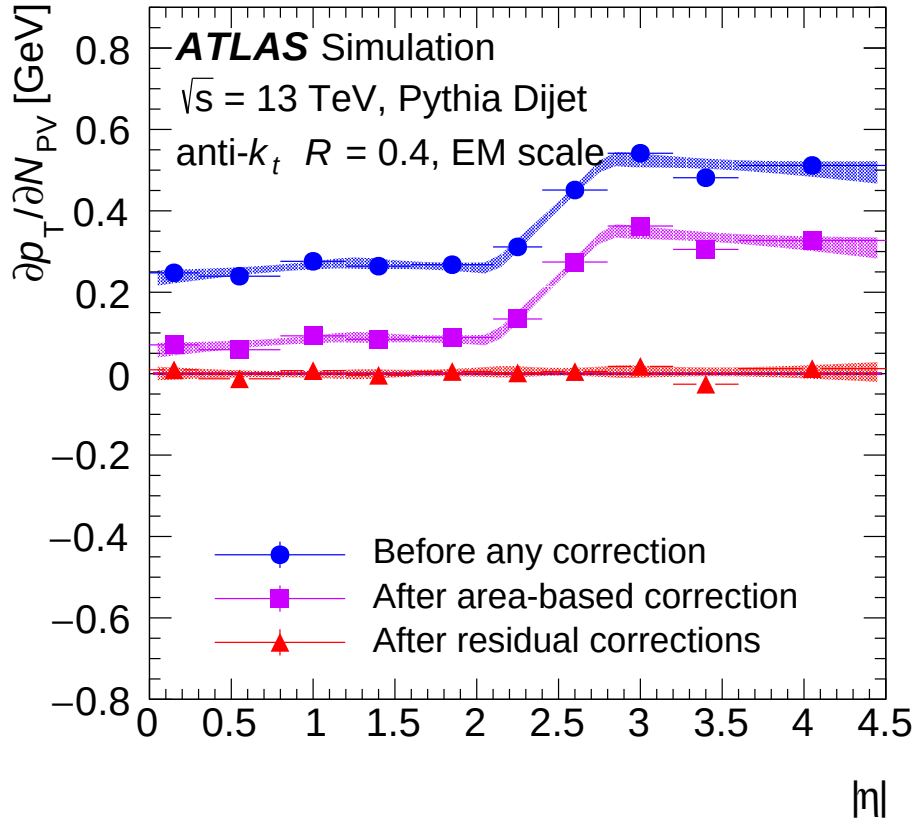


Figure 3–14 The average amount of pile-up energy added per reconstructed primary vertex N_{PV} for a small- R jet, shown before and after corrections. The blue line represents the uncorrected jets, purple after the ρA_{jet} area correction, and red post- α and β adjustments^[77].

Following pile-up subtraction, jets are calibrated against MC truth information to address energy losses in hadronic showers, which may not be fully detectable due to the detector’s inactive volumes or energy absorbed in nuclear binding within strong force interactions. This calibration aligns reconstructed jets with their corresponding truth jets by determining the response ratio X_{reco}/X_{truth} and applying corrections in detailed bins of η and energy. This process is vital for both small- R and large- R jets to ensure accurate energy and mass measurements, as depicted for small- R jets in Figure 3–15.

The final step involves refining and validating these calibrations with data-derived factors to account for any discrepancies between the MC simulations and actual measurements. This is crucial for ensuring accurate jet energy and mass representations in ATLAS analyses.

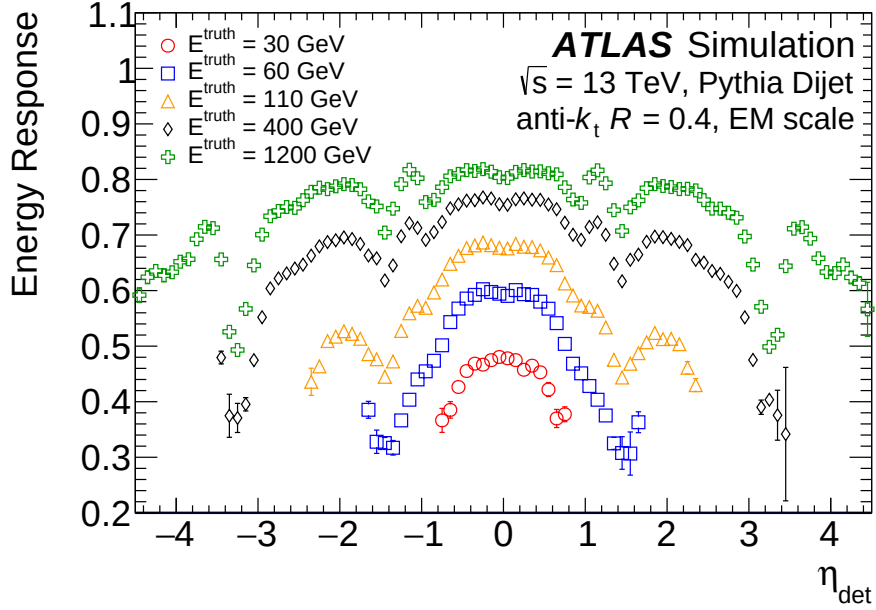


Figure 3–15 The energy response, $E_{\text{reco}}/E_{\text{true}}$, for small- R jets, illustrating the calibration back to the truth scale. The inverse of this response sets the average jet calibration factor^[77].

3.4.3.3 Jet tagging

Following calibration, the next step involves examining the substructure of jets, specifically the angular distribution of energy within each jet. This analysis is crucial for determining the jet's origin and is particularly valuable for distinguishing between boosted massive hadronic particle decays and QCD dijet/multijet production. While the jet mass is an intuitive substructure variable already covered under calibration, it can be refined through the inclusion of tracking data, resulting in the track-assisted mass $m_{\text{TA}} = m_{\text{track}} \times \frac{p_T^{\text{calo}}}{p_T^{\text{track}}}$. This provides complementary data to the calorimeter-based mass m_{calo} , leading to the formulation of the combined mass m_{comb} as follows:

$$m_{\text{comb}} = Am_{\text{calo}} + Bm_{\text{TA}}, \quad \text{where} \quad A = \frac{\sigma^{-2}(m_{\text{calo}})}{\sigma^{-2}(m_{\text{calo}}) + \sigma^{-2}(m_{\text{TA}})} \quad \text{and} \quad B = \frac{\sigma^{-2}(m_{\text{TA}})}{\sigma^{-2}(m_{\text{calo}}) + \sigma^{-2}(m_{\text{TA}})},$$

with $\sigma(m_x)$ denoting the Jet Mass Resolution (JMR) for each mass definition x ^[78]. This refined measure significantly enhances JMR, crucial for jet tagging to effectively separate physical processes. Figure 3–16 displays the combined mass distributions for QCD, W-jet, and top-jet, highlighting how sharper peaks reduce background interference in signal peaks.

Beyond jet mass, other substructure variables are also significant for differentiating be-

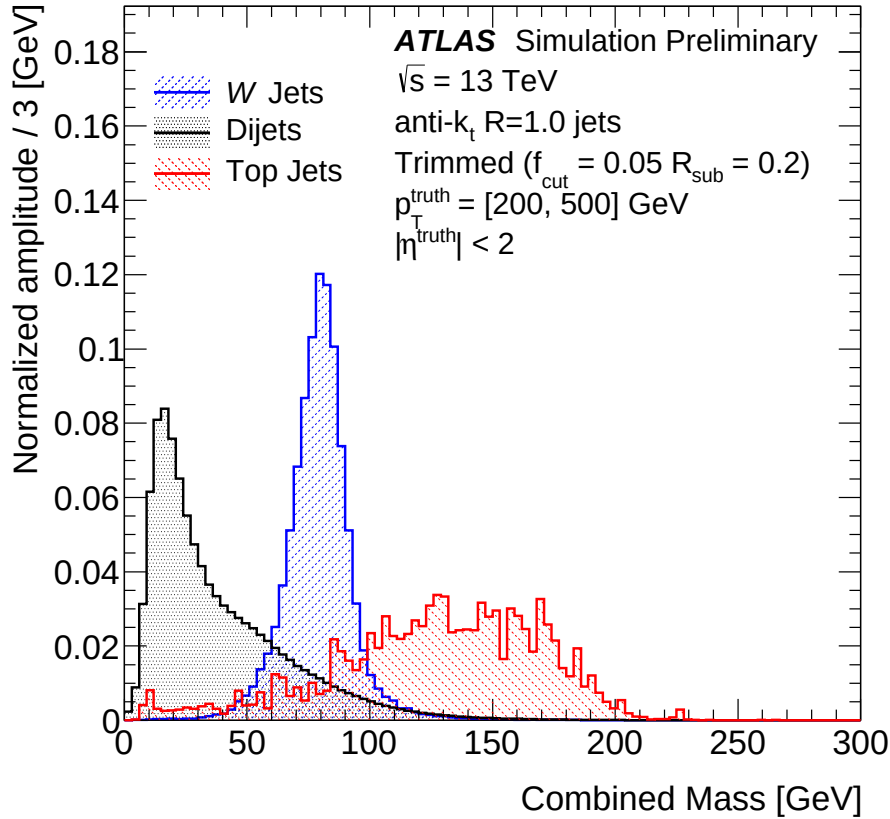


Figure 3–16 Distribution of combined jet mass m_{comb} , showcasing the effective separation between QCD jets, W-boson jets, and top-quark jets^[79].

tween QCD jets and jets from hadronically decaying massive particles. Optimal variables vary with the target process, leading to distinct tagging approaches for W-bosons and top-quarks as shown in Figures 3–17 and 3–18. Advanced machine learning techniques such as Boosted Decision Trees (BDTs) and Deep Neural Networks (DNNs), utilizing about ten substructure variables, have shown performance improvements. For instance, W-tagging benefits by approximately 25% from BDTs or DNNs, while top-tagging efficiency doubles with these methods^[79].

H-tagging ($H \rightarrow b\bar{b}$ identification) predominantly relies on b-tagging to minimize the extensive QCD background. Additional cuts on jet mass and other substructure variables enhance sensitivity^[80], with H-tagging efficiency for various selections depicted in Figure 3–19. In terms of QCD rejection, a single b-tag achieves a background rejection factor of about

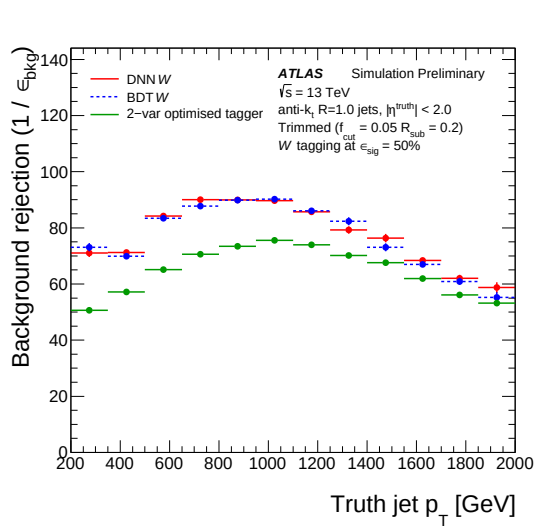


Figure 3–17 Comparison of W-tagging performance at a fixed 50% signal efficiency, using either two-variable optimized taggers or more complex BDTs and DNNs^[79].

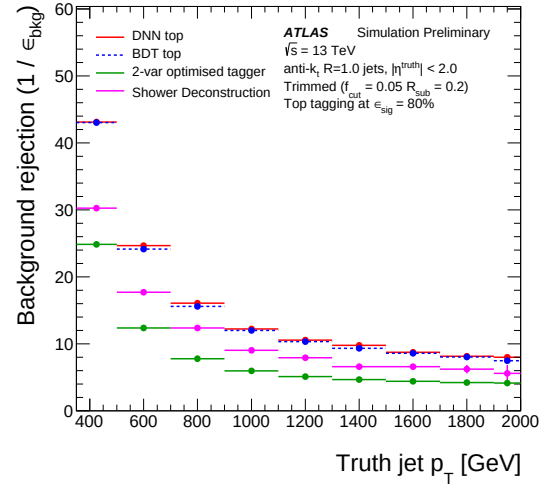


Figure 3–18 Comparison of top-tagging performance at a fixed 80% signal efficiency, illustrating the efficiency gains from using two-variable taggers versus BDTs and DNNs^[79].

50, which increases to 200 with two b-tags, 600 with a mass cut, and over 1000 with further substructure adjustments.

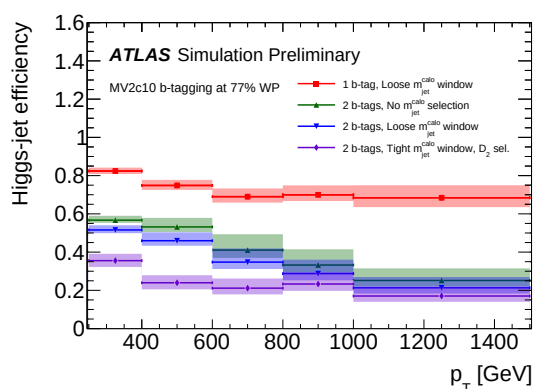


Figure 3–19 H-tagging signal efficiency for various tagging cuts, with corresponding QCD jet rejection factors for each option listed in the text^[80].

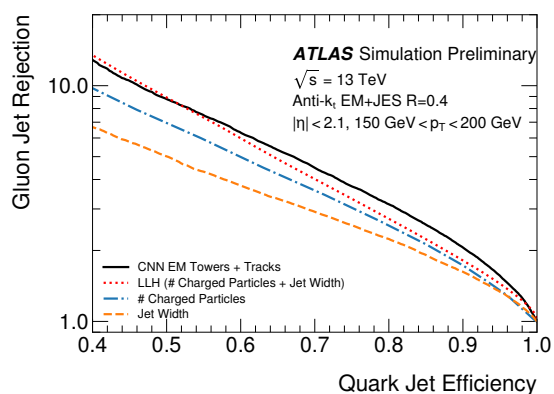


Figure 3–20 Performance of non-top-quark versus gluon discrimination using track multiplicity, jet width, their combination, and a Convolutional Neural Network (CNN)^[81].

Chapter 4 Observation and Differential Measurement of Wgamma Process with ATLAS Detector

4.1 Introduction

The initial investigation in this thesis examines the scattering between two vector bosons, $VV \rightarrow VV$, where V represents W , Z , or γ . These reactions allow for probing and investigating the electroweak interactions within the framework of the Standard Model (SM). They are especially receptive to the interactions among three or four gauge bosons, offering a pathway to uncover potential new phenomena that extend beyond the SM.

The processes of electroweak $VVjj$ production ($EWVVjj$) at the tree level can be categorized into non-vector boson scattering (non-VBS) and VBS. For the sake of gauge invariance, the VBS diagrams that contribute at $O(\alpha_{EW}^4)$ at tree level cannot be isolated from the non-VBS diagrams, hence, they are regarded as the signal for this analysis.

The processes $VVjj$, with VV decaying into leptons—for instance, electroweak production of like-sign WW , $WZjj$, and $ZZjj$ —are established in various reports^[10-15]. Prior to this report, the $W\gamma jj$ channel had not been reported in ATLAS. Conversely, the CMS team^[82] has declared their discovery with an observed (expected) significance of 5.3 (4.8) σ for $EWW\gamma jj$ in the $l\nu\gamma jj$ end state.

The diagrams below 4–1 illustrate select representative diagrams for the signal and background processes under study. In this particular analysis, the focus is on the electroweak production of $W\gamma jj$. Both VBS and non-VBS productions are considered as the signal, with the principal background being the QCD production of $W\gamma jj$, which is shown in the final diagram.

The differential cross-section is evaluated using several variables like m_{jj} , p_T^{jj} , $\Delta\phi_{jj}^{\text{signed}}$, p_{T_l} , $M_{W\gamma}$, and $\Delta\phi_{l\gamma}^{\text{signed}}$, which are all sensitive to the VBS process and to dimension-8 operators in the context of an Effective Field Theory (EFT). These indicators are of particular interest for the identification of anomalous Quartic Gauge Couplings (aQGC). Following the extraction of the EW signal via a binned log-likelihood fit, a Bayesian unfolding method is utilized to adjust these observables for detector effects.

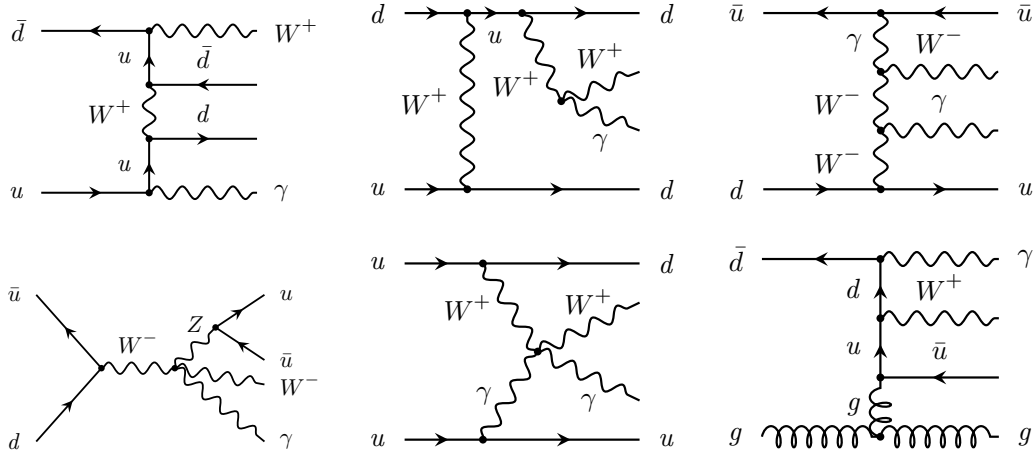


Figure 4–1 From left to right the diagrams show: (i) Electroweak $W\gamma jj$ production without self-interaction of gauge bosons. (ii) EW $W\gamma jj$ non-VBS production featuring triple gauge boson interactions (Bremsstrahlung). (iii) $W\gamma$ VBS with triple gauge boson couplings. (iv) EW $W\gamma jj$ non-VBS occurring via a three-boson interaction with quartic gauge couplings. (v) $W\gamma$ VBS with quartic gauge boson couplings. (vi) QCD $W\gamma jj$ production.

4.2 Event Simulation with Monte Carlo

4.2.1 Monte Carlo Methodology

In this analysis, Monte Carlo (MC) simulations are pivotal for modeling both the signal and selected background events. These simulations are integral for defining the selection criteria of the analysis and for the assessment of systematic uncertainties. Occasionally, they are utilized within control regions for the derivation of data-driven fake estimates (refer to sections on data-driven estimates of jets masquerading as electrons and jet-induced muon fakes) and for the validation of such estimates (refer to the MC closure tests in the section on jet-induced photon fakes). All MC samples are generated using version 21.2.194 of the ATLAS Athena software, adopting the STDM4 standard model derivation and ptg4 4460. The exhaustive enumeration of MC samples is detailed in appendix A.1. Table 4–1 provides a synopsis of the event generators deployed.

4.2.2 Signal and background simulation

The nominal electroweak $W\gamma jj$ sample is produced with *Sherpa*2.2.12^[83] at leading order. The matrix element calculation is done with *NNPDF*3.1 pdf set^[84].

Process	Prompt/Non-prompt	Generator	ME Accuracy	PDF	Shower & Hadronization	Parameter Tune
EW $W\gamma jj$	Prompt	Madgraph5	LO	NNPDF3.1 LO	Pythia8+EvtGen	A14
		Sherpa 2.2.12	LO	NNPDF3.0 NLO	Sherpa	Default
QCD $W\gamma jj$	Prompt	Sherpa 2.2.11	NLO	NNPDF3.0 NLO	Sherpa	default
		Madgraph5	NLO	NNPDF3.0 NLO	Pythia8+EvtGen	A14
EW $Z\gamma jj$	Prompt	Madgraph5	LO	NNPDF3.1 LO	Pythia8+EvtGen	A14
QCD $Z\gamma jj$	Prompt	Sherpa 2.2.11	NLO	NNPDF3.0 NLO	Sherpa	default
$t\bar{t}\gamma$	Prompt	Madgraph5	LO	NNPDF2.3 LO	Pythia8+EvtGen	A14
$tW\gamma$	Prompt	Madgraph5	LO	NNPDF3.0 NLO	Pythia8+EvtGen	A14
$tq\gamma$	Prompt	Madgraph5	LO	NNPDF3.0 NLO	Herwig7+EvtGen	Default
Single Top	Non-Prompt	Powheg	NLO	NNPDF3.0 NLO	Pythia8+EvtGen	A14
W+jets	Non-Prompt	Sherpa 2.2.11	NLO	NNPDF3.0 NNLO	Sherpa	Default
Z+jets	Non-Prompt	Sherpa 2.2.11	NLO	NNPDF3.0 NNLO	Sherpa	Default
Diboson	Non-Prompt	Sherpa 2.2.12	NLO	NNPDF 3.0 NNLO	Sherpa	Default
Dijet	Non-Prompt	Pythia8	LO	NNPDF2.3 LO	Pythia8+EvtGen	A14
EW Wjj	Non-Prompt	Sherpa 2.2.1	LO	NNPDF3.0 NNLO	Sherpa	default
EW Zjj	Non-Prompt	Sherpa 2.2.1	LO	NNPDF3.0 NNLO	Sherpa	default
$t\bar{t}$	Non-Prompt	Powheg	NLO	NNPDF3.0 NLO	Pythia8+EvtGen	A14
tW	Non-Prompt	Powheg	NLO	NNPDF3.0 NLO	Pythia8+EvtGen	A14

Table 4–1 Overview of Monte Carlo (MC) simulation tools employed for event replication in this study. Comprehensive explanations and bibliographic citations are detailed within the main text.

MC representations of immediate backgrounds serve as models for analytical fitting, whereas representations of delayed backgrounds are restricted to control zones for empirical falsification estimations or for validating these estimations through consistency trials.

Additional samples of the electroweak $W\gamma jj$ and $Z\gamma jj$ processes are generated using MadGraph5^[85] at the leading order. For the calculations of the matrix elements, the NNPDF3.1 PDF set^[84] is employed. Subsequently, the parton level events are processed by Pythia8, which incorporates parton showering, hadronisation, and the underlying event dynamics. The A14 set of tuned parameters^[86] is utilized in Pythia8. Additionally, EvtGen^[87] is applied to model the decay properties of bottom and charmed hadrons.

A significant discrepancy is observed in the total cross sections for the electroweak $W\gamma jj$ signal samples between Sherpa and MadGraph. Specifically, Sherpa reports a cross section of 1.78 nb, while MadGraph shows a higher value of 2.52 nb. Given the more recent data from Sherpa, it is designated as the default for analyses. However, due to the unresolved nature of this discrepancy, both expected significances and fiducial cross sections are presented for each sample.

The dominant background in this study stems from events featuring a leptonically decaying W , a photon, and two jets originating from strong interactions. This background is

simulated using Sherpa 2.2.11^[83]. The matrix element for events with up to two partons is computed at next-to-leading order, while for 2 to 4 partons, the computation reverts to leading order. The Comix^[88] and OpenLoops^[89-90] libraries are utilized for generating parton-level predictions. Additionally, the CKKW matching procedure^[91] is employed to merge different final state topologies. The NNPDF3.0 PDF set at next-to-leading order is used for these calculations. Sherpa with default settings handles parton showering, hadronisation, and the underlying event dynamics. This simulation serves as the nominal estimate for the QCD background. The same generator setup is also applied to produce the QCD $Z\gamma jj$ sample for QCD background estimation and the W +jets and Z +jets samples for the Monte Carlo closure test of the jet-to-photon misidentification rate.

A secondary QCD $W\gamma jj$ sample is employed to assess the systematic uncertainties associated with the generator choice in the estimation of the QCD $W\gamma jj$ background. This sample is generated with MadGraph5 at next-to-leading order using the NNPDF3.0 PDF set at NLO^[84]. Pythia8 is utilized for parton showering, hadronisation, and handling the underlying event dynamics with the A14 tuning parameters^[86]. Moreover, EvtGen is used to simulate the decay properties of bottom and charmed hadrons^[87].

Backgrounds from $tW\gamma$, $tq\gamma$, and $t\bar{t}\gamma$ events are simulated using MadGraph5 at leading order. The NNPDF2.3 PDF set at leading order is employed for the $t\bar{t}\gamma$ sample, whereas the NNPDF3.0 PDF set at next-to-leading order is utilized for the $tW\gamma$ and $tq\gamma$ samples. Pythia8 with the A14 tune and EvtGen are used for parton showering, hadronisation, underlying event activity, and the decay properties of bottom and charmed hadrons in the $t\bar{t}\gamma$ and $tW\gamma$ samples. For the $tq\gamma$ sample, Herwig7 with default settings simulates the parton showering, hadronization, and underlying event activity.

Backgrounds from single top t -channel production are generated using Powheg at next-to-leading order, employing the NNPDF3.0 PDF set at the same order. Pythia8 with the A14 tune and EvtGen are again used for parton showering, hadronisation, and underlying event activity, as well as for modeling the decays of bottom and charmed hadrons. This configuration also produces backgrounds from $t\bar{t}$ events and events involving a single top and a W boson. The overlap between tW and $t\bar{t}$ diagrams is addressed using the DR scheme, which sets the amplitude of overlapping diagrams to zero.

Diboson and dijet events are simulated for data-driven estimates of jets faking leptons.

The diboson sample is generated using Sherpa 2.2.2 at next-to-leading order with the NNPDF3.0 PDF set at next-to-next-to-leading order, while Sherpa handles the showering, hadronization, and underlying event activity with default settings. The dijet sample is produced with Pythia8 at leading order using the NNPDF2.3 PDF set at leading order, with Pythia8 and EvtGen used for parton showering, hadronisation, and underlying event activity.

Electroweak Wjj and Zjj events, employed in cross-checks of the jet-to-photon misidentification estimate, are generated at next-to-leading order using Sherpa 2.2.1. The NNPDF3.0 PDF set at next-to-next-to-leading order is used for these simulations. For parton showering, hadronization, and underlying event activity, Sherpa with default parameter tunes is utilized.

All Monte Carlo simulations are processed through the GEANT4 simulation^{GEANT4} of the ATLAS detector, and reconstructed using the same algorithms as the data. Discrepancies in trigger, reconstruction, isolation, identification, and tagging efficiencies between the data and Monte Carlo are adjusted for on an event-by-event basis using scale factors. Multiple proton-proton interactions within the same or nearby bunch crossings (pileup) are simulated with Pythia8 using the A3 tune and the NNPDF2.3LO PDF set. These simulated pileup events are added to the primary Monte Carlo samples and reweighted to ensure the average number of proton-proton interactions in the simulations aligns with the observed data.

4.2.3 Sample Overlap Removal

Samples containing n photons in the matrix element undergo cuts on the photon's transverse momentum and ΔR with the lepton to properly fill the phase space. These samples need to be merged with samples containing $n - 1$ photons in the matrix element, complemented by additional photons from the showering process that are not subject to these cuts. This integration, however, risks double counting when photons from the showering pass the kinematic cuts designated for the photons in the dedicated samples. To mitigate this issue, an overlap removal procedure is implemented across all $X\gamma$ and X sample pairs, which includes our signal $W\gamma$ and VBF W , electroweak $Z\gamma$ and VBF Z , QCD $W\gamma$ and W +jets, QCD $Z\gamma$ and Z +jets, $t\gamma$ and $t\bar{t}$, as well as $tW\gamma$ and tW . The overlap removal is conducted using the VGammaORTool^[92].

4.2.4 Data

The analysis utilizes the complete Run 2 dataset acquired by the ATLAS detector from 2015 to 2018 during proton-proton (pp) collisions at a center-of-mass energy of $\sqrt{s} = 13$ TeV, provided by the LHC. The data are required to satisfy single lepton trigger conditions and various data quality criteria, which ensure proper operation of the detector throughout the data collection period. The runs that meet these criteria are documented in good run lists. The dataset corresponds to an integrated luminosity of 139 fb^{-1} . The associated uncertainty with this measurement of integrated luminosity is reported as 1.7% ^[93].

- GoodRunsLists/data15_13TeV/20170619/data15_13TeV.periodAllYear_DetStatus-v89-pro21-02
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- GoodRunsLists/data16_13TeV/20180129/data16_13TeV.periodAllYear_DetStatus-v89-pro21-01
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- GoodRunsLists/data17_13TeV/20180619/data17_13TeV.periodAllYear_DetStatus-v99-pro22-01
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- GoodRunsLists/data18_13TeV/20190318/data18_13TeV.periodAllYear_DetStatus-v102-pro22-04
_Unknown_PHYS_StandardGRL_All_Good_25ns_TriggerNo17e33prim.xml

4.3 Event Selection

Since we have introduced how the objects are reconstructed in the ATLAS detector in section 3.4, one can define a set of selections applied on these objects appears in one event. In this analysis, baseline event selections are decided after optimization which follows the rules:

- The event reconstructs at least one vertex candidate. The primary vertex is identified as the one with the greatest sum of p_T^2 from its associated tracks.
- The event includes at least two jets, one tight and isolated lepton, and a minimum of one tight and isolated photon. The tag jets, used for calculating dijet variables, are the

two jets with the highest p_T .

- There is an absence of a second lepton of the same flavor that meets loose identification criteria.
- The event exhibits missing transverse energy greater than or equal to 30 GeV.
- The angular separation between the leading jet (or the second jet) and the missing transverse energy, $\Delta\Phi(j1(2), \text{MET})$, is greater than 0.4.
- The transverse mass of the W boson is at least 30 GeV.
- The mass of the photon-lepton system, $M_{l\gamma}$, deviates from the Z boson mass by at least 10 GeV: $|M_Z - M_{l\gamma}| > 10 \text{ GeV}$.
- The two leading jets each have $p_T > 50 \text{ GeV}$ and are separated by a $\Delta R > 0.4$.
- The event does not contain any b-tagged jets.
- The mass of the dijet, formed by the two leading jets, is at least 500 GeV.

In the neural network distribution analysis, an additional criterion of $\Delta Y(jj) > 2$ is implemented. For the differential extraction process, the threshold for M_{jj} is raised to 1 TeV. Conversely, in the analysis of $\Delta Y(jj)$, the $\Delta Y(jj) > 2$ requirement is omitted, and the M_{jj} criterion is adjusted to 700 GeV.

The event yields along with the Monte Carlo predicted yields for both the electron and muon channels are detailed in Table A–2 and Table A–3 in appendix A.3, respectively. It is important to note the observed discrepancies between the actual event yields and the total predicted yields; these can be attributed to the exclusion of Monte Carlo fake backgrounds in the tables. These fake backgrounds are instead estimated using data-driven methods as detailed in Section 4.4.

4.4 Background Estimation

4.4.1 Jet fake photons

4.4.1.1 The template fit method

The template fit method leverages the distinct distribution shapes of isolation energy in tight and non-tight data events identified as photons. The isolation energy is defined by the equation:

$$E_{iso} = E_T^{cone40} - 0.022 \cdot pT \quad (4-1)$$

To determine the count of jets mimicking tight and isolated photons, the approach in each bin is as follows:

- The isolation distribution of tight, truth-matched photons from Monte Carlo simulations is used to derive a prompt photon template shape. This fitting utilizes the Sherpa electroweak $W\gamma jj$ and Sherpa QCD $W\gamma jj$ Monte Carlo samples that include a real photon, chosen for their substantial statistical data.
- A template shape for a jet faking a photon is obtained by fitting the isolation distribution of non-tight data.
- A probability density function (pdf) is constructed by summing the templates of the prompt photon and the jet faking photon. The normalization is adjusted to match data containing a reconstructed tight photon. During this fitting, the template parameters are allowed to vary but are constrained by multivariate Gaussians determined by the optimal fit parameters and their uncertainties from the template shape extraction. This procedure ensures the propagation of statistical uncertainties from the template fit to the final result.
- The component of the jet faking photon is integrated up to an isolation threshold of 2.45 GeV to estimate the yield of jets that fake tight and isolated photons.

4.4.1.2 Jet fake photon uncertainties

Four sources of uncertainty on the jet faking photon background are considered:

1. Statistical error on the jet faking photon yield
2. Real photon subtraction from the control region
3. Photon loose identification definition systematic
4. Real photon isolation modelling uncertainty.

Complete study of jet fake photon uncertainties are recorded in appendix A.4.

4.4.1.3 Jet fake photon results

The background of jet faking photons is determined using a template fit method. The uncertainties incorporated in this method include: statistical uncertainties from the data and Monte Carlo used in the fit; systematic uncertainties due to real photon leakage into the jet faking photon-enriched control region; variations based on the choice of loose photon identification working point; and uncertainties in the modeling of real photon isolation within the Monte Carlo simulations. Systematic variations and their corresponding uncertainties are quantified using a bootstrapping procedure. The resulting jet faking photon yields, which are utilized for fitting the neural network, are depicted in Figure 4–2. The ratio panel in the figure illustrates the size of the variation relative to the nominal yield. It should be noted that in estimating the yield in the signal region, half of the data is used, and these events are utilized twice as part of the blinding strategy.

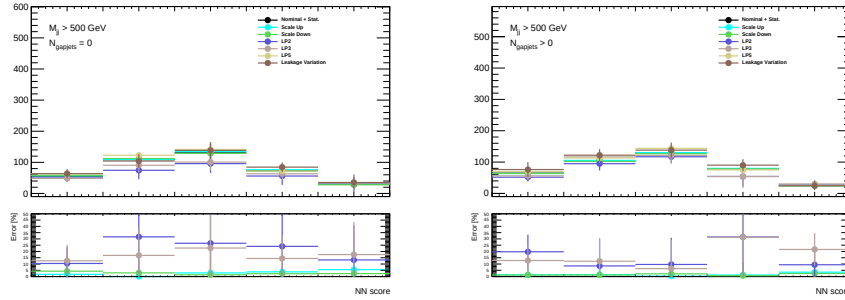


Figure 4–2 Distribution of jet faking photon NN scores and associated uncertainties.^[94]

4.4.2 Jet fake electron

4.4.2.1 Fake factor method

In scenarios where a prompt photon coincides with jet production, misidentification of jets as leptons (electrons or muons) may contaminate the signal region. The likelihood that a hadronic jet is erroneously reconstructed as a lepton may be underestimated by Monte Carlo (MC) simulations. Consequently, we adopt a data-driven approach to quantify the impact of misidentified hadronic jets. True leptons typically satisfy stringent quality criteria, whereas misidentified leptons, or ‘fake leptons,’ often fail to meet these high-quality standards, including isolation and identification requirements.

Estimation of the fake lepton background is performed utilizing a jet-enriched dataset acquired by the ATLAS detector. The dataset employed for calculating the fake factor requires passing a relaxed selection criteria that maintains all nominal analysis selections except the lepton quality filters. Events containing high-quality leptons, characterized by stringent identification (tight-id) and isolation (tight-iso) criteria, are classified as 'tight' events. The analysis proceeds by distinguishing between 'loose' and 'tight' samples, facilitating the definition of fake efficiency, ϵ , and fake factor, F , as described in Equations 4–2 and 4–3 respectively.

The notations used are elucidated as follows:

- ϵ represents the fake efficiency.
- N_e^{loose} denotes the count of fake lepton events passing the baseline selection without stringent lepton quality checks.
- N_e^{tight} indicates the count of fake lepton events that comply with both the baseline and strict lepton quality criteria.
- F symbolizes the fake factor.

$$\epsilon = \frac{N_e^{\text{tight}}}{N_e^{\text{loose}}} \quad (4-2)$$

$$F = \frac{\epsilon}{1 - \epsilon} \quad (4-3)$$

This analysis further refines the fake factor for jets faking leptons by examining dijet samples. We compute this by the ratio of the number of jets meeting tight lepton selection criteria to those that only satisfy anti-tight lepton criteria, adjusted across various lepton transverse momentum (p_T) and pseudorapidity ranges. Corrections are applied to account for prompt lepton contamination based on MC simulations. The fake lepton background within the signal region is subsequently estimated as follows:

$$N_{\text{fakelep}} = F_{e/\mu} \times (N_{e/\mu\text{-data}}^{\text{anti-tight}} - N_{e/\mu\text{-prompt lepton}}^{\text{anti-tight}}) \quad (4-4)$$

Defining 'loose' electrons is critical for accurate estimation of the jet fake electron factor using the fake factor methodology. This definition influences both the statistical reliability and the purity of the dataset utilized in estimating F . The purity of the jet-enriched sample pivotal to calculating F has been rigorously validated. Figure 4–3 illustrates the distribution within the dijet control region, predominantly comprising dijet events, which constitute approximately 80% of this region.

The definitions of electron types used in this analysis are as follows:

- Tight Electron
 - $p_T > 20 \text{ GeV}$
 - $|\eta| < 2.5$
 - $|d_0/\sigma_{d_0}| < 5$
 - $|z_0 \times \sin(\theta)| < 0.5 \text{ mm}$
 - Iso-Tight, Id-Tight
- Loose Electron
 - $p_T > 20 \text{ GeV}$
 - $|\eta| < 2.5$
 - $|d_0/\sigma_{d_0}| < 5$
 - $|z_0 \times \sin(\theta)| < 0.5 \text{ mm}$
- Anti-Tight Electron
 - passes Loose Electron criteria
 - fails Tight Electron criteria

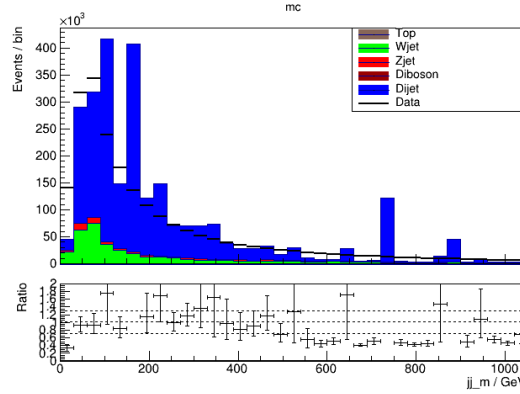


Figure 4–3 Distribution of components within the dijet control region.^[94]

4.4.2.2 Fake factor measurements with dijet sample

A dijet data sample serves as the basis for measuring the jet fake electron factors, whereas a Z+jets data sample, although evaluated, was excluded from this application due to its low jet purity and insufficient statistical power.

The selection criteria for the dijet sample used in the fake factor analysis stipulate that each event must contain at least one jet and one lepton. The lepton must trigger at least one of

the un-prescaled electron or muon triggers employed in the analysis, which are summarized in Table 4–2. Employing the same triggers ensures consistency in defining the anti-tight region, as articulated in Equation 4–4. The leading jet in these dijet events must have a transverse momentum $p_T > 30$ GeV and meet specific quality standards. The events are further refined by requiring the missing transverse momentum E_T^{miss} to be less than 20 GeV and the reconstructed transverse invariant mass of the $W(\rightarrow l\nu)$ system to also be below 20 GeV, effectively excluding $W(\rightarrow l\nu) + jets$ events. The angular separations $|\Delta\phi(l, jet)|$ and $|\Delta R(l, jet)|$ are analyzed to further minimize contamination from other processes, thereby enhancing the purity of the di-jet control region. The complete event selection criteria for dijet events used in calculating lepton fake factors are listed in Table 4–3.

Lepton Triggers
HLT_24_lhmedium_L1EM20VH
HLT_e60_lhmedium
HLT_e120_lhloose
HLT_e26_lhtight_nod0_ivarloose
HLT_e60_lhmedium_nod0
HLT_e140_lhloose_nod0
HLT_mu20_iloose_L1MU15
HLT_mu26_ivarmedium
HLT_mu50

Table 4–2 Un-prescaled lepton triggers used in the analysis.

Data collected over the entire Run-2 period is utilized to compute the fake factors. Figure 4–4 displays a comparison between data and MC simulations in both the tight and anti-tight regions. Although both regions are predominantly influenced by dijet production, the fraction of dijet events is smaller in the tight region due to the stringent electron quality required, making it challenging for jet fake electrons to be classified as such.

Prompt leptons from processes like $W(\rightarrow l\nu) + jets$, $Z(\rightarrow ll) + jets$, and top-related events are subtracted from the data in both regions. The residual events in the tight region are considered as jet fake electrons that meet the tight selection criteria, thereby forming the numerator in the fake factor calculation. Conversely, events remaining in the anti-tight region constitute the denominator. Both the numerator and denominator are tabulated in a 2-D histogram against electron p_T and η .

Dijet Event Selection

GRL

Trigger

$$N_l = 1 \text{ and } p_T^l > 20 \text{ GeV}$$

$$N_{jet} \geq 1 \text{ and } p_T^{jet} > 30 \text{ GeV}$$

B-jet veto

$$E_T^{\text{miss}} < 20 \text{ GeV}$$

$$m_T^W < 20 \text{ GeV}$$

$$|\Delta\phi(l, jet)| > 2.5$$

$$|\Delta R(l, jet)| > 3.8$$

Tight or Loose

Table 4–3 Dijet event selection criteria for the fake factor calculation, optimized to suppress non-dijet event contributions.

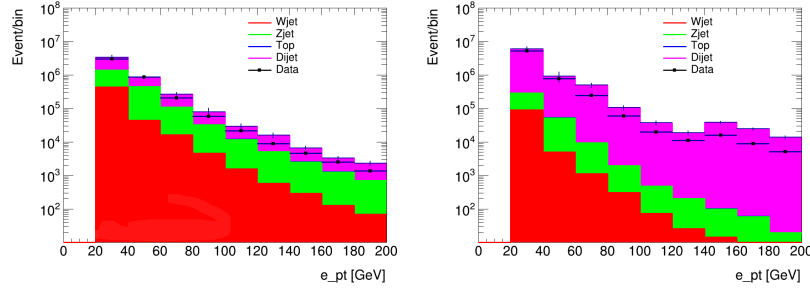


Figure 4–4 Left: Data-MC comparison in the tight region, showing contributions from dijet, W/Z+jets, and minor top-related processes. Right: The anti-tight region is predominantly dominated by dijet events. In the fake factor calculations, non-dijet processes are subtracted from real data collected from collisions. The remaining events in the tight region serve as the numerator, while those in the anti-tight region serve as the denominator.^[94]

Lepton fake factors are finally estimated as a function of lepton p_T and η . Table 4–4 enumerates the electron fake factors across different p_T and η bins.

4.4.2.3 Application of the fake factor

The distribution of fake leptons is determined utilizing the fake factors previously derived. Specifically, for fake electrons within each designated tight region, a corresponding anti-tight region is defined by relaxing the electron isolation and identification criteria. All other selection parameters for this anti-tight region remain consistent with those defined for the tight region. The distribution of fake electrons in the tight region is subsequently calculated

Fake Factor			
$\eta \backslash p_T$	$p_T[20, 40]$	$p_T[40, 140]$	$p_T[140, 1000]$
$\eta[2, 2.5]$	0.494 ± 0.004	0.807 ± 0.011	0.158 ± 0.003
$\eta[1.52, 2]$	0.394 ± 0.004	0.762 ± 0.012	0.223 ± 0.005
$\eta[1.37, 1.52]$	0.241 ± 0.020	0.367 ± 0.054	0.136 ± 0.048
$\eta[1, 1.37]$	0.409 ± 0.005	0.774 ± 0.023	0.279 ± 0.010
$\eta[0.5, 1]$	0.437 ± 0.005	0.796 ± 0.021	0.323 ± 0.013
$\eta[0, 0.5]$	0.401 ± 0.005	0.784 ± 0.025	0.314 ± 0.016

Table 4–4 Fake factor for electron in each p_T and η bin.

by applying the fake factor to the distribution of fake-enriched electrons identified within the anti-tight region. Concurrently, contributions from prompt electrons are subtracted from the observed data in the anti-tight region, utilizing Monte Carlo (MC) simulated events to correct for this contamination.

4.4.2.4 Systematic uncertainties

The estimation of jet fake electrons using the dijet sample incorporates multiple sources of systematic uncertainties, which are enumerated as follows:

1. **Statistical Uncertainty:** This is influenced by the event yield in the corresponding anti-tight regions. The nominal event yield for each anti-tight region is determined by subtracting the prompt Monte Carlo (MC) components from the data. Statistical uncertainties are then automatically propagated by ROOT histograms.

2. **Sample Composition Differences:** Variations in composition between the dijet and $\gamma + jets$ samples can affect the fake factor estimation. The truth compositions of both $\gamma + jets$ and dijet samples, predominantly composed of photon conversions (background electrons originating from converted photons) and Dalitz decays (decay of an electrically neutral pseudoscalar meson into a dilepton pair and a photon)^[95], are analyzed post-baseline selections without quality cuts on electrons. Contributions from heavy flavor jets also play a minor role in the composition of fake electrons. Systematic uncertainties due to the compositional differences in the fake factor between $\gamma + jets$ and dijet processes are considered. Figures 4–5 and 4–6 illustrate the compositions and electron fake factors from simulated dijet and $\gamma + Jets$ events respectively.

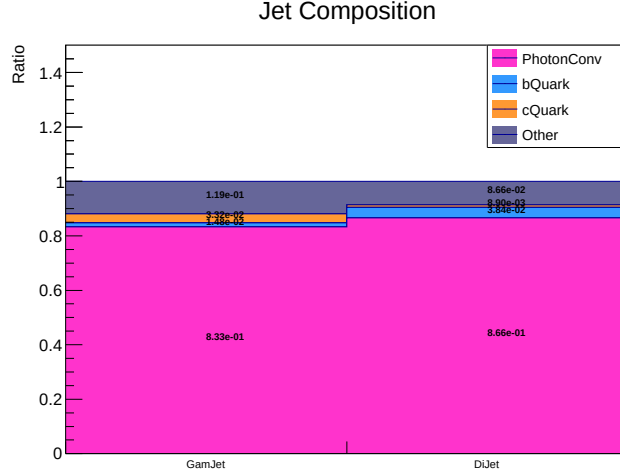


Figure 4–5 Jet composition in dijet and $\gamma + Jets$ samples.^[94]

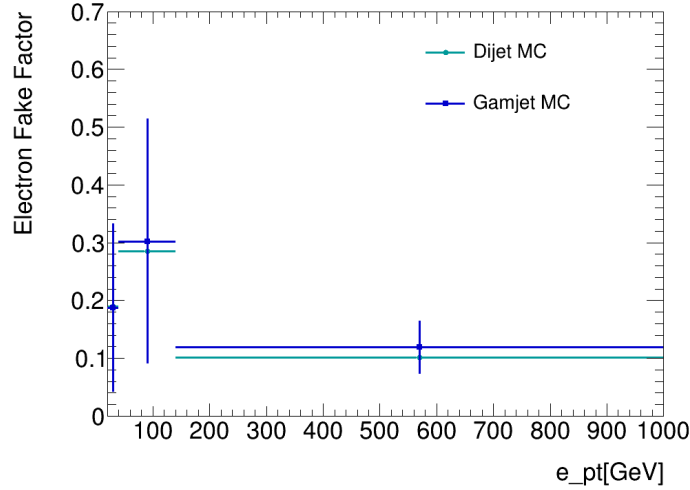


Figure 4–6 Electron fake factor closure test from simulated events.^[94]

3. Selection Cut Variations: Variations in the selection criteria for the dijet sample, such as $E_T^{\text{miss}} < 20$ GeV, $m_T^W < 20$ GeV, and $p_T^{\text{jet}} > 30$ GeV, are potential sources of systematic uncertainty. These cuts are varied by 5 GeV to assess their impact on the fake factors, with results tabulated in Table 4–5.

4. Prompt Lepton Subtraction: The final jet fake electron distribution is obtained by applying electron fake factors to the corresponding anti-tight regions, with prompt composition subtracted using MC simulations. Sherpa and MadGraph are utilized to simulate the QCD induced $W\gamma$ process, which is a significant background in the EW $W\gamma$ VBS analy-

sis. The Sherpa-simulated QCD sample is considered nominal, while the MadGraph sample serves as an alternative; the difference in the final jet fake electron distribution is accounted for as systematic uncertainty due to the prompt background subtraction.

5. Different $p_T - \eta$ Binning: The nominal $p_T - \eta$ binning for calculating the electron fake factor is potentially a source of systematic uncertainty. Given the robust statistics provided by the dijet sample, the fake factor is recalculated with refined p_T bins to examine the impact of distribution correlations with p_T . An alternative p_T binning and the corresponding fake factors are documented in Table 4–6.

6. Scale Factors for W/Z+jets Processes: The Wjets and Zjets processes are predominant in the dijet regions used for fake factor calculations. Variations in the yield of these background processes due to applied scale factors can affect the nominal fake distributions. Theoretical uncertainties associated with W/Z+jets events are thus included and analyzed.

fake factor	$p_T[20, 40]$	$p_T[40, 140]$	$p_T[140, 1000]$
nominal	0.378 ± 0.004	0.599 ± 0.012	0.148 ± 0.005
MET-down	0.393 ± 0.005	0.628 ± 0.014	0.152 ± 0.005
MET-up	0.364 ± 0.004	0.586 ± 0.010	0.148 ± 0.004
m_T^W -down	0.372 ± 0.005	0.590 ± 0.013	0.150 ± 0.005
m_T^W -up	0.382 ± 0.004	0.615 ± 0.011	0.147 ± 0.004
p_T^{jet} -down	0.378 ± 0.004	0.599 ± 0.012	0.148 ± 0.005
p_T^{jet} -up	0.362 ± 0.004	0.587 ± 0.011	0.148 ± 0.005

Table 4–5 Systematic variations of fake factor for electrons in p_T bins

η	$\eta[0, 0.5]$	$\eta[0.5, 1]$	$\eta[1, 1.37]$	$\eta[1.37, 1.52]$	$\eta[1.52, 2]$	$\eta[2, 2.5]$
p_T						
$p_T[20, 40]$	0.363 ± 0.012	0.375 ± 0.012	0.358 ± 0.011	0.179 ± 0.042	0.335 ± 0.007	0.442 ± 0.007
$p_T[40, 50]$	0.680 ± 0.086	0.635 ± 0.077	0.765 ± 0.067	0.306 ± 0.138	0.592 ± 0.039	0.693 ± 0.025
$p_T[50, 60]$	0.984 ± 0.219	0.666 ± 0.182	0.735 ± 0.114	0.577 ± 0.255	0.754 ± 0.059	0.756 ± 0.041
$p_T[60, 70]$	0.337 ± 0.119	0.404 ± 0.064	0.450 ± 0.051	0.413 ± 0.197	0.489 ± 0.031	0.498 ± 0.027
$p_T[70, 80]$	0.383 ± 0.098	0.511 ± 0.092	0.467 ± 0.071	0.313 ± 0.129	0.499 ± 0.036	0.554 ± 0.032
$p_T[80, 90]$	0.494 ± 0.127	0.514 ± 0.104	0.503 ± 0.102	-0.012 ± 0.420	0.402 ± 0.047	0.487 ± 0.045
$p_T[90, 100]$	0.488 ± 0.159	0.681 ± 0.137	0.436 ± 0.090	0.064 ± 0.212	0.465 ± 0.045	0.520 ± 0.042
$p_T[100, 140]$	0.697 ± 0.140	0.622 ± 0.092	0.428 ± 0.056	0.349 ± 0.205	0.432 ± 0.029	0.431 ± 0.021
$p_T[140, 1000]$	0.245 ± 0.038	0.187 ± 0.023	0.215 ± 0.016	0.070 ± 0.081	0.150 ± 0.008	0.114 ± 0.005

Table 4–6 Alternative p_T binning and corresponding fake factors for electron fake estimation

4.4.2.5 Summary of Jet Fake Electron Estimation

The contribution of the jet fake electron background is determined by applying the electron fake factor to the corresponding anti-tight regions as described by Equation 4–4. The prompt contributions within these regions are subtracted using Monte Carlo (MC) simulations that utilize truth information to identify real electrons.

Figure 4–7 displays the estimated yields of jet fake electrons and the associated systematic uncertainties. The plots incorporate systematic terms in a stacked format, providing a visual breakdown of the different contributing factors.

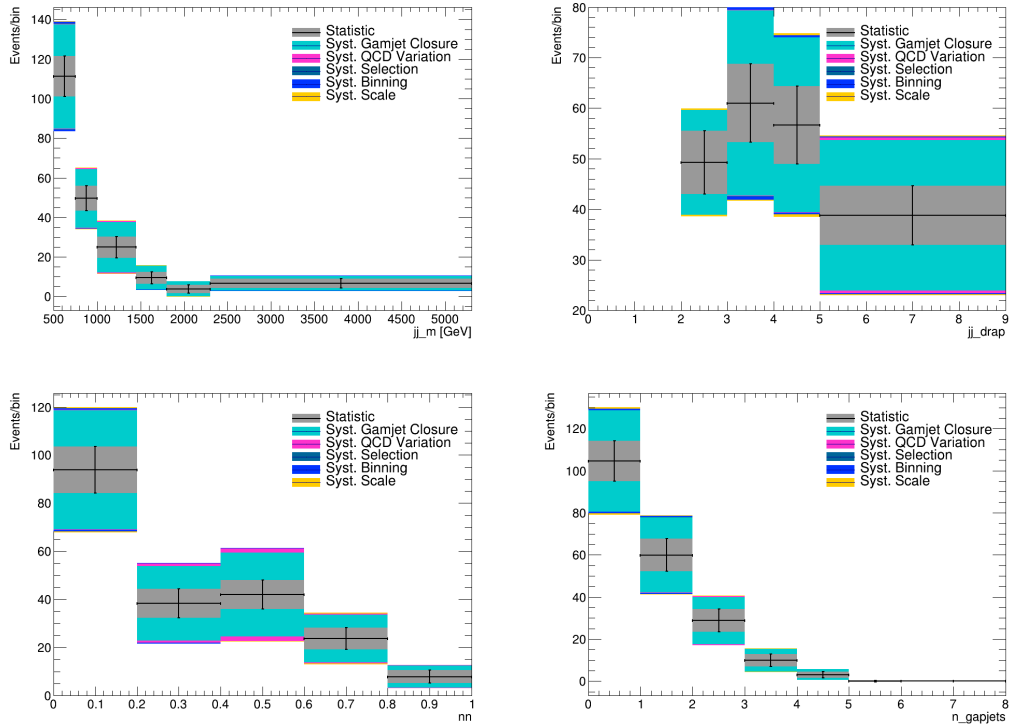


Figure 4–7 Jet Fake Electron Contribution in jj_m . Plots are drawn with systematic terms added in stack format.^[94]

The distribution of jet fake electrons is also analyzed across various kinematic variables of interest, such as $\Delta(Y)_{jj}$, NN score, and $N_{gapjets}$, with corresponding results illustrated in the same figure, respectively.

4.4.2.6 Electron Validation Region

To validate the fake factor method employed for estimating jet fake electrons, a validation region (VR) closely resembling the signal region is selected by inverting the missing transverse energy and transverse mass of the W boson criteria from the signal region. An anti-tight region is similarly defined by relaxing the stringent isolation and identification requirements for electrons.

Comparative analyses between the data and MC are conducted, with results depicted in Figure 4–8. The MC data includes estimations of jet fake electron contributions with systematic uncertainties and contributions from other truth-matched background processes. The comparison demonstrates agreement within one sigma error bars between the data and the stacked MC, indicating the robustness of the fake factor method.

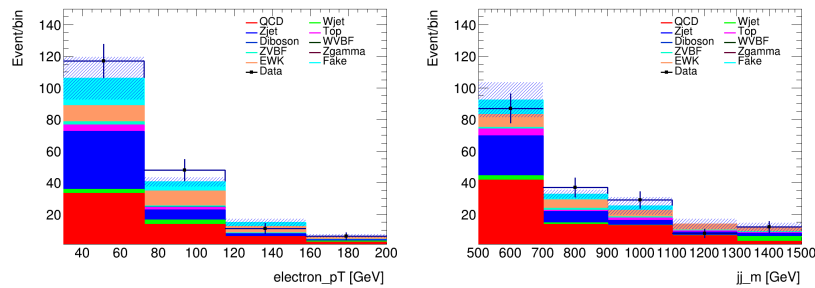


Figure 4–8 Estimation of jet fake electron distribution in the validation region using the fake factor method. Left image shows the distribution versus electron p_T , and the right image illustrates the distribution versus m_{jj} .^[94]

4.4.3 Jet fake muon

In this analysis, the strategy for identifying jet-induced fake muons parallels that used for jet-induced fake electrons. However, the likelihood of jets being misidentified as muons is considerably lower than their misidentification as electrons. Consequently, this section will omit a detailed exposition on the fake factor method and will be concise. Detailed description could be found in appendix A.5.

4.4.3.1 Fake muon estimation in signal regions

The estimated fake factor for jets misidentified as muons in dijet events has been applied to the signal and control regions of the VBS $W\gamma jj$ analysis. This application incorporates

the systematic uncertainties discussed previously. The outcomes, including distributions and yields, are displayed in Figures 4–9.

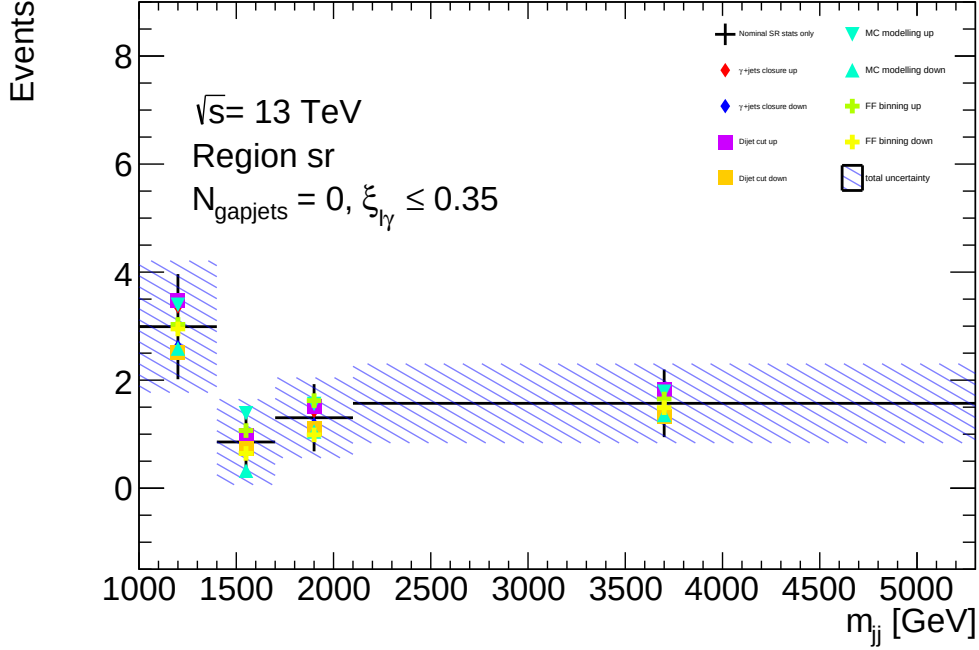


Figure 4–9 Distribution of fake muons for the invariant mass m_{jj} in the signal region, used for signal extraction.^[94]

4.4.4 Lepton faking photons

4.4.4.1 Introduction

Analysis of Figure 4–10 and Figure 4–11 reveals a significant presence of misidentified photons within the Zjets, Wjets, and Diboson Monte Carlo (MC) samples, even after applying baseline selection criteria. Predominantly, the misidentified photons are categorized as electrons or background photons, as illustrated in the corresponding right panels of the figures. The background photons primarily originate from light mesons, particularly π^0 and from final state radiation (FSR) photons. These backgrounds are estimated using the jet-to-photon fake rate method. Notably, in the electron channel of the Zjets MC samples, a substantial number of isolated electrons are erroneously classified as photons.

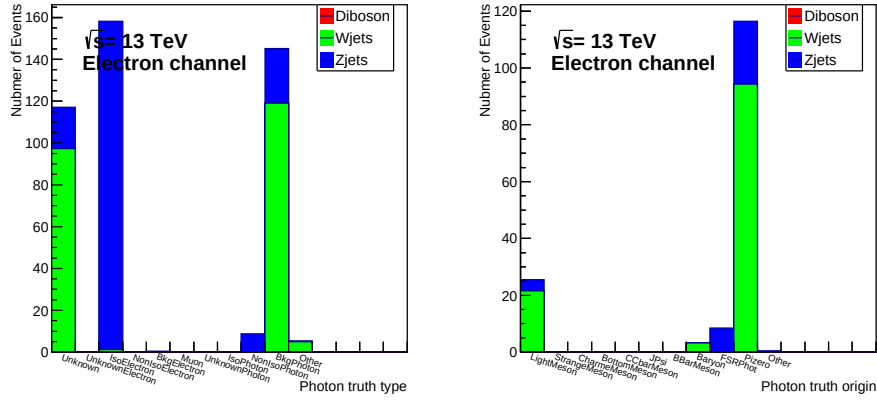


Figure 4–10 Left panel: Distribution of the truth type of photons in Zjets, Wjets, and Diboson MC samples for the electron channel post-baseline selection. Right panel: Distribution of the truth origin of photons, classified as photons, in Zjets, Wjets, and Diboson MC samples for the electron channel post-baseline selection.^[94]

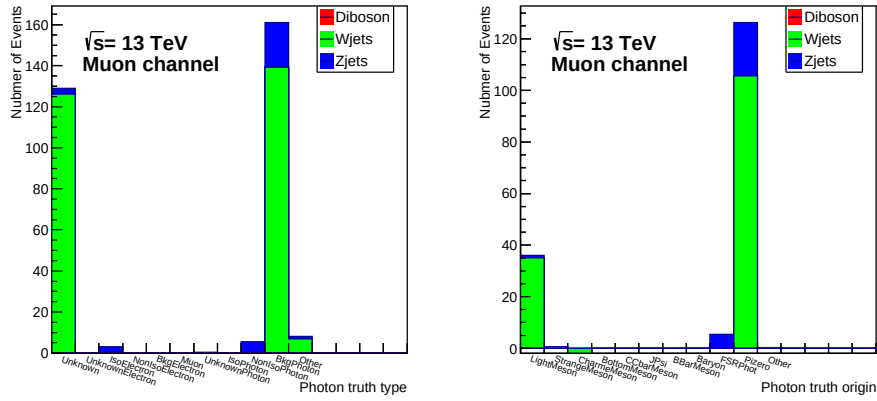


Figure 4–11 Left panel: Distribution of the truth type of photons in Zjets, Wjets, and Diboson MC samples for the muon channel post-baseline selection. Right panel: Distribution of the truth origin of photons, classified as photons, in Zjets, Wjets, and Diboson MC samples for the muon channel post-baseline selection.^[94]

It is feasible that photons could be erroneously reconstructed or identified as electrons due to inefficiencies in tracking or inaccurate alignment between the track and the energy cluster in the calorimeter, as noted by^[96]. To estimate this misidentification, a data-driven approach is utilized rather than relying solely on Monte Carlo simulations. This methodology involves determining the electron to photon fake rate by measuring it in a control region. This control

region is defined by modifying the photon requirements to corresponding electron criteria, either partially or entirely. The fake rate is ascertained using two additional control regions: one that is enriched in actual electrons and another that predominantly contains electron to photon fakes. The expression for the fake rate is formalized as follows:

$$F_{e \rightarrow \gamma} = \frac{N_{\gamma}^{reco} \epsilon_{\gamma}}{N_e^{reco} \epsilon_e} \quad (4-5)$$

Here, N_{γ}^{reco} and N_e^{reco} represent the number of events in regions enriched with fake and real samples, respectively, while ϵ_{γ} and ϵ_e denote the identification efficiencies for photons and electrons, respectively. Subsequently, the determined fake rate is applied to a different control region, where the standard selection criteria for the signal region are adjusted by substituting photons with electrons that have similar transverse momentum (p_T), isolation, and identification requirements. It is crucial that the electron and photon object selection criteria, including trigger requirements in the control regions for fake rate determination, closely align with those in the control and signal regions where the fake rate is subsequently applied.

4.4.4.2 Selection

CRee and CReg The real and fake enriched control regions, denoted as CRee and CReg, respectively, are established by employing a tag-and-probe method similar to that used in the fake factor calculation for identifying a Z boson. The tag electron is required to coincide with the lowest unprecaled single electron trigger. The probe in this setup can be either an electron or a photon. In the CRee region, the probe is an electron, whereas in the CReg region, it is a photon. To ensure high trigger efficiency, the p_T of the tag electron is set at a minimum of 30 GeV, while the p_T threshold for the probe electron is reduced to 22 GeV to align with the photon selection criteria. Both CRee and CReg control regions impose a veto on additional baseline electrons or photons to eliminate ambiguities concerning the source of the electron or electron-to-photon fake associated with the Z boson, and to prevent overlap with other control regions where the fake rate is applied. The detailed selection criteria are summarized in Table 4–7.

Tag electron	Probe electron	Probe photon	Other selections
$p_T > 30 \text{ GeV}$	$p_T > 22 \text{ GeV}$	$p_T > 22 \text{ GeV}$	$m_T^{W(e\nu)} < 20 \text{ GeV}$
$ \eta < 2.5$	$ \eta < 2.37$	$ \eta < 2.37$	$E_T^{miss} < 20 \text{ GeV}$
e_isoTightVarRad	e_isoTightVarRad	gam_isoTight	
e_idTight	e_idTight	gam_idTight	
$ z_0 \times \sin \theta < 5 \text{ mm}$	$ z_0 \times \sin \theta < 5 \text{ mm}$		
$ d_0/\sigma_{d_0} < 3$	$ d_0/\sigma_{d_0} < 3$		
pass single electron triggers	opposite charge with tag electrons		

Table 4–7 Definitions of tag and probe electrons and probe photons for the CRee and CReg control regions.

4.4.4.3 Fake rate estimation

In Z boson decays into two electrons, there exists a potential for each electron to be misreconstructed as a photon. The tag and probe methodology necessitates that the final state includes at least one electron that meets the criteria of the "tag" selection. Assuming the total count of $Z \rightarrow ee$ events is denoted as N , the reconstructed events can be categorized as follows: N_{ee}^{reco} representing events with two electrons, $N_{e\gamma}^{reco}$ for events with one electron and one photon, and $N_{\gamma\gamma}^{reco}$ for events with two photons.

$$N = N_{ee} + N_{e\gamma} + N_{\gamma\gamma} \quad (4-6)$$

$$N = N_{ee}^{reco} + N_{e\gamma}^{reco} + N_{\gamma\gamma}^{reco} \quad (4-7)$$

$$N_{e_{\text{tag}}e_{\text{tag}}}^{reco} = \epsilon_e^2 N_{e_{\text{tag}}e_{\text{tag}}} \quad (4-8)$$

$$N_{e_{\text{tag}}e_{\text{probe}}}^{reco} = \epsilon_e^2 N_{e_{\text{tag}}e_{\text{probe}}} \quad (4-9)$$

$$N_{e_{\text{tag}}\gamma_{\text{probe}}}^{reco} = \epsilon_e \epsilon_\gamma (2N_{e_{\text{tag}}e_{\text{tag}}} + N_{e_{\text{tag}}e_{\text{probe}}}) \quad (4-10)$$

$$F_{e \rightarrow \gamma} = \frac{\epsilon_\gamma}{\epsilon_e} = \frac{N_{e_{\text{tag}}\gamma_{\text{probe}}}^{reco}}{2N_{e_{\text{tag}}e_{\text{tag}}}^{reco} + N_{e_{\text{tag}}e_{\text{probe}}}^{reco}} \quad (4-11)$$

The subscript "tag" indicates that the electron passes the stringent "tag" selection criteria, whereas "probe" refers to the electron or photon undergoing the less stringent "probe" selection. It's critical to note that particles passing the "probe" criteria might also fulfill the "tag" selection. This method allows for the calculation of the fake rate of electrons being misidentified as photons by dividing the number of events with one photon and one electron by the number of events with two electrons. Significantly, in scenarios where both electrons pass the "tag" selection, their weights are doubled to adjust for their potential dual tagging.

The fake rate is meticulously determined across 25 bins—divided into five bins each for the probe's transverse momentum (p_T) and pseudorapidity ($|\eta|$). Within each bin, a fit to the invariant mass of the paired objects is conducted to discern the signal and background contributions. A double-sided crystal ball function models the signal, while an exponential function describes the background. The parameters for both functions are left adjustable. In cases where the probe meets the tag criteria in the CRee scenario, both electrons are theoretically capable of mimicking a photon, thereby contributing twice to the fake rate's denominator. Separate histograms and fits are generated by interchanging the roles of tag and probe for each event where the probe also qualifies as a tag. Detailed information could be found in appendix A.6.

Tables 4–8 and 4–9 delineate the criteria for tagging and probing electrons in both the electron and muon channels. Selection processes focus on events featuring one tag electron or muon and one probe electron. Subsequently, a two-dimensional (2D) fake factor, dependent on the probe electron's transverse momentum (p_T) and pseudorapidity (η), is applied. In cases where the probe electron also meets the tag criteria in the electron channel, it is pertinent to double the event weights to correctly account for these occurrences. Importantly, the reconstruction of the W boson leverages the tag lepton's higher p_T , ensuring a precise measurement.

Signal electron	probe electron	Other selections
$p_T > 30 GeV$	$p_T > 22 GeV$	$m_T^{W(e\nu)} > 30 GeV$
$ \eta < 2.5$	$ \eta < 2.37$	$E_T^{miss} > 30 GeV$
$ z_0 \times \sin\theta < 5 mm$	$ z_0 \times \sin\theta < 5 mm$	$N_{jet} \geq 2$
$ d_0/\sigma_{d_0} < 3$	$ d_0/\sigma_{d_0} < 3$	$p_T^{j0} > 50 GeV$
e_isoTightVarRad	e_isoTightVarRad	$p_T^{j1} > 50 GeV$
e_idTight	e_idTight	$m_{jj} > 500 GeV$
pass single electron triggers		$ M_Z - M_{ee} > 10 GeV$

Table 4–8 Definitions of tag and probe electrons in electron channel.

Signal muon	probe electron	Other selections
$p_T > 30 GeV$	$p_T > 22 GeV$	$m_T^{W(\mu\nu)} > 30 GeV$
$ \eta < 2.5$	$ \eta < 2.37$	$E_T^{miss} > 30 GeV$
$ z_0 \times \sin\theta < 0.5 mm$	$ z_0 \times \sin\theta < 5 mm$	$N_{jet} \geq 2$
$ d_0/\sigma_{d_0} < 3$	$ d_0/\sigma_{d_0} < 3$	$p_T^{j0} > 50 GeV$
mu_isoPflowTight_VarRad	e_isoTightVarRad	$p_T^{j1} > 50 GeV$
mu_idTight	e_idTight	$m_{jj} > 500 GeV$
pass single muon triggers		

Table 4–9 Definitions of tag and probe electrons in muon channel.

4.4.4.4 Systematics

The estimation of the electron to photon fake rate is based entirely on empirical data, incorporating five distinct sources of systematic uncertainties:

1. **Fitting Range Variability:** The fitting range is adjusted by ± 5 GeV to evaluate its impact on uncertainty. The nominal and varied ranges are:
 - Nominal: 71 - 111 GeV
 - Up variation: 66 - 116 GeV
 - Down variation: 76 - 106 GeV

The related uncertainties are depicted in Figure 4–12.

2. **Integration Window Variability:** The window of integration for signal extraction is also varied by ± 5 GeV:
 - Nominal: 81 - 101 GeV
 - Up variation: 76 - 106 GeV
 - Down variation: 86 - 96 GeV

Uncertainties related to these variations are shown in Figure 4–12.

3. **Variations in η Binning:** The fake rate's η binning is adjusted by adding or subtracting two bins from the nominal binning, excluding the calorimeter crack region (1.37 to 1.52):

- Nominal: 0.0 - 0.5 - 1.0 - 1.37/1.52 - 2.0 - 2.37
- Up variation: 0.0 - 0.33 - 0.66 - 1.0 - 1.37/1.52 - 1.8 - 2.1 - 2.37
- Down variation: 0.0 - 0.7 - 1.37/1.52 - 2.37

Uncertainties are illustrated in Figure 4–13.

4. **Variations in p_T Binning:** The binning for the fake rate's p_T is similarly varied:

- Nominal: 22 - 30 - 40 - 50 - 60 - 1000
- Up variation: 22 - 27 - 33 - 38 - 45 - 55 - 65 - 1000
- Down variation: 22 - 35 - 50 - 1000

Figure 4–13 showcases the associated uncertainties.

5. **Fitting Function Variations:** The choice of fitting function for signal and background is alternated to gauge the sensitivity of the results to the functional form:

- Nominal: Double-sided crystal ball function for signal and exponential for background
- Signal variation: Gaussian with a double-sided exponential for signal and exponential for background
- Background variation: Double-sided crystal ball for signal and a 4th order Bernstein polynomial for background

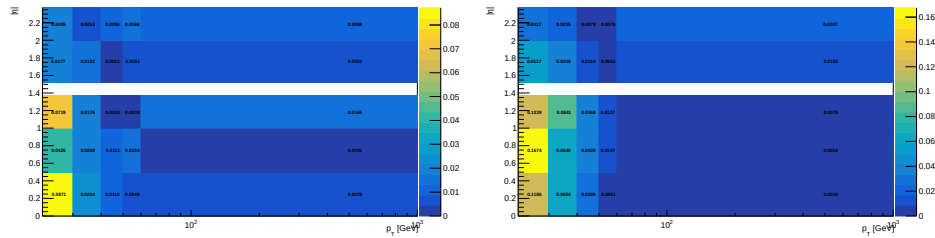


Figure 4–12 Fake rate's uncertainty of varying the range of the fitting and integration window.^[94]

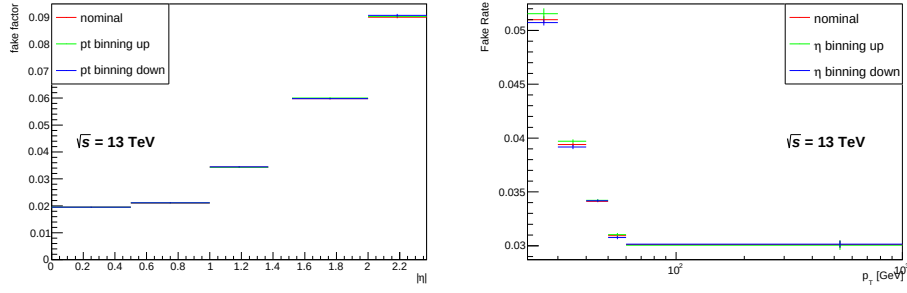


Figure 4–13 Fake rate's uncertainty of varying the binning in p_T and η .^[94]

4.4.4.5 Estimation in Signal and control regions

The comparison plots, illustrating the data-driven estimates of electron faking photon events against MC samples, including Zjets, Wjets, and Diboson, where photons are misidentified as electrons after baseline selections, are depicted in Figure 4–14. Notably, within the signal and control regions that apply a Z veto, the data-driven assessments reveal a higher incidence of electron faking photon events compared to these three MC samples, both in the electron and muon channels. This discrepancy suggests that these MC samples may underestimate the electron faking photon background.

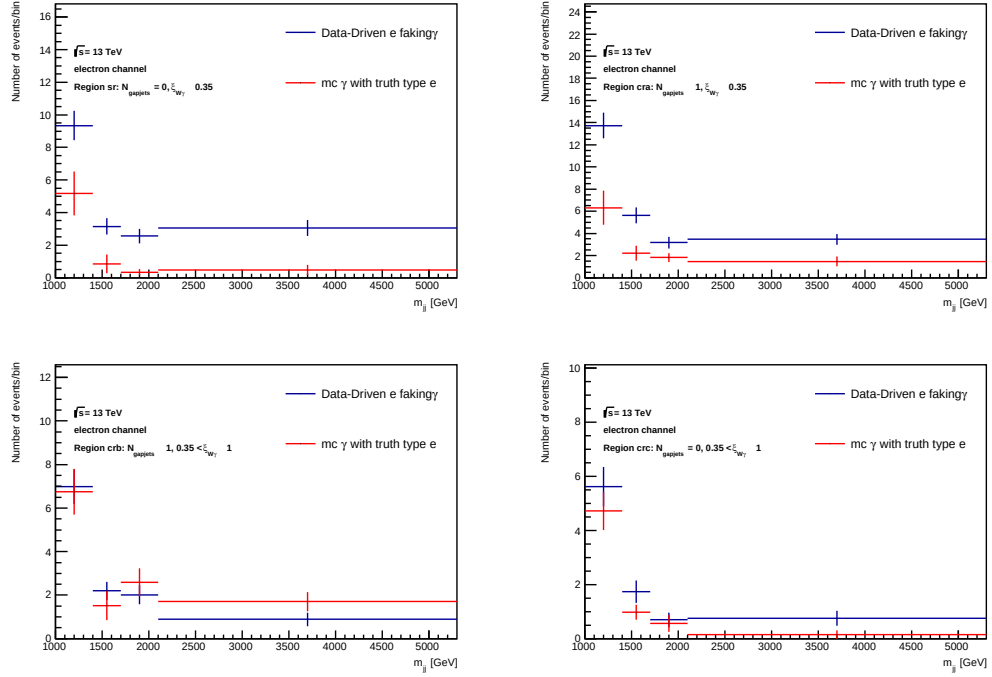


Figure 4–14 m_{jj} distributions of the electron faking photon events estimated in signal and control regions in the electron channel. This comparison underlines the discrepancies between data-driven results and MC simulations, indicating potential underestimation of the electron faking photon background by the MC samples.^[94]

4.4.5 Pileup Background

Unlike the stringent selection criteria for leptons, there is no explicit requirement concerning the point of origin for photons due to the general challenge in accurately measuring this attribute in most events. Consequently, it is plausible for a photon from a disparate pp interaction within the same LHC bunch crossing to merge with a W +jet event from the primary vertex, thus masquerading as a signal event. In Monte Carlo simulations, truth information for pileup overlay events is not retained, resulting in pileup photons being assigned a truth type and origin of 0 by the MC truth classifier tool. Similarly, photons emitted at large angles from jets, which fail truth matching, also receive a truth type and origin of 0. To circumvent the use of these potentially misleading events, the background contribution from pileup photons is estimated using a data-driven method, as implemented in the $Z(l\ell)\gamma$ analysis.

The fundamental assumption of this data-driven method is that the distribution of the

spatial discrepancy, specifically the z position difference between the primary vertex and the photon (derived from calorimeter pointing), exhibits distinct shapes for photons originating from pileup compared to those from the hard scatter. To enhance the accuracy of photon pointing resolution, and thus the reliability of this method, only converted photons that have interacted with the silicon pixel detector are employed. These converted photons exhibit significantly improved resolution due to the precise spatial information provided by the pixel hits. For photons that have registered hits in the pixel detector, the $\Delta z(\gamma, PV)$ distribution is notably more sharply defined.

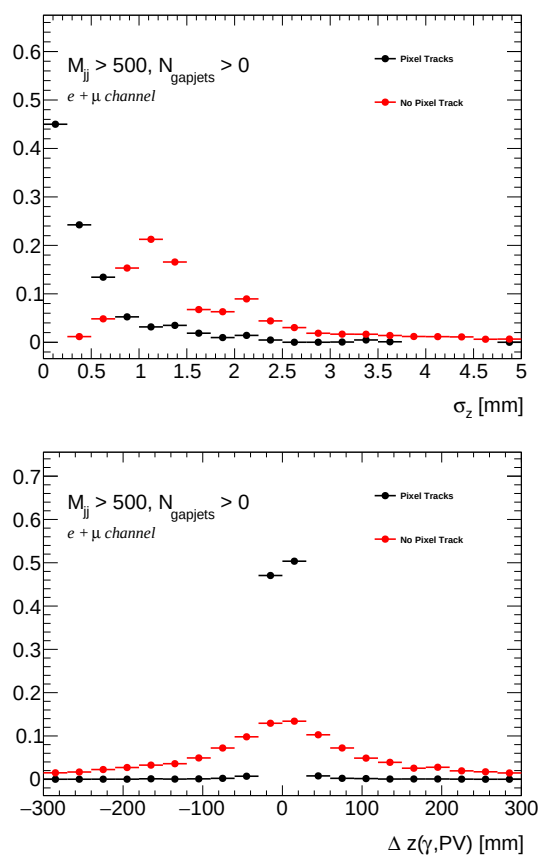


Figure 4–15 Photon pointing resolution and Δz between the photon pointing z and the primary vertex for converted photons matched with pixel tracks and for photons with no pixel tracks.^[94]

The distribution of $\Delta z(\gamma, PV)$ within the data from the control region, where $N_{\text{gapjets}} > 0$, is depicted in Figure 4–16.

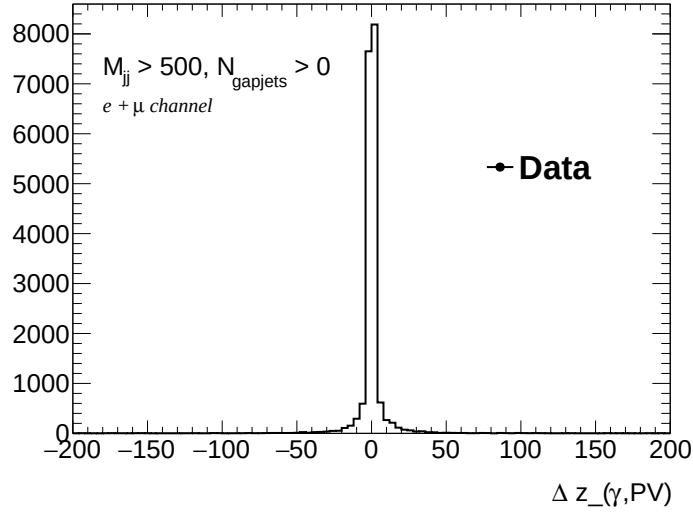


Figure 4-16 $\Delta z(\gamma, PV)$ in data in the control region.^[94]

The $\Delta z(\gamma, PV)$ distribution is distinctly sharply peaked at zero, indicating that well-resolved photons have been selected and that the majority of events feature a reconstructed photon originating from the hard scatter. In contrast, for pileup photons, the $\Delta z(\gamma, PV)$ distribution is modeled as the difference of two uncorrelated Gaussians, each with a width of 35 mm—reflecting the longitudinal spread of photon bunches in the LHC. Consequently, this distribution should exhibit a Gaussian profile with a width of $35 \text{ mm} \times \sqrt{2} = 50 \text{ mm}$. This theoretical prediction is empirically verified by generating toy models based on Gaussians with a width of 35 mm and fitting the resulting difference between these distributions, as illustrated in Figure 4-17.

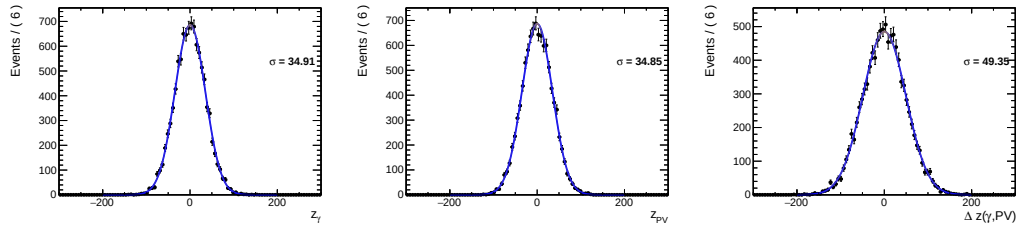


Figure 4-17 To illustrate the distribution resulting from the difference between two uncorrelated Gaussians each with a width of 35 mm, toy models are generated. This simulation aims to demonstrate that the resulting distribution is itself a Gaussian with a calculated width of $\sqrt{2} \times 35 \text{ mm} = 49.5 \text{ mm}$, approximately 50 mm. This approach provides a practical demonstration of how combining two such Gaussians affects the resultant distribution width.^[94]

Using the Gaussian properties of the pileup distribution, the fraction of pileup events in the data, denoted as f_{PU} , can be quantitatively determined by the following equation:

$$f_{PU} = \frac{N_{data}^{|\Delta z| > 50mm} - N_{MC}^{|\Delta z| > 50mm} \times C}{N_{data} \times 0.32}. \quad (4-12)$$

The normalization constant, C , is determined by comparing the QCD $W\gamma$ and EW $W\gamma$ simulations to observed data. This comparison is essential to confirm that C adequately scales the Monte Carlo simulations to match the data. The comparative analysis, illustrated in Figure 4–18, reveals no discrepancies in the $\Delta z(\gamma, PV)$ distribution for the QCD sample, suggesting the model’s accuracy. However, discrepancies are noted within the signal sample; these are primarily observed in a control region characterized by a sparse presence of signal events. Currently, the estimation solely utilizes the QCD sample. The inclusion of the signal sample for this estimation in the signal region may be considered post-data unblinding.

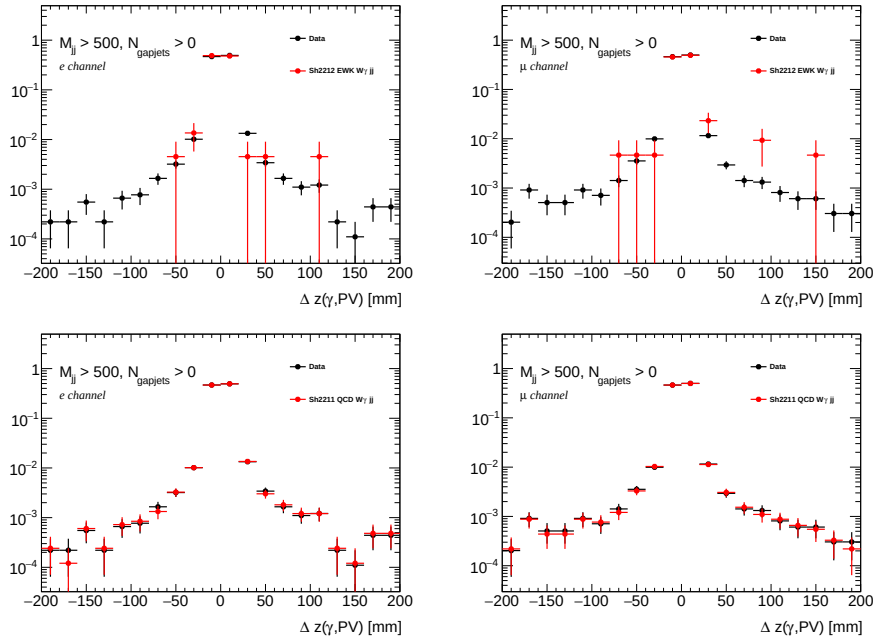


Figure 4–18 Modelling of the $\Delta z(\gamma, PV)$ in the sherpa EWK $W\gamma jj$ sample and QCD $W\gamma jj$ sample.^[94]

In the control region, the normalization factor is determined to be 1.58 ± 0.08 , aligning with the normalization factor applied in the inclusive $Z\gamma$ analysis. This consistency supports the reliability of the normalization process. The calculated result for the pileup fraction is subsequently presented as follows:

$$f_{pu} = 0.79 \pm 0.70\% \quad (4-13)$$

The pileup background includes a component where photons, originating from pileup jets, are misreconstructed. This aspect is already considered in the data-driven estimate for jets impersonating photons. To prevent double counting, this estimate is conducted using a sample of inclusive prompt photon events, which is derived from data collected via prescaled single photon triggers. The purity of photons in this sample is assumed to be equivalent to that in pileup events. These photons are subjected to the same baseline selection criteria and are required to undergo conversion in the silicon pixel tracker.

Utilizing this photon purity, the fraction of pileup photons in the data is calculated to be $0.45 \pm 0.39\%$. This value is adjusted for data from which non-prompt backgrounds have been subtracted. Currently, this calculation and its application are confined to the control region used for the neural network fit. In control regions with high M_{jj} , the pileup fraction is consistent with zero, attributed to larger statistical errors arising from the limited number of events that feature high-resolution photons. The pileup fraction calculation will be extended to the signal region following the data unblinding.

4.5 Observation of $W\gamma jj$ process

4.5.1 Overview of the NN fit

The extraction of the electroweak (EW) component is achieved through a profile likelihood fit applied to the output distribution of the neural network, using TRExFitter version 4.22. Detailed explanations of the fit are provided in later sub-sections. Additionally, a secondary fit using the $\Delta\eta_{jj}$ distribution serves as a cross-check for the primary neural network output fit.

The primary objective of these fits is to determine the signal strength parameter, defined as $\mu_{EW} = \frac{N_{EW}^{meas}}{N_{EW}^{exp}}$, where N_{EW}^{meas} and N_{EW}^{exp} represent the measured and expected number of events, respectively. This parameter is estimated in both the control region (0 jets) and the signal region (greater than 0 jets) within the rapidity gap of the two leading jets. The normalization of the QCD $l\nu\gamma$ template is also adjusted in these regions.

Incorporating additional Monte Carlo backgrounds, such as top and $ll\gamma$ events, these

are input into the fit with constrained variations reflecting their uncertainties. Data-driven estimates of fake backgrounds are similarly incorporated. Two different fitting methods are employed: one using the neural network output, and another using the rapidity gap, both of which target the sensitive variable for the analysis.

The likelihood functions for both the neural network distribution and $\Delta\eta_{jj}$ fits are formulated as follows:

$$L(n|\mu_{EW}, \mu_{QCD}, \theta) = \prod_i \text{Pois}(n_i|\nu_i(\mu_{EW}, \mu_{QCD}, \theta)) \prod_k f_k(a_k|\theta_k) \quad (4-14)$$

where μ_{EW} and μ_{QCD} represent the signal strength and the QCD normalization, respectively. Here, n_i and ν_i denote the observed and expected number of events in the i^{th} bin. The parameters θ encapsulate the nuisance parameters that quantify the impact of various systematic uncertainties within the model, expressed through the constraint terms $f_k(a_k|\theta_k)$.

The fit seeks to minimize the test statistic, defined by the negative log-likelihood (NLL):

$$\text{NLL}(\mu_{EW}, \hat{\mu}_{EW}, \hat{\theta}, \hat{\theta}) = -2 \ln \frac{L(\mu, \hat{\theta})}{L(\hat{\mu}, \hat{\theta})} \quad (4-15)$$

The significance of the measurement is evaluated based on the NLL for the background-only hypothesis ($\mu_{EW} = 0$):

$$Z_{\text{meas}} = \sqrt{\text{NLL}(\mu_{EW} = 0)} \quad (4-16)$$

The NLL is minimized using the TRExFitter software package.

4.5.2 Neural network configuration

A neural network (NN) is trained using TensorFlow^[97] and Keras^[98] on the Sherpa signal sample alongside all prompt background Monte Carlo (MC) samples, including QCD $W\gamma jj$, $Z\gamma jj$, and top backgrounds. The training dataset comprises events that meet the signal region selection criteria: $M_{jj} > 500$ GeV, $\Delta Y(jj) > 2$, and no jets in the rapidity gap between the two leading transverse momentum jets. This setup establishes a naturally signal-rich region for the neural network training and a QCD-rich background control region characterized by events with more than one jet in the rapidity gap. It was observed that including the number of jets in the rapidity gap as a training variable resulted in the neural network disproportionately relying on this feature. Consequently, this variable is integrated into the selection to encourage the neural network to utilize a broader range of training variables more effectively.

To maximize the use of the available MC data in the analysis, two separate neural networks are trained: one on MC events with odd event numbers and another on those with even event numbers. This approach ensures that the events not used in the training of one network are employed for the evaluation and validation of the other. The neural network output score for the data is then determined by averaging the output values of the two networks when applied to the data. The training employs a binary cross-entropy loss function, with each event's loss being weighted by its normalized event weight. Furthermore, the total background cross-section within the training region is normalized to match that of the signal, enhancing the robustness of the training process.

The neural network is specifically trained to discriminate between signal and background based on a set of 13 kinematic variables. These variables are chosen for their potential to differentiate the characteristics of signal events from those typically observed in background events. The list below details each variable and its relevance to the analysis:

- $\xi_{l\gamma}$ • $pT_{l\gamma}$ • $|\Delta\phi(l\gamma, jj)|$ • $\Delta R(l, \gamma)$
- pT_{γ} • η_{j_0} • $\Delta R(l\gamma, jj)$
- pT_l • M_W^T • $\Delta R(\gamma, j_0)$
- pT_{j_0} • $|\Delta\eta(j_0, j_1)|$ • ξ_{γ}

The neural network is structured to consist of an initial batch normalization layer, followed by three densely connected hidden layers containing 512 nodes each. Each node in these layers employs a LeakyReLU activation function, defined as:

$$f(x) = \begin{cases} 0.01x, & \text{if } x < 0 \\ x, & \text{otherwise} \end{cases} \quad (4-17)$$

The output layer, which is densely connected to the last hidden layer, utilizes a sigmoid activation function to output probabilities, expressed as:

$$f(x) = \frac{1}{1 + e^{-x}} \quad (4-18)$$

The model is optimized using the Adam learning rate optimizer^[99] with an initial learning rate of 3×10^{-5} . The structure of the network—specifically the number of hidden layers, the number of nodes per layer, and the learning rate—was optimized through a grid search. This

process involved training multiple models with varying configurations to determine the architecture that minimizes loss on validation data. The results of this grid search are summarized in Table 4–10, with the best-performing parameters highlighted in bold.

Hyper-parameter	Values
Number of hidden layers	2, 3 , 4, 5, 7
Nodes per layer	64, 128, 256, 512 , 1024
Learning rate	1×10^{-5} , 3×10^{-5} , 1×10^{-4} , 3×10^{-4} , 1×10^{-3}

Table 4–10 Summary of hyper-parameter grid search. The optimal values are shown in boldface.

To prevent overtraining, an early stopping mechanism is employed with a patience parameter set to 10 epochs. Furthermore, the neural network training does not differentiate between electron and muon channels. A comparative analysis of the input variable distributions between these channels showed negligible differences, thereby eliminating the need for separate network training for each channel.

4.5.3 NN training

The training and validation losses for the neural networks trained on even and odd event number Monte Carlo samples are illustrated in Figure 4–19. This comparison helps to assess the model’s learning curve and its generalization capabilities across different data subsets.

The neural network trained on even event numbers exhibits a larger generalization gap, which is the difference between the training and validation losses, compared to the network trained on odd event numbers. However, it is observed that the increases in training performance do not come at the cost of validation performance, as the validation losses remain stable or decrease. The overall similarity in network performance on training and validation sets, as shown in Figure 4–20, suggests that neither network suffers from overfitting.

To quantify the discriminatory power of the neural networks, the area under the receiver operating characteristic curve (AUC) is used. The ROC curves for both models are displayed in Figure 4–21, where both networks achieve an AUC of 0.75.

The influence of each training variable on the model’s performance was further examined by training the network with and without each variable. The variable resulting in the most significant drop in AUC when omitted was deemed the most important. The rankings of the training variables, averaged over five iterations, are shown in Table 4–11. The consistency in

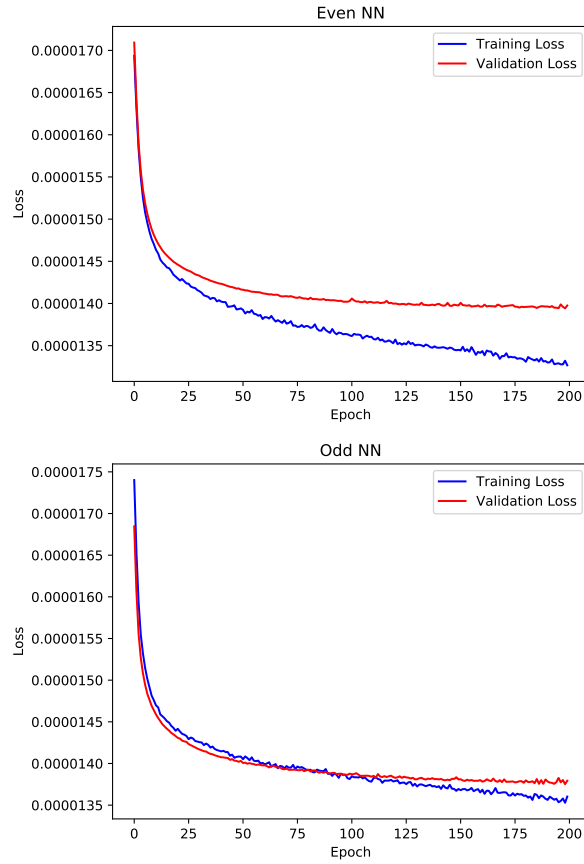


Figure 4–19 Loss curves for the neural network trained on even event number MC (left) and odd event number MC (right).^[94]

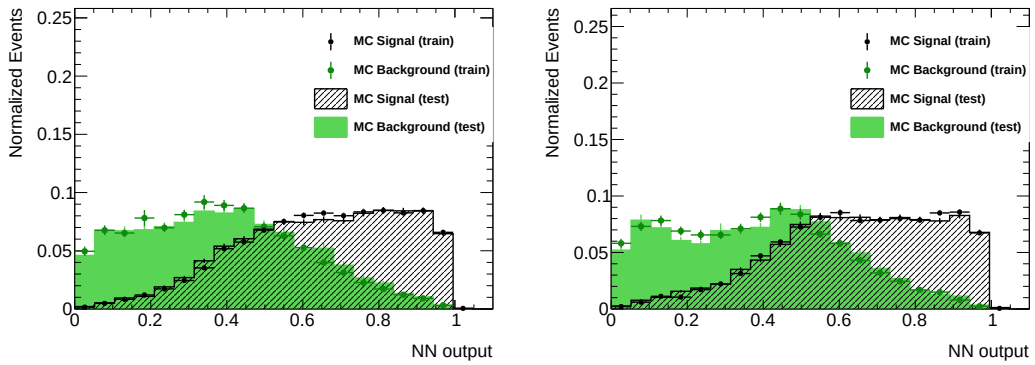


Figure 4–20 Signal and background shapes in the neural network output distribution for training and validation samples, trained on even event number MC (left) and odd event number MC (right).^[94]

variable importance between the two neural networks confirms that both models are capturing

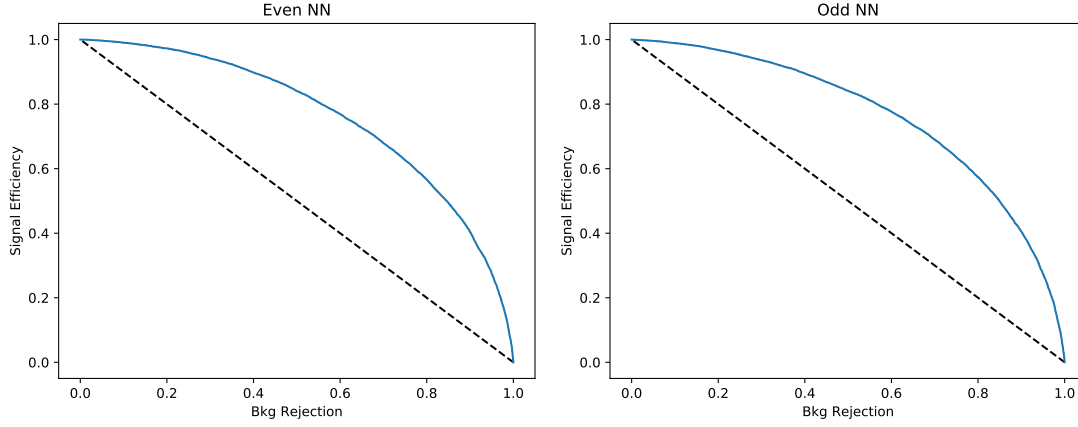


Figure 4-21 Receiver operating characteristic curves for the neural network trained on even event number MC (left) and odd event number MC (right).^[94]

the same underlying physics.

Training Variable	Even AUC_{N-1}/AUC_N	Odd AUC_{N-1}/AUC_N
$\xi_{l\gamma}$	0.96	0.96
$\Delta\eta_{jj}$	0.96	0.96
$\Delta R(l\gamma, jj)$	0.98	0.98
pT_γ	0.99	0.99
pT_l	0.99	0.99
ξ_γ	0.99	0.99
$\Delta R(j_0, \gamma)$	0.99	0.99
$\Delta R(l, \gamma)$	0.99	0.99
$pT_{l\gamma}$	1.0	1.0
$\Delta\phi(l\gamma, jj)$	1.0	1.0
M_W^T	1.0	1.0
pT_{j_0}	1.0	1.0
η_{j_0}	1.0	1.0

Table 4-11 Ranking of training variables by impact on AUC.

4.5.4 Expected signal strength

Expected results are derived utilizing an Asimov dataset in the signal region, alongside actual data in the control region. The Asimov dataset is constructed by fitting a background-only model to the data in the control region. This fit yields the QCD normalization factor and the nuisance parameters, which are subsequently used to simulate the Asimov data for the

signal region. A combined fit of the signal and background models is then performed using the actual data from the control region and the Asimov dataset from the signal region.

Given that the pileup background constitutes a percentage of the real data within each bin, incorporating it in the signal region before unblinding would compromise the blinding protocol. Therefore, the pileup background template in the signal region is initially set to zero and will be assessed and included once unblinding occurs.

The comparison between data and Monte Carlo simulations in the control region, both prior to and following the fit used to generate the Asimov dataset, is illustrated in Figure 4–22.

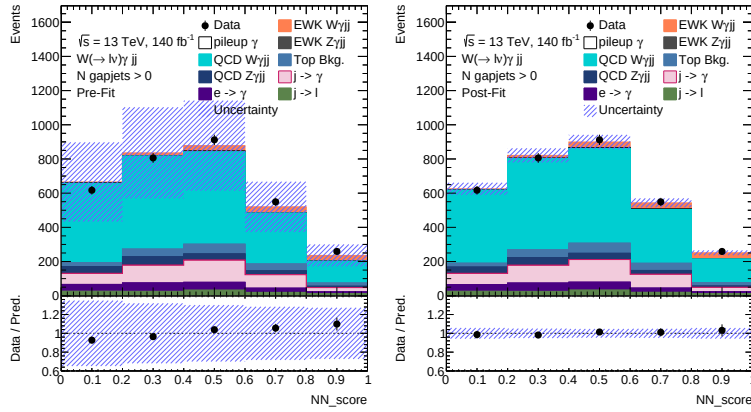


Figure 4–22 Control region only fit used in constructing the Asimov dataset on which the expected results are based.^[94]

4.6 Signal Extraction

4.6.1 Introduction

4.6.2 Overview

This section describes the extraction of the EW $W\gamma jj$ differential event yield in m_{jj} , $p_{T,jj}$ and $\Delta\phi_{jj}^{\text{signed}}$. This is achieved using a data-driven method which uses signal and control regions in a binned log-likelihood fit. This fit is used to constrain both the shape and normalization of the strong $W\gamma jj$ background during the extraction of the EW $W\gamma jj$ event yield. The extracted yields are unfolded to produce differential cross sections in Section 4.7. The differential cross-sections are derived for the combined electron and muon channels. We are

unable to derive separate lepton channel distributions due to statistical limitations.

4.6.3 Methodology

The analysis employs a binned maximum likelihood fit to investigate the differential production of $EW-W\gamma jj$. This fitting procedure incorporates three control regions (3CR) to enhance the precision of the measurements.

$$L = \prod_{r,i} \text{Pois}(N_{ri}^{\text{data}} | \gamma_{ri} \nu_{ri}(\alpha)), \quad (4-19)$$

where N_{ri}^{data} is the observed number of events, ν_{ri} represents the expected number of events from simulations, and γ_{ri} are nuisance parameters accounting for MC statistical uncertainties.

The expected number of events, ν_{ri} , is formulated as:

$$\nu_{ri} = \mu_i \nu_{ri}^{\text{EW,MC}} + \nu_{ri}^{\text{strong}} + \nu_{ri}^{\text{non-}W\gamma,\text{MC}} + \nu_{ri}^{\text{fakes}}, \quad (4-20)$$

where $\nu_{ri}^{\text{EW,MC}}$ and $\nu_{ri}^{\text{non-}W\gamma,\text{MC}}$ are MC predictions for the electroweak $W\gamma$ production and other background processes, respectively. ν_{ri}^{fakes} includes data-driven background estimates.

The strength of the EW signal, denoted by μ_i , is a free parameter in the fit, reflecting the modification required to match the observed data. The ν_{ri}^{strong} term is detailed in:

$$\nu_{\text{CRA},i}^{\text{strong}} = b_{\text{L},i} \nu_{\text{CRA},i}^{\text{strong,MC}}, \quad (4-21)$$

$$\nu_{\text{CRB},i}^{\text{strong}} = b_{\text{H},i} \nu_{\text{CRB},i}^{\text{strong,MC}}, \quad (4-22)$$

$$\nu_{\text{SR},i}^{\text{strong}} = b_{\text{L},i} f(x_i) \nu_{\text{SR},i}^{\text{strong,MC}}, \quad (4-23)$$

$$\nu_{\text{CRC},i}^{\text{strong}} = b_{\text{H},i} f(x_i) \nu_{\text{CRC},i}^{\text{strong,MC}}. \quad (4-24)$$

This approach uses the SR to denote the Signal Region, and CRA, CRB, and CRC as the Control Regions, applying different constraints to improve the fit accuracy. Each region contributes uniquely, allowing the model to adapt based on the characteristics of each region and thereby refine the overall fit.

Choice of model parameters A decision was made to employ the *CRA method* in this analysis, where the bin-dependent factors b_i are shared between the Control Region A (CRA) and the Signal Region (SR). This choice, although not unique, avoids the complexities of using Control Region B (CRB), where both N_{gapjets} and $\xi_{W\gamma}$ are inverted, crossing two phase-space boundaries. In the CRA method, the residual correction, $f(x)$, is shared between

Control Region C (CRC) and the SR. Alternatively, in the *CRC method*, $f(x)$ would be shared between CRA and the SR.

The equivalence of these configurations, demonstrated by the VBF-Z 13TeV analysis, hinges on the symmetry of the regions and parameters. Under the assumption that b_L is only constrained by CRA (except for μ_{EW}), the post-fit QCD background in CRA is determined solely by the data and MC predictions specific to that region:

$$v_{CRA,i}^{\text{strong}} = b_{L,i} v_{CRA,i}^{\text{strong,MC}} \approx N_{CRA,i}^{\text{data}} - v_{CRA,i}^{\text{EW,MC}} - v_{CRA,i}^{\text{other,MC}}, \quad (4-25)$$

assuming $\mu_{EW} = 1$ for simplicity, though the symmetry holds otherwise.

Defining the ratio $X(r, i)$ as:

$$X(r, i) = \frac{N_{ri}^{\text{data}} - v_{ri}^{\text{EW,MC}} - v_{ri}^{\text{other,MC}}}{v_{ri}^{\text{strong,MC}}}, \quad (4-26)$$

we approximate $b_{L,i} \approx X(\text{CRA}, i)$, and similarly for the high centrality region, $b_{H,i} \approx X(\text{CRB}, i)$.

The function $f(x_i)$, representing the adjustment needed for CRC, is approximated by:

$$f(x_i) \approx \frac{X(\text{CRC}, i)}{X(\text{CRB}, i)}, \quad (4-27)$$

leading to the strong background correction in the SR:

$$b_{L,i} f(x_i) = \frac{X(\text{CRA}, i) X(\text{CRC}, i)}{X(\text{CRB}, i)}. \quad (4-28)$$

If the CRC method were applied instead, the roles of the control regions would be commuted, but the resulting expression for the background correction remains the same, proving the methods' approximate equivalence. Consequently, the signal extraction procedure is conducted using both CRA and CRC methods for thorough validation.

4.6.4 Input simulations

The $v_{ri}^{\text{EW,MC}}$ terms are estimated using the Sherpa 2.2.11 EW- $W\gamma jj$ samples for the precise definitions of the samples mentioned here. which contain events for the EW production of a $W(l\nu)$ and a γ in association with jets generated using Sherpa 2.2.11 (EW $W\gamma jj$). The Madgraph5 EW- $W\gamma jj$ samples are used to define the generator choice uncertainties from the signal MC estimates. The $v_{ri}^{\text{strong,MC}}$ terms are estimated using two different MC samples. These

are the Madgraph5 QCD- $W\gamma jj$ samples and the Sherpa 2.2.11 QCD- $W\gamma jj$ samples which contain events for the QCD- $W\gamma jj$ production of a W and a γ generated using MG5+Pythia8 and Sherpa 2.2.11 respectively. It is known from previous analyses which extract an EW signal in a VBF/VBS enhanced phasespace that the irreducible strong background is poorly modelled. This highlights the importance of deriving data-driven corrections to the strong background in order to reduce the overall modelling uncertainties on the measurement. To facilitate this, two QCD- $W\gamma jj$ samples are used to reduce the overall model dependence of the measurement and to enable the quantifying of the systematic uncertainty due to choice of MC generator.

The Sherpa 2.2.11 sample is chosen as the nominal QCD $W\gamma jj$ sample. The choice of Sherpa 2.2.11 QCD $W\gamma jj$ as the nominal sample is a result of the approximately 2.3-times superior statistical precision¹ of the Sherpa compared to the Madgraph QCD- $W\gamma jj$ samples. Using the Madgraph QCD- $W\gamma jj$ sample as the nominal would result in a larger MC statistical uncertainty on the measurement and would also degrade the statistical resolution of the experimental systematic uncertainties and QCD- $W\gamma jj$ theory uncertainties.

The choice of the nominal extracted yield (also called the “central value” in this chapter) is given by

$$N_{EW, \text{Nominal}} \equiv \langle N_{EW,i} \rangle, \quad (4-29)$$

where the index i runs over 10000 pseudo-experiments, termed *bootstraps*, where for each bootstrap, the Asimov **and** all MC templates are fluctuated in all CRs and the SR before performing the signal extraction. For the Asimov, the bin contents for each bootstrap is sampled from a Poisson distribution of mean equal to the bin content. The reason for taking the average over bootstraps, rather than just the nominal values for the templates and Asimov, is that we avoid issues with systematics e.g. generator modelling which can potentially result in the nominal value lying far away from the mean of the pseudo-experiments.

The $v_{ri}^{\text{non-}W\gamma, \text{MC}}$ terms are estimated using a collection of samples: The EW production of Z and a γ in association with jets; the corresponding QCD- $Z\gamma$ production process; single top production processes in S and T channels; W -top production; $t\bar{t}$ production; $t\bar{t}\gamma$ production; $tW\gamma$ production; EW production of a $W(l\nu)$ in association with two jets; Z production in

¹ This value is calculated by comparing the $\frac{\sqrt{\text{sum-of-weights}^2}}{\text{sum-of-weights}}$ values for the events passing the baseline event selection criteria.

association with jets; and the EW production of a Z in association with jets.

Each MC event must pass the baseline selection criteria outlined in section 4.3 in addition to being split up into SR and Control Regions. For each event, the MC weight is scaled by the electron, photon, muon, PRW, JVT, B-tagging and trigger scale factors. To estimate the expected number of events in data from the MC, the weights were additionally scaled by the production cross-sections and integrated luminosity of the sample. The resulting weight is then divided by the sum of all MC weights for the process.

The fit templates including all of the above contributions for m_{jj} are shown in Figure 4–23.

4.6.5 Construction of Asimov dataset and binning optimization

To ensure the integrity of the analysis and avoid potential biases, such as parameter tuning to force a match between the data and the MC simulations, the data in the Signal Region (SR) remains blinded. Instead, an Asimov dataset is constructed to evaluate the expected number of events in the control regions and to validate the likelihood fit procedure. The expected number of events for the Asimov dataset is calculated using the formula:

$$N_{ri}^{\text{Asimov}} = \sum_s v_{ri}^{s,\text{MC}}, \quad (4-30)$$

where the index s encompasses the non- $W\gamma$, EW- $W\gamma jj$, and QCD- $W\gamma jj$ MC templates. For the QCD- $W\gamma jj$ component, the nominal Sherpa 2.2.11 sample is employed. The statistical uncertainty associated with the Asimov dataset is represented by $\sqrt{N_{ri}^{\text{Asimov}}}$.

Furthermore, the Asimov dataset along with the MC templates are crucial in determining the optimal binning for observables. A key criterion for this binning strategy is to ensure a uniform relative statistical precision across bins for the extracted EW yield. This uniformity is assessed by fitting the Signal, QCD- $W\gamma$, and non- $W\gamma$ templates—each incorporating their respective MC statistical uncertainties—to the Asimov dataset. Although the central values derived from the Asimov dataset will align with the sum of the templates, this fitting process allows for the appropriate propagation of MC and Asimov uncertainties through the analytical framework. This methodological approach facilitates a robust estimation of the expected statistical precision for the extracted EW yield.

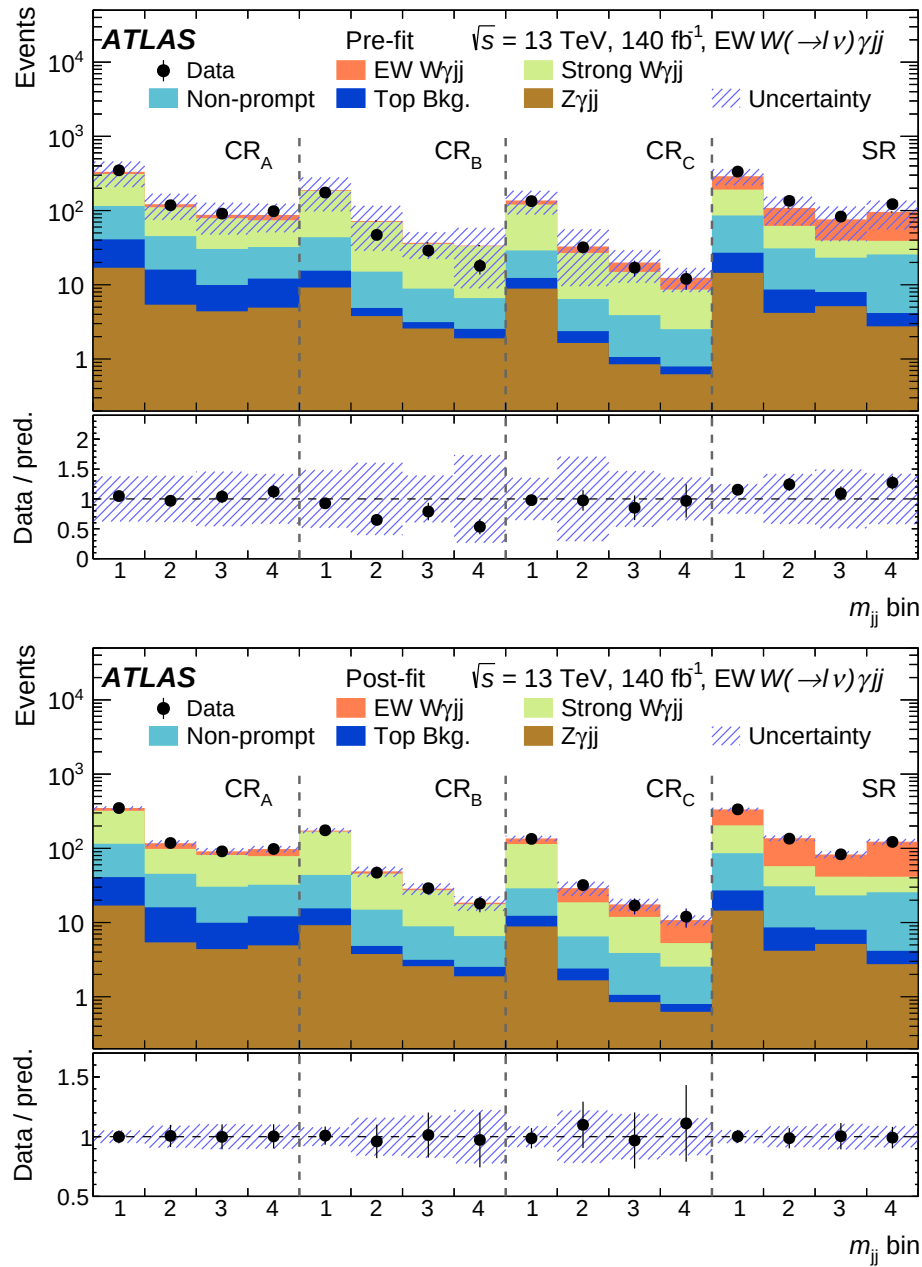


Figure 4–23 Prefit and postfit MC templates and unblinded data in the SR and three CRs for m_{jj} . The uncertainty bands are calculated from combined statistical and systematic uncertainties and show the uncertainty on the entire stack before and after the fit. Before the fit, the uncertainty is dominated by the QCD scale uncertainties. After the fit, the normalisation of the scale uncertainties get constrained, and the uncertainty is dominated by the statistical precision of the data. The top backgrounds include ttgamma, tWgamma, and tqgamma backgrounds. $Z\gamma jj$ backgrounds include the EW and QCD production modes of $Z\gamma+jj$ production. Non-prompt backgrounds refer to the data-driven estimates described in sections 4.4.^[94]

4.6.6 Uncertainties

Uncertainties impacting the extracted EW yield are categorized into two types: systematic and statistical. Systematic uncertainties are further divided into theoretical uncertainties, which influence the shape and normalization of the MC background and signal samples, and experimental uncertainties, which impact event reconstruction. These systematic uncertainties are designed to be **correlated** across both control and signal regions, meaning that systematic changes are applied to the SR and CRs simultaneously prior to the construction of the likelihood and the extraction of the EW yield. It is important to note that the random number seeds used in the bootstrapping process are selected based on the run-number. Since the SR and CRs do not overlap, different random number seeds are utilized for each toy scenario in these regions. Statistical uncertainties are derived by generating toy distributions and creating a new likelihood function for each, with separate random seeds allocated for each SR and CR to ensure these uncertainties are **uncorrelated** between these regions.

An exhaustive list of experimental uncertainties, which includes predominant factors such as Jet Energy Scale (JES) and Jet Energy Resolution (JER), is documented. The theoretical uncertainties encompass PDF and scale uncertainties for the QCD, EW, and specific non- $W\gamma$ backgrounds, along with α_s uncertainties for the QCD, EW, and QCD- $Z\gamma$ backgrounds; renormalization and factorization scale uncertainties for the EW and QCD- $W\gamma$ background, as well as uncertainties from generator choice for the QCD $W\gamma jj$ background. Not accounted for are the systematic uncertainties arising from the interference between the QCD- $W\gamma jj$ and EW $W\gamma$ production processes and uncertainties related to luminosity.

This section elaborates on how these uncertainties influence the derived EW signal, providing a detailed analysis of their effects.

A detailed analysis on how these uncertainties influence the derived EW signal is documented in appendix A.7

4.6.7 Results

4.6.7.1 Asimov Results

Figure 4–24 displays the final extracted signal for the EW yields with total systematic and statistical uncertainties derived from the analysis.

Tables recording all final extracted yields and uncertainties using the nominal method

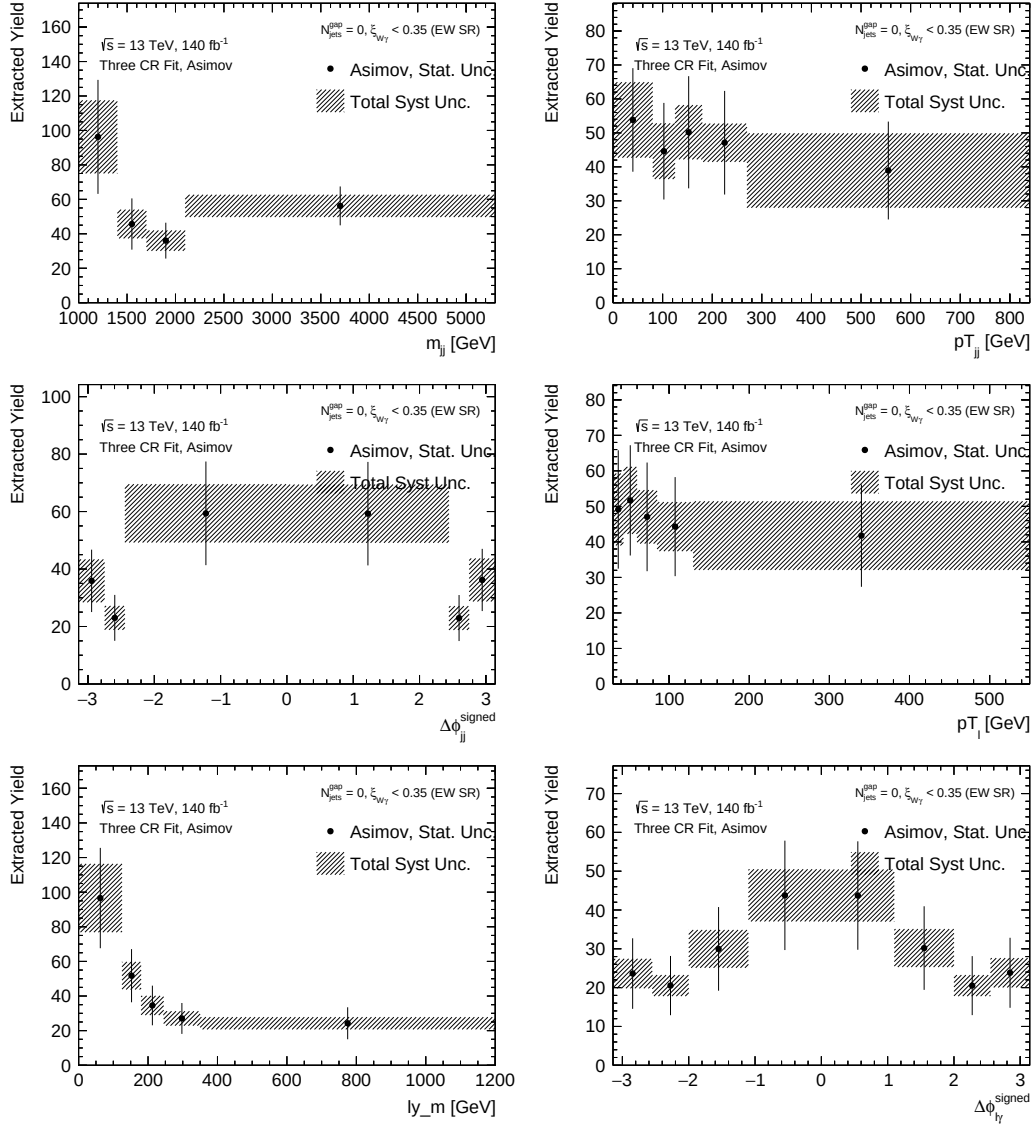


Figure 4–24 Extracted EW $W\gamma jj$ yield in the signal region, detailing statistical uncertainties derived from Asimov data and systematic uncertainties post-smoothing.^[94]

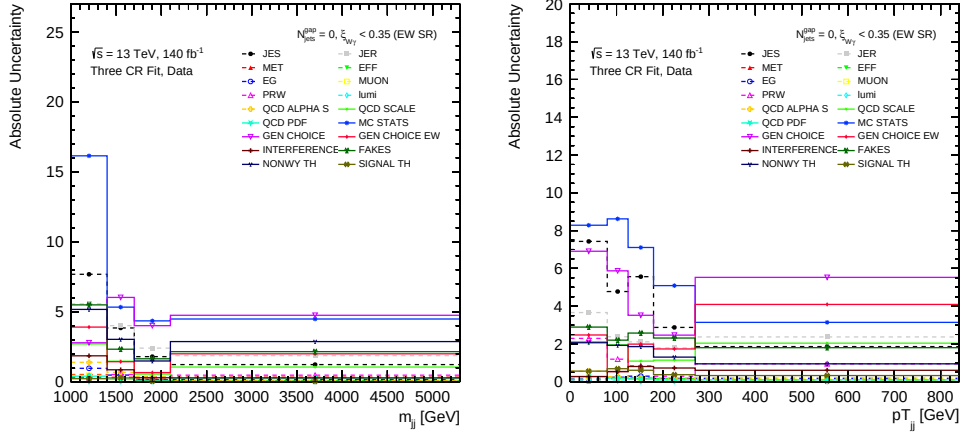


Figure 4–25 Absolute systematic uncertainty values on the extracted EW yield from data.^[94]

could be found in appendix A.7.

4.6.7.2 Data Results

Extracted data yield distributions for m_{jj} and $p_{T,jj}$ are shown in figure 4–25

4.7 Correction of Detector Effects

Detector effects such as efficiency, acceptance, and limited resolution can distort the distributions of physical observables. The goal of experimental physics analysis is to reconstruct the true distributions of these observables. Unfolding is a procedure used to correct for these detector effects and measure the truth-level spectrum based on observed physics data.

In this analysis, the signal distributions described in Section 4.6 are unfolded to estimate the underlying truth distribution. The region considered for unfolding is the Signal Region (SR), as defined in Section 4.6, which corresponds to our fiducial region described in Section 4.3 with constraints $m_{jj} > 1$ TeV and $N_{\text{gapjets}} = 0, \xi_{l\gamma} < 0.35$.

Various techniques are utilized across analyses with the ATLAS detector. For this analysis, we employ iterative Bayesian unfolding as detailed by D’Agostini in^[100] and implemented in the RooUnfold framework^[101]. The statistical and systematic uncertainties are estimated by unfolding the Asimov extracted yields from the signal extraction section. Enhancements have been made to the RooUnfold package to better integrate with the Asimov yields.

The unfolding methodology using iterative Bayesian techniques is outlined in Section 4.7.1.

Section 4.7.2 details the inputs for Bayesian unfolding, while Section A.8.1 discusses the technical closure tests of the method. Sections 4.7.4 and 4.7.5 present the statistical and systematic uncertainties, and the results of the unfolding of the Asimov extracted yields, respectively.

4.7.1 Iterative Bayesian unfolding

Different unfolding methods are utilized in ATLAS analyses, with iterative Bayesian unfolding being commonly employed. The method is detailed in D’Agostini’s seminal work. This approach seeks to infer the truth-level distribution $\mathbf{x}$ from the measured distribution $\mathbf{y}$. Conceptually, the bin contents of histograms can be viewed as vectors, and the impact of detector distortions can be represented by a matrix $\mathbf{A}$. This relationship is expressed as:

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{y} \quad (4-31)$$

Here, $\mathbf{A}$ is known as the response or smearing matrix, encapsulating information on how the detector transforms the true distribution into the measured one. The challenge of unfolding lies in solving Equation 4–31 to derive $\mathbf{x}$ from $\mathbf{y}$. Direct inversion of $\mathbf{A}$ is generally impractical due to issues of non-invertibility and the conceptual errors highlighted by D’Agostini.

A more detailed look at the relationship can be framed in terms of probabilities:

$$t_i = \sum_j P(T_i|M_j)m_j = \sum_j \theta_{ij}m_j \quad (4-32)$$

Here, $P(T_i|M_j)$ and θ_{ij} represent the probability that an event measured in bin j truly belongs in bin i . m_j is the measured distribution’s probability for bin j , and t_i is the corresponding truth-level distribution’s probability for bin i .

Applying Bayes’ theorem offers a way forward:

$$\theta_{ij} = P(T_i|M_j) = \frac{P(M_j|T_i)P(T_i)}{\sum_i P(M_j|T_i)P(T_i)} = \frac{a_{ji}P(T_i)}{\sum_i P(M_j|T_i)P(T_i)} \quad (4-33)$$

In this equation, $P(M_j|T_i) = a_{ji}$ are the elements of the response matrix from Equation 4–31, and $P(T_i)$ is the prior probability of an event in truth bin i .

The response matrix is constructed using Monte Carlo simulations that track events passing both truth-level and reconstruction-level criteria. However, not all events that pass reconstruction-level criteria contribute to the response matrix—some fail at the truth-level and vice versa, necessitating fiducial and efficiency corrections.

Once these corrections are applied, the measured distribution m_j is inputted into the unfolding formula. However, the results can be biased by the initial choice of prior distribution. To mitigate this, the unfolding process is iteratively applied, with each iteration using the output of the previous as the new prior. The iterative process is formalized as:

$$t_{i,n} = \sum_j \frac{a_{ji} P(t_{i,n-1})}{\sum_i P(M_j | t_{i,n-1}) P(t_{i,n-1})} m_j, \quad n \geq 1, \quad t_{i,0} := T_i \quad (4-34)$$

where $t_{i,n}$ represents the probability for truth bin i after n iterations, with $t_{i,0}$ initially set to the Monte Carlo truth distribution T_i . While increasing iterations reduces bias from the prior, it may enhance statistical fluctuations. The balance between bias reduction and statistical accuracy generally dictates using fewer than 10 iterations; currently, two iterations are employed after a dedicated optimization.

4.7.2 Inputs for iterative Bayesian unfolding

The Asimov extracted yields from the electroweak Monte Carlo (MC) distribution, as detailed in the signal extraction section, serve as inputs for the unfolding process. The response matrix, crucial for this unfolding, is constructed using SHERPA electroweak MC samples. Unfolding is carried out across the designated signal regions for various observables: m_{jj} , p_T^{jj} , and $\Delta\phi_{jj}$. The signal region is delineated by conditions $N_{jets}^{gap} = 0$ and $\xi_{W\gamma} < 0.35$, with event selection based on the baseline criteria outlined in the event selection section. I will only show the distribution of m_{jj} in this section for technical details. But the final results for all variables will be shown in the final section.

Response matrices, as depicted in Figure 4–26, are generated by requiring events to satisfy both truth-level and reconstruction-level selections. Notably, the response matrix for $\Delta\phi_{jj}$ is symmetrized by averaging the four contents corresponding to each truth-reco pair. This matrix predominantly exhibits a diagonal correlation between the reconstructed and truth-level distributions, indicating that the effects of symmetrization are minimal and can be disregarded.

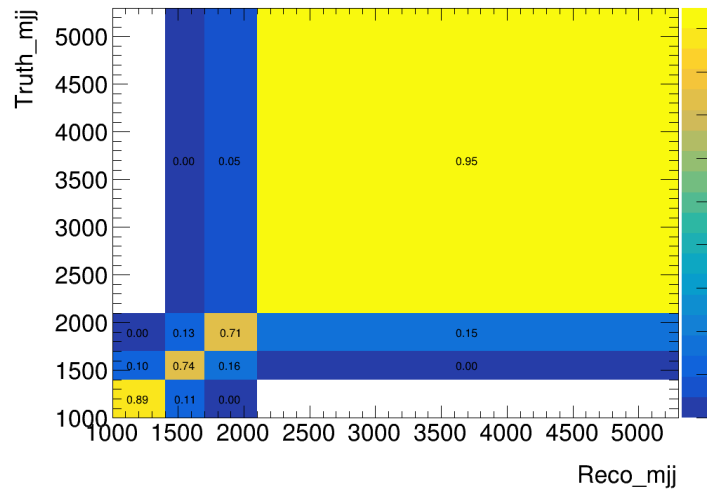


Figure 4–26 Response matrices for m_{jj} in SR selections. Electron and muon channel combined electroweak signal samples are used to build the migration matrices.^[94]

As once mentioned in Section 4.7.1, not all events that pass reconstruction-level selections are eligible for the unfolding matrix. Prior to conducting the iterative unfolding process, a fiducial correction must be applied to the reconstruction-level distribution. Similarly, an efficiency correction is required for the truth-level distributions after unfolding; this correction is implemented internally by the RooUnfold package. Figure 4–27 illustrates the fiducial correction factors, which are computed by dividing the projected distribution from the response matrix by the reconstruction-level MC distribution. These fiducial correction factors generally exceed 60%.

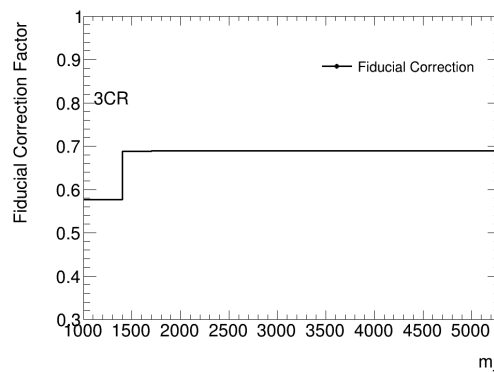


Figure 4–27 Fiducial correction factors for the nominal unfolding procedure of m_{jj} in signal region selections.^[94]

4.7.3 Closure tests

In this analysis, three kinds of closure tests are implemented.

The technical closure test, as discussed in Section A.8.1, plays a crucial role in verifying the accuracy of the unfolding framework. For this test, we feed the unfolding framework with the exact reconstruction-level distribution of the electroweak (EW) $W\gamma$ MC sample. The unfolded distribution is then compared with the truth-level EW $W\gamma$ MC sample to ensure consistency.

Additionally, a closure test concerning MC shape effects is conducted using an alternative signal sample generated with MadGraph. This test, often referred to as a hidden variable test, evaluates the impact of elements not included in the CP detector simulation uncertainties. The methodology behind this test is detailed in Section A.8.2.

A data-driven closure test, described in Section A.8.3, assesses the bias inherent in the unfolding process. In this test, the MC distribution is reweighted to align with actual data. The unfolded distribution is then compared to the reweighted truth-level distribution to evaluate the accuracy of the unfolding procedure.

The detailed description of these closure tests could be found in appendix A.8

4.7.4 Statistical and systematic uncertainties

4.7.4.1 Statistical Uncertainty

Statistical uncertainties in the electroweak (EW) signal extraction are evaluated using the bootstrap method, as detailed in the signal extraction section. This method involves the generation of 10,000 bootstrap samples for each statistical variation, enabling a robust estimation of statistical uncertainty. After unfolding, the mean values and the root mean square (RMS) of each bin are calculated to determine the uncertainty.

The influence of statistical errors from both MC components (EW, QCD, Non- $W\gamma$, Fakes) and Asimov data is quantified using a similar bootstrap approach. For this purpose, 10,000 bootstrap toys are generated for each component. Following figure displays one set of unfolded bootstrap results for m_{jj} , illustrating how statistical uncertainties are propagated through the analysis.

Each of the 10,000 bootstrap toys is subjected to iterative Bayesian unfolding, with the RMS of the unfolded values in each bin representing the uncertainty. Figure 4–29 showcases

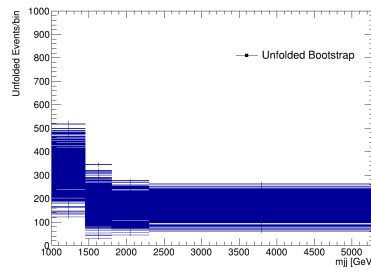


Figure 4–28 An example of 10,000 unfolded bootstraps of m_{jj} for Asimov Data, used to estimate statistical uncertainty. The RMS of each bin is considered as the relative uncertainty, with mean values for the first and fourth bins at 392.00 and 193.96, respectively, and RMS values at 77.98 and 37.57. Consequently, statistical uncertainties of 19.89% and 19.37% are assigned to the first and fourth bins, respectively.^[94]

the relative statistical uncertainties for m_{jj} across the various components such as EW, QCD, Non-Wy, Fakes, and Asimov Data distributions.

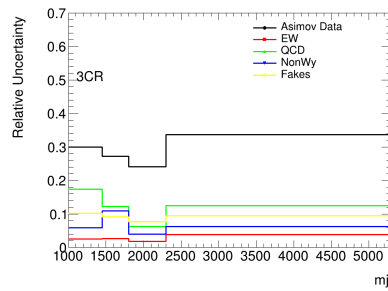


Figure 4–29 Statistical uncertainties for m_{jj} in the combined electron and muon channels after SR selections and unfolding for full Run II Asimov data. Results are presented for a 3CR fit.^[94]

4.7.4.2 Experimental Uncertainty

Experimental uncertainty is quantified by unfolding the extracted electroweak (EW) yield under the influence of various systematic uncertainties. For each source of systematic uncertainty, a corresponding shift is applied to the Monte Carlo (MC) templates. The response matrices and fiducial corrections are subsequently derived from SHERPA + PYTHIA8 EW MC samples, with each element adjusted to reflect the same systematic shifts.

The range of experimental uncertainties considered in this analysis, resulting from these adjustments, is shown in Figures 4–30. These figures illustrate the impacts of various systematic shifts on the unfolding process, providing a visual representation of how each systematic

source affects the final unfolded results.

Following figure is showing JET uncertainties after unfolding:

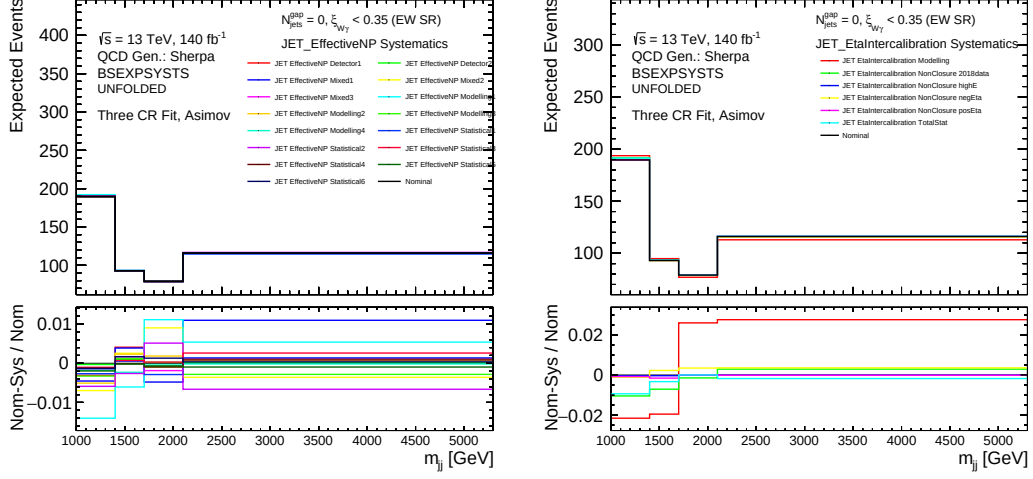


Figure 4–30 JET uncertainties for m_{jj} in the electron and muon combined channel after SR selections and unfolding for full RunII Asimov data.^[94]

Figure 4–31 in the following is showing JER uncertainties after unfolding:

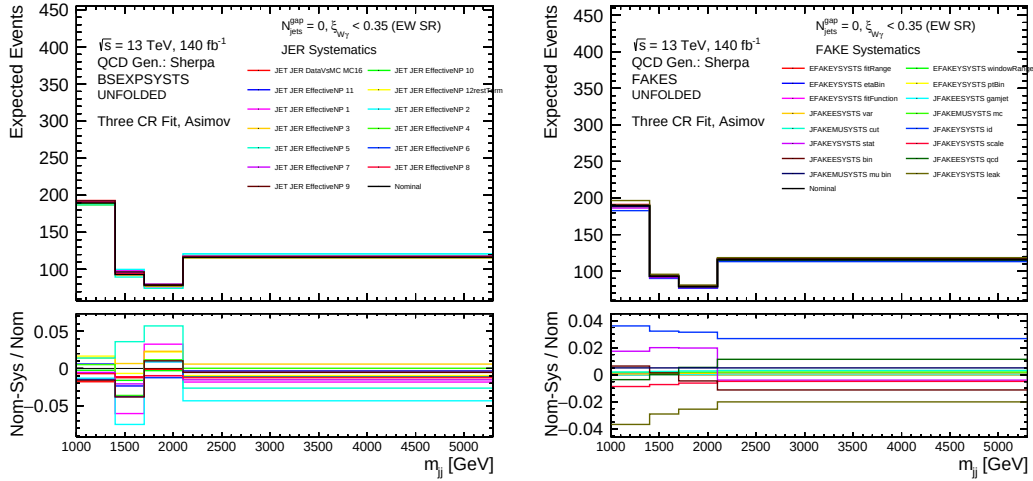


Figure 4–31 JER and other systematic uncertainties for m_{jj} in the electron and muon combined channel after SR selections and unfolding for full RunII Asimov data.^[94]

4.7.4.3 Theory Uncertainties

Our analysis incorporates at least two distinct sources of systematic uncertainty for each Monte Carlo sample: uncertainties arising from missing higher order terms in the cross-section computation and uncertainties associated with the parton distribution functions (PDFs) used in the simulations.

To assess the impact of missing higher order terms, scale variations are employed. These variations address the potential inaccuracies in the perturbative expansion of the partonic cross section due to truncated terms. For each Monte Carlo sample, six variations of the scale are considered, while off-diagonal variations are excluded from this analysis to maintain focus on primary effects. This method provides a structured approach to quantify theoretical uncertainties.

The effects of these scale uncertainties on the unfolded results are visualized in Figure 4–32. These figures illustrate how scale variations influence the unfolding process, showcasing the differential impact across various bins and observables analyzed.

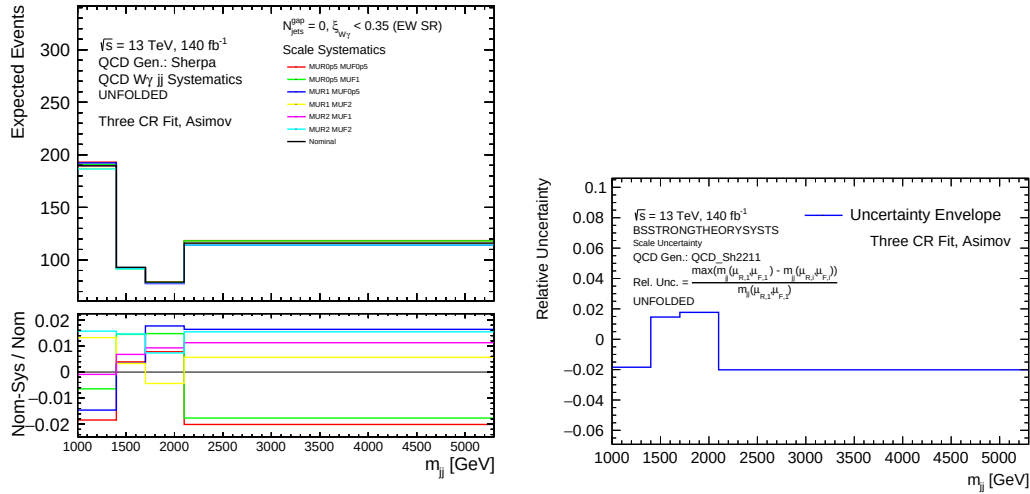


Figure 4–32 Effect of variations of the renormalization and factorization scales on the predicted QCD background in the signal region. The uncertainties for m_{jj} is shown here.^[94]

PDF uncertainties are estimated by varying the PDFs used, relative uncertainties are shown in the following figures 4–33:

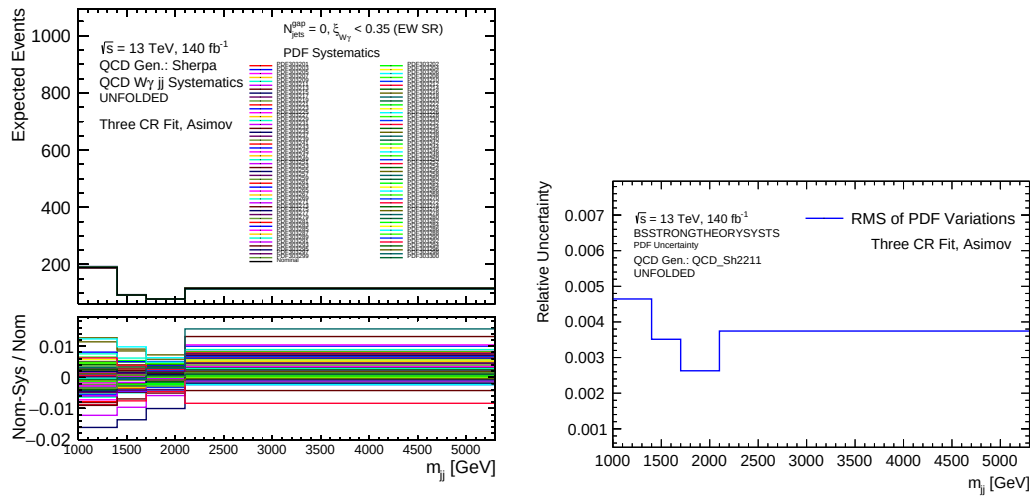


Figure 4-33 The effect of variations of the underlying PDF on the predicted signal and backgrounds on m_{jj} . RMS of PDF variations are also summarized.^[94]

4.7.5 Unfolding results

Distribution of all variables are shown in this section.

4.7.5.1 Asimov results

This section presents the unfolded Asimov yields and differential distributions for electroweak (EW) components within the signal region (SR). Total systematic uncertainties are derived by computing the quadratic sum of the statistical, experimental, and theoretical uncertainties described in the preceding sections. Figures 4–36 and 4–37 provide comprehensive summaries of these analyses, showcasing the unfolded results and the aggregation of uncertainties respectively.

A detailed examination of absolute systematic uncertainties is conducted across all variables involved in the signal extraction and subsequent unfolding process. The absolute uncertainties for each variable, post-unfolding, are methodically listed and illustrated in the referenced figures. Additionally, to facilitate a robust comparison of uncertainties before and after the unfolding process, the fractional uncertainty for each variable is calculated and visually depicted. This analysis extends to both the Asimov dataset and the unblinded results, offering an exhaustive perspective on the uncertainties affecting the study.

All systematic uncertainties discussed are summarized in Figure 4–34. This summary will also be included in HEPDATA for reference and further scholarly use.

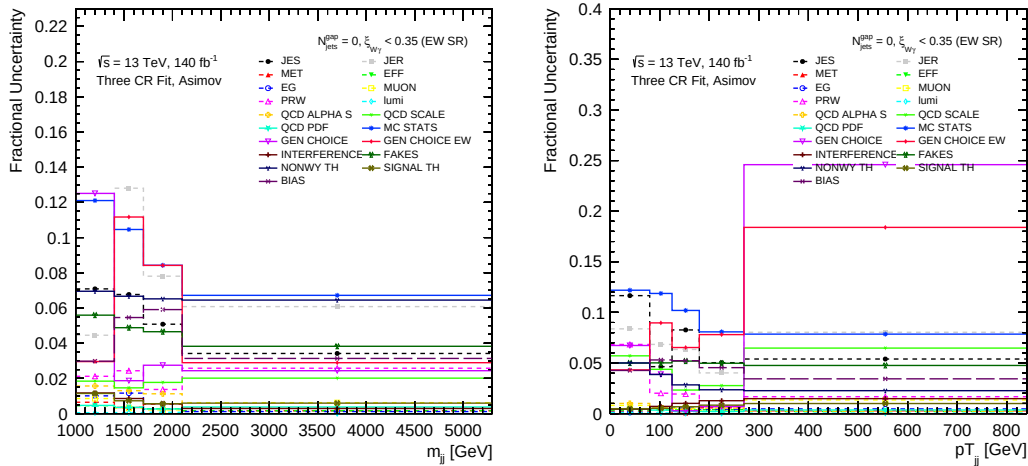


Figure 4–34 Systematic uncertainties for 3CR fits with all the terms added up in quadrature. m_{jj}, p_T^{jj} distributions are shown for electron and muon channel combined.^[94]

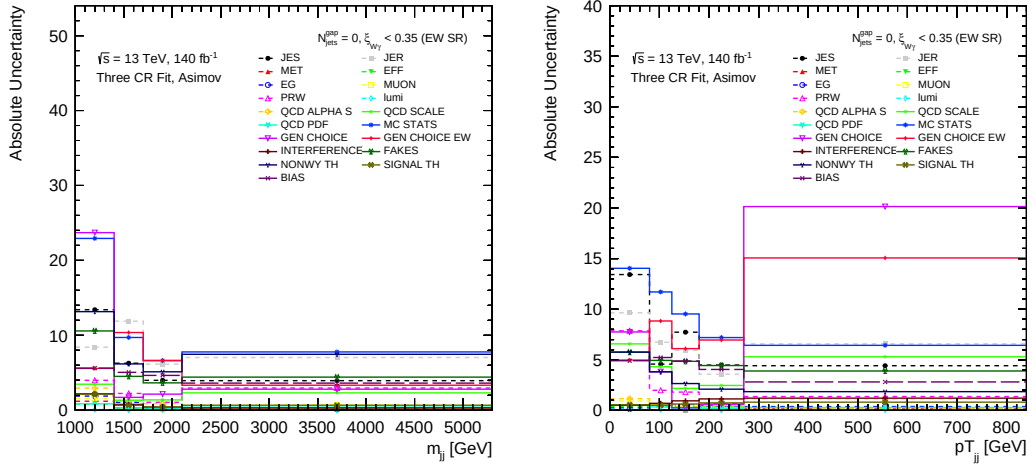


Figure 4–35 Absolute systematic uncertainties on the unfolded extracted yield for 3CR fits with all the terms added up in quadrature. m_{jj}, p_T^{jj} distributions are shown for electron and muon channel combined.^[94]

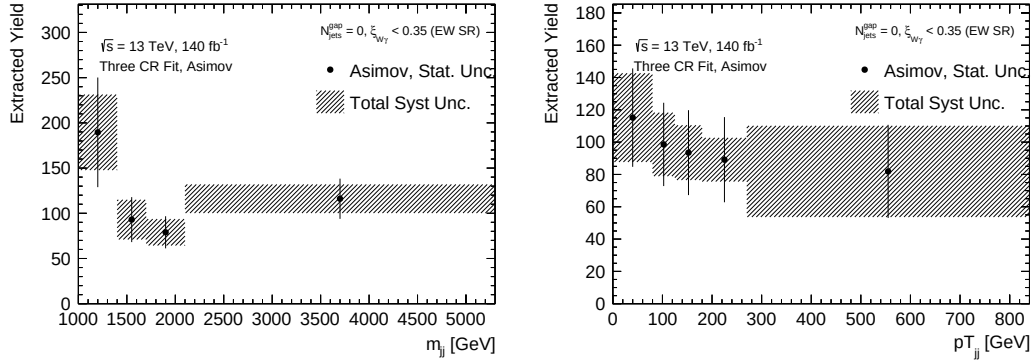


Figure 4–36 Expected EW $W\gamma$ yields of m_{jj}, p_T^{jj} in the electron and muon combined channel after SR selections, extractions and unfolding procedure.^[94]

4.7.5.2 Data results

This section details the unblinded unfolded yields and differential distributions for electroweak (EW) components within the signal region (SR). Total systematic uncertainties are derived by computing the quadratic sum of the statistical, experimental, and theoretical uncertainties discussed in the previous sections. Figure 4–40 and Figure 4–41 provide comprehensive overviews of these results, illustrating the unfolded distributions and summarizing the associated uncertainties.

Figure 4–38 consolidates all the systematic uncertainties detailed earlier. The contents of

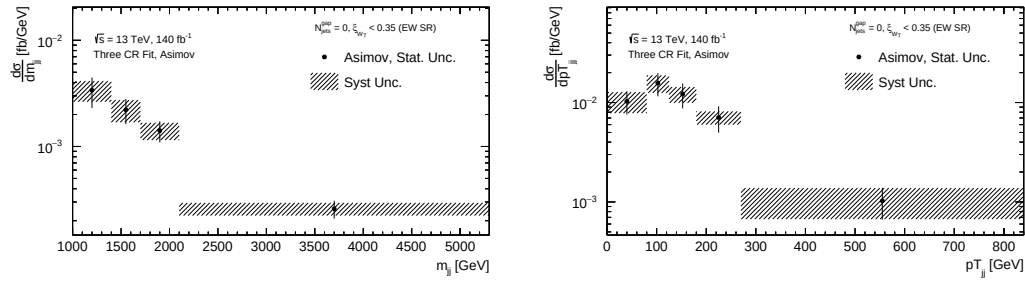


Figure 4–37 Nominal unfolded EW $W\gamma$ differential distribution of m_{jj}, p_T^{jj} in the electron and muon combined channel after SR selections extractions and unfolding procedure.^[94]

this figure, along with the systematic uncertainty data, will be documented and made available in HEPDATA for broader accessibility and reference within the scientific community.

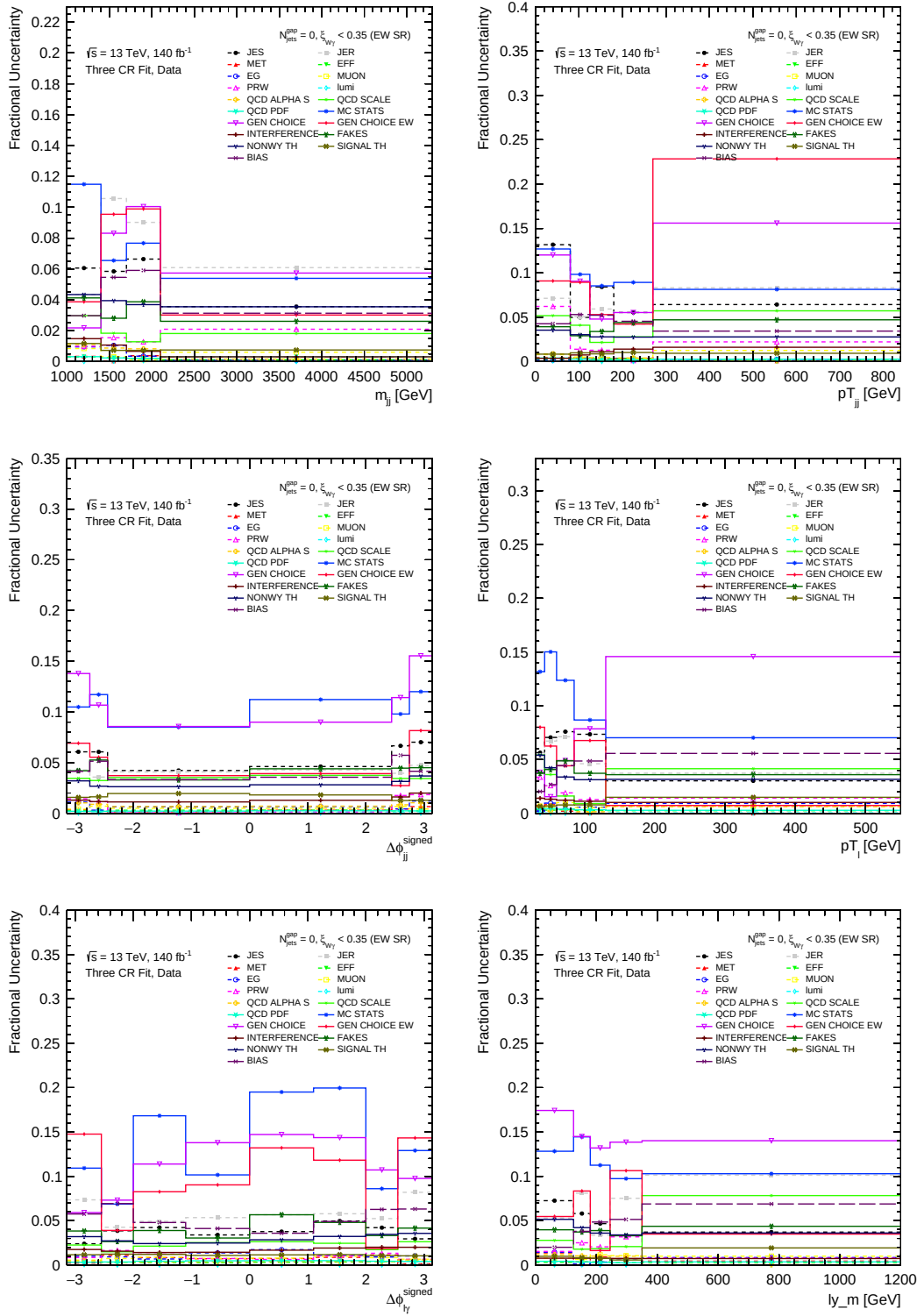


Figure 4-38 Systematic uncertainties for 3CR fits with all the terms added up in quadrature. $m_{jj}^{jj}, p_T^{jj}, \Delta\phi_{jj}^l, p_T^l, m_{l\gamma}$ and $\Delta\phi_{l\gamma}$ distributions are shown for electron and muon channel combined.^[94]

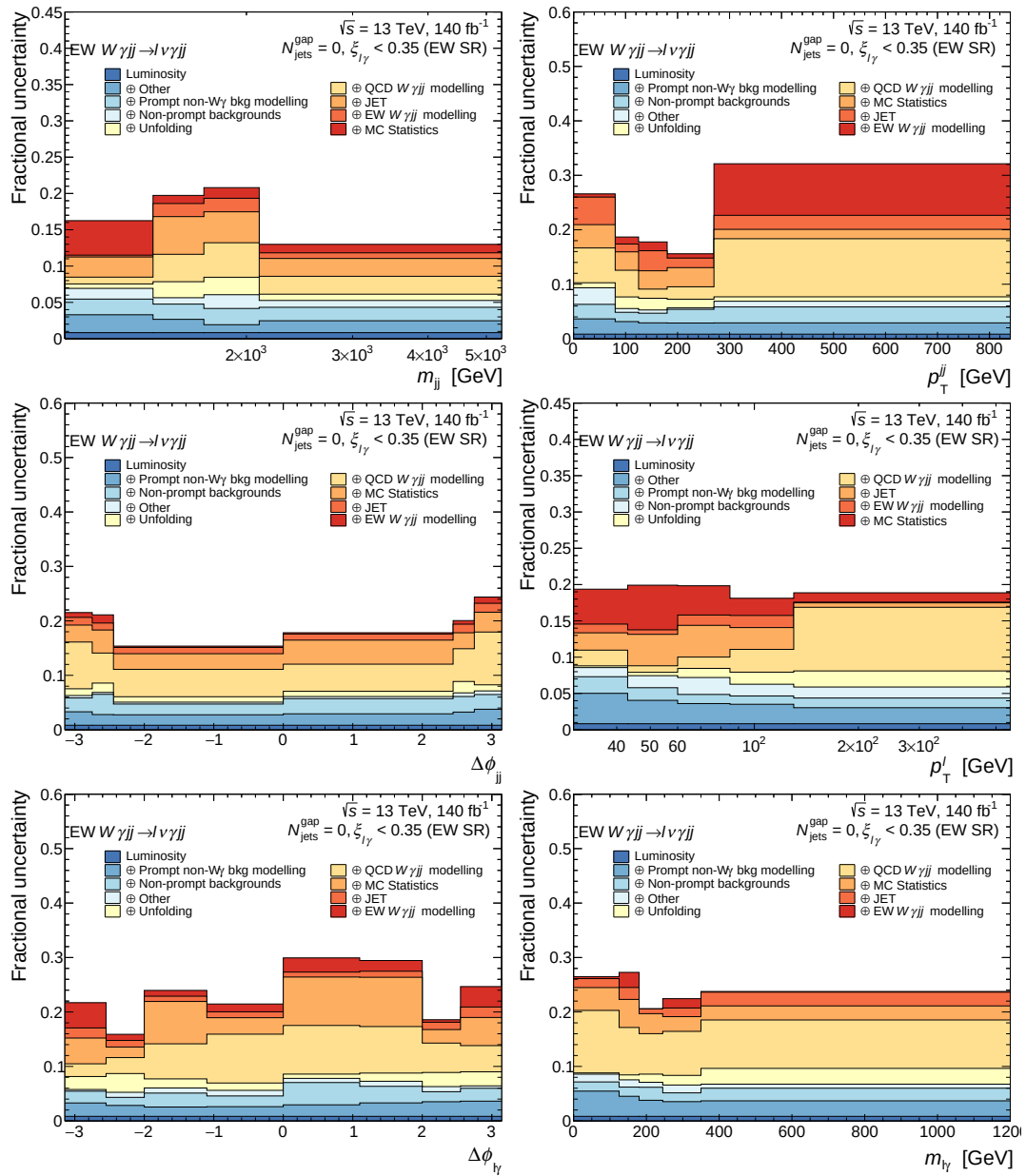


Figure 4–39 Fractional systematic uncertainties on the unfolded differential cross-sections derived using data. NB: These are the same uncertainties (but presented as a stack rather than individual histograms) presented in Figure 4–38, with the addition of the flat luminosity uncertainty.^[94]

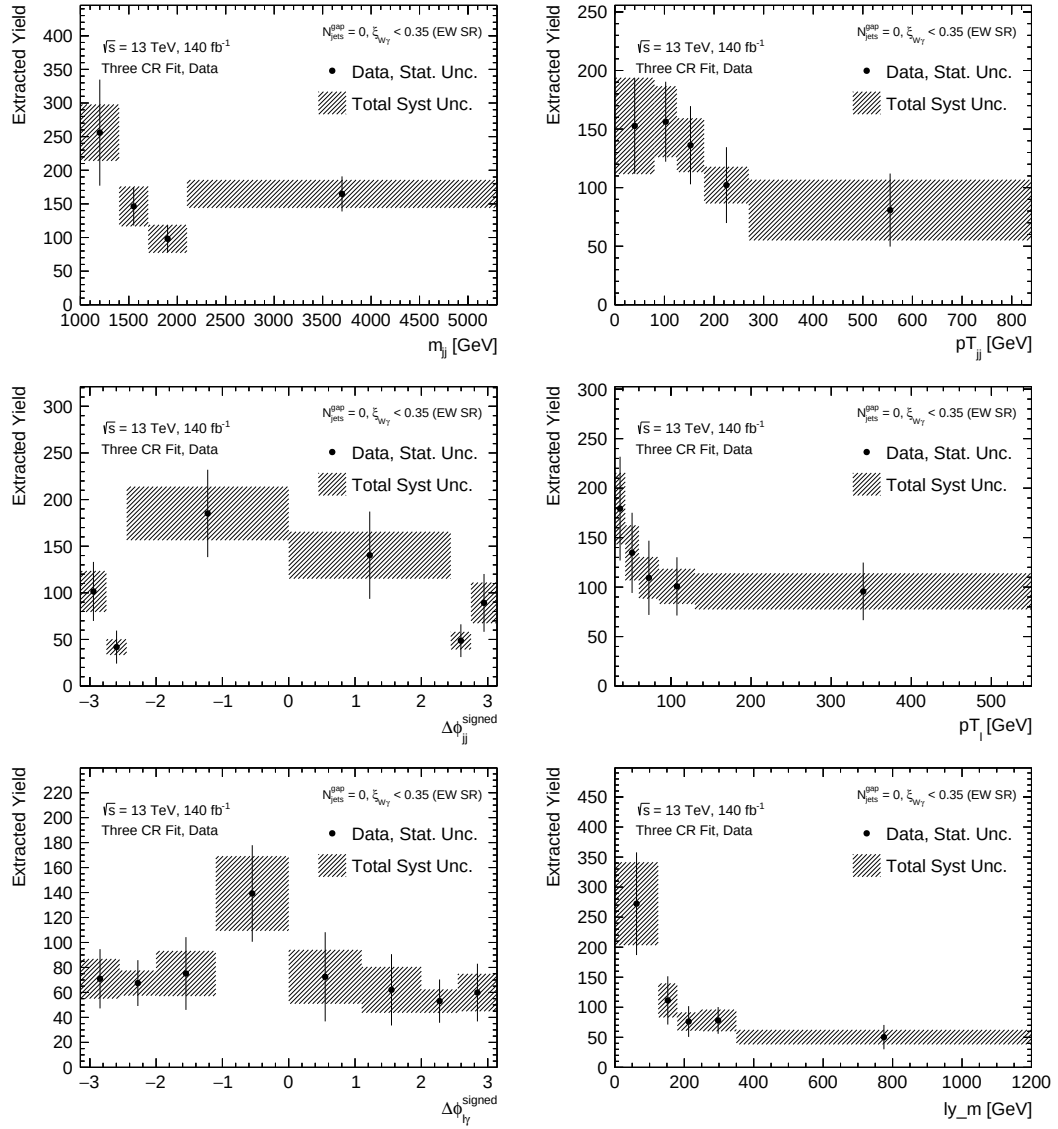


Figure 4-40 Unblinded EW $W\gamma$ yields of $m_{jj}, p_T^{jj}, \Delta\phi_{jj}, p_T^l, m_{l\gamma}$ and $\Delta\phi_{l\gamma}$ in the electron and muon combined channel after SR selections, extractions and unfolding procedure.^[94]

4.8 Systematic Uncertainties

In this section, we discuss the systematic uncertainties affecting the Monte Carlo predictions in our analysis. Those uncertainties basically consist of theoretical uncertainties and experimental uncertainties. Theoretical uncertainties are those which have influence over shape and normalization of the MC background and signal samples. Experimental uncertainties have affects over the event reconstruction process. Detailed description of systematic uncertainties could be found in appendix A.9.

4.8.1 Treatment of uncertainties in fit

Each discussed source of uncertainty is represented by a nuisance parameter θ , constrained by a standard Gaussian distribution (mean 0, width 1). Additionally, a nuisance parameter for each bin of the fit is created to address the effect of limited Monte Carlo statistics, employing a Poisson constraint for the statistical uncertainties of the Monte Carlo. All nuisance parameters are permitted to vary to minimize the negative log-likelihood. A post-fit mean value significantly distant from 0 suggests a deviation in the expected value of the uncertainty, while an error smaller than one indicates that the data has sufficient statistical power to constrain the uncertainty's magnitude.

Experimental uncertainties on Monte Carlo backgrounds are correlated across processes and regions. In contrast, PDF and α_S uncertainties are correlated across regions but maintained uncorrelated across different processes. Since scale uncertainties account for missing higher orders in the perturbative expansion of the partonic cross section, they are not inherently correlated across regions and are thus treated independently.

In the fitting process, the normalization of theory uncertainties on the signal sample is excluded as the normalization of the signal sample is adjusted to match the data.

4.9 EFT Interpretation

The couplings between gauge bosons are precisely defined by the $SU(2) \times U(1)$ gauge symmetry inherent in the electroweak sector of the Standard Model (SM). Deviations from the expected SM cross-sections could signify new physics phenomena beyond the Standard Model.

Measurements of multi-boson processes provide a basis for verifying the SM and iden-

tifying any signs of physics beyond the Standard Model. These can be quantitatively assessed in a model-independent way using Effective Field Theory (EFT), which extends the SM Lagrangian to include higher-order operators that adhere to the symmetries of Lorentz invariance and gauge invariance:

$$\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \sum_{n=5}^{\infty} \frac{f_n}{\Lambda^{n-4}} O_n \quad (4-35)$$

Here, f_n represents the coupling constants, O_n denotes operators of dimension $n > 4$, and Λ is the scale at which new physics emerges. In this framework, new particles are not explicitly included; instead, their effects are integrated through these higher-order operators and any anomalous standard model couplings. The coefficients f_n can be derived from more comprehensive high-energy theories, thus constraints on f_n through measurements can limit the range of potential new physics theories. It is important to note that the validity of this effective theory is confined to energies below the new physics scale, typically expected around the electroweak symmetry breaking scale.

The lowest order operators that affect quartic boson couplings are dimension-8. Table 4–12 lists the 18 dimension-8 operators along with the quartic boson couplings they influence. The analysis discussed in this paper is particularly sensitive to the $WW\gamma\gamma$ and $WW\gamma Z$ couplings, both of which exist at tree level within the SM. All of the operators could be found in appendix A.18.

	WWWW	WWZZ	WW γZ	WW $\gamma\gamma$	ZZZZ	ZZZ γ	ZZ $\gamma\gamma$	Z $\gamma\gamma\gamma$	$\gamma\gamma\gamma\gamma$
$O_{S,0}, O_{S,1}$	✓	✓			✓				
$O_{M,0}, O_{M,1}, O_{M,6}, O_{M,7}$	✓	✓	✓	✓	✓	✓	✓		
$O_{M,2}, O_{M,3}, O_{M,4}, O_{M,5}$		✓	✓	✓	✓	✓	✓		
$O_{T,0}, O_{T,1}, O_{T,2}, O_{T,3},$	✓	✓	✓	✓	✓	✓	✓	✓	✓
$O_{T,4}, O_{T,5}, O_{T,6}, O_{T,7}$		✓	✓	✓	✓	✓	✓	✓	✓
$O_{T,8}, O_{T,9}$					✓	✓	✓	✓	✓

Table 4–12 Dimension-8 operators and the quartic vertices they affect.^[102]

4.9.1 Event Generation

Monte Carlo samples for the electroweak production of a W boson and a photon, including contributions from the dimension-8 operators discussed earlier, are generated using MadGraph along with the Eboli model^[103]. To circumvent the necessity of generating a multitude of Monte Carlo samples for each coupling value of interest, the linear and quadratic terms are produced separately. This method enables each sample to be simply reweighted by

the coupling value of interest, or its square, to derive the predictions for any specific coupling value. This approach also facilitates independent examinations of the linear and quadratic contributions.

The validity of this decomposition method is confirmed by generating decomposed samples using a notably large coupling value and comparing the aggregated results to those from a single sample where the Standard Model and EFT contributions are generated concurrently. The effectiveness of this decomposition closure is illustrated in Figure 4–42 for the $T0$ operator.

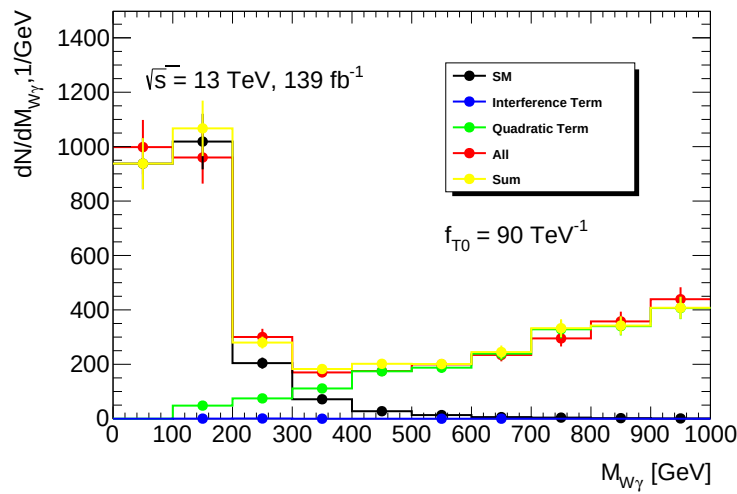


Figure 4–42 Verification of Sample Decomposition Strategy. The label "All" represents a sample in which the Standard Model and EFT contributions are jointly generated. The label "Sum" denotes the aggregate of the separately generated Standard Model, linear, and quadratic terms.

In the validation process of the sample decomposition, the scaling of cross sections for both linear and quadratic terms with respect to the coupling constants is confirmed. This involves generating interference and exclusive anomalous quadruple gauge coupling (aQGC) terms for the $T7$ operator at varying coupling strengths. The accurate scaling relationship of the cross section with coupling values is depicted in Figure 4–43.

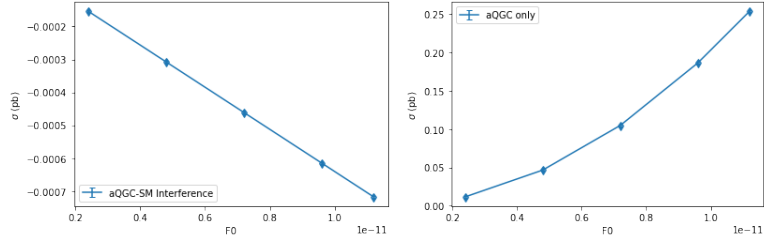


Figure 4-43 Scaling of the cross section of the interference term and aQGC-only term with the coupling value. The correct linear and quadratic dependences are observed.

As with the MadGraph signal samples, the EFT Monte Carlo samples are generated at leading order. The NNPDF3.0 NLO PDF set is utilized, and parton-level events are showered using Pythia8. The detector response is subsequently simulated using Geant4.

4.9.2 Statistical Model

In this analysis, one-dimensional limits are established for each coupling individually. Specifically, a statistical model that parameterizes a single aQGC coupling is fitted to the data, with all other couplings set to zero. The model for the differential cross section in terms of variable X for a given coupling c is expressed as:

$$\frac{d\sigma^i}{dX}(c) = \frac{d\sigma_{\text{SM}}^i}{dX}(1 + \delta\theta) + c \cdot \frac{d\sigma_{\text{int}}^{(i)}}{dX}(1 + \delta\theta) + c^2 \cdot \frac{d\sigma_{\text{quad}}^i}{dX}(1 + \delta\theta) \quad (4-36)$$

where i denotes the bin index, and σ_{SM} , σ_{int} , and σ_{quad} represent the Monte Carlo predicted cross sections for the Standard Model, linear, and quadratic terms, respectively. The parameter $\delta\theta$ is a nuisance parameter that accounts for uncertainties in both the Standard Model and EFT predictions. Scale uncertainty is considered as an uncertainty affecting both the Standard Model and EFT predictions. An additional nuisance parameter, defined by the shape differences between the MadGraph and Sherpa predictions of the Standard Model process, affects only the Standard Model prediction.

This statistical model is then fitted to the unfolded data using a maximum likelihood method, defined as:

$$\mathcal{L}(c, \vec{\theta}) = \frac{1}{\sqrt{(2\pi)^k \cdot |V|}} \exp\left(-\frac{1}{2}\chi^2(c, \vec{\theta})\right) \prod_{\vec{\theta}} \mathcal{G}(\vec{\theta}) \quad (4-37)$$

where the χ^2 statistic assesses the fit between the statistical model and the unfolded results:

$$\chi^2(c, \vec{\theta}) = [y - f(c, \vec{\theta})]^T V^{-1} [y - f(c, \vec{\theta})] \quad (4-38)$$

In this formula, y represents the unfolded measurement, $f(c, \vec{\theta})$ denotes the model prediction, $\vec{\theta}$ is a vector of nuisance parameters, $\mathcal{G}(\theta)$ is a unit Gaussian at value θ , k typically stands for the number of measurements or bins, and V is the $k \times k$ covariance matrix. The covariance matrix is constructed from the statistical uncertainty derived from toy simulations. Measurement uncertainties can be incorporated directly into the covariance matrix or treated as additional nuisance parameters. Opting to treat uncertainties as nuisance parameters tends to yield more conservative limits, which are adopted as the default for this analysis.

4.9.3 Limit Setting

The likelihood function described above is employed to construct a profile likelihood ratio test statistic:

$$q(c_x) = -2 \log \frac{\mathcal{L}(c, \hat{\hat{\theta}})}{\mathcal{L}(\hat{c}, \hat{\hat{\theta}})} \quad (4-39)$$

where $\mathcal{L}(c, \hat{\hat{\theta}})$ represents the unconditional maximum likelihood and $\mathcal{L}(\hat{c}, \hat{\hat{\theta}})$ is the maximum likelihood evaluated at a specific value of c .

Wilke's theorem posits that in the large sample limit, where the likelihood function approaches a Gaussian form, the test statistic adheres to a χ^2 distribution characterized by m degrees of freedom, where m represents the number of free parameters in the model. Under the assumption that Wilke's theorem is applicable, the quantiles of the χ^2 distribution can be utilized to establish a 95% confidence region as follows:

$$\int_0^{q(c)} \chi^2(m=1) dq = 95\% \quad (4-40)$$

The process of setting limits is demonstrated through a scan of the test statistic as a function of the coupling of interest, specifically for the T0 operator, as shown in Figure 4-44. In this figure, the coupling values corresponding to a test statistic that encompasses 95% of the χ^2 cumulative distribution are marked with a dotted line. The calculated 95% confidence interval for this coupling is $[-2.40, 2.44]$.

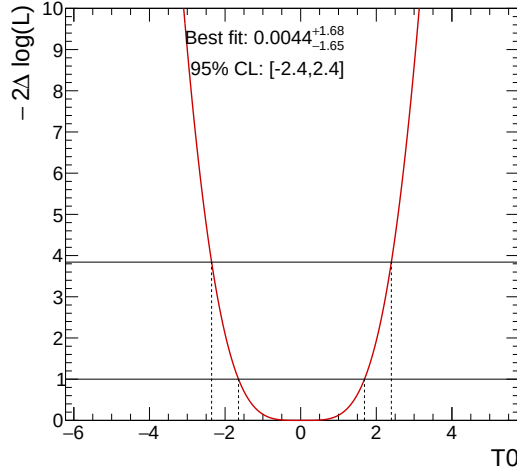


Figure 4-44 Likelihood scan of coupling of the T0 operator using a fit of the p_{jj}^T distribution to asimov data.

The validity of Wilke's theorem can be verified through pseudo-experiments, where N toy datasets are generated by fluctuating nuisance parameters and systematic uncertainties around their central values. Both unconditional and conditional fits are performed to compute the test statistic. Ideally, the test statistic should conform to a χ^2 distribution at the 95% confidence interval bounds. Any deviation from this distribution can be used to assess the extent to which the limits, set using the χ^2 cumulative distribution function, may be over or under covering. Figure 4-45 illustrates the distribution of test statistics for pseudo-experiments conducted by fitting the T0 operator coupling to the p_{jj}^T distribution. This figure confirms that at the boundaries of the 95% confidence interval, Wilke's theorem is upheld, and the test statistic adheres to a χ^2 distribution.

Toys are utilized to set limits and validate the coverage of Wilke's theorem. At each scan point, 1000 toy distributions are analyzed. The proportion of fits where the test statistic exceeds the value obtained from a true distribution fit is graphed as a function of the parameter of interest. The 95% confidence level (CL) interval is defined at points where the fraction of toys exceeding the nominal test statistic is 5%. This toy-based scan is illustrated alongside the scan of the T0 parameter for 1000 toys at 200 scan points in Figure 4-46. The limits determined using toys for the T0 operator are $[-2.4, 2.4]$, which align with the asymptotic assumption given the granularity of the scan. With Wilke's theorem validated, the asymptotic assumption is employed for stating limits.

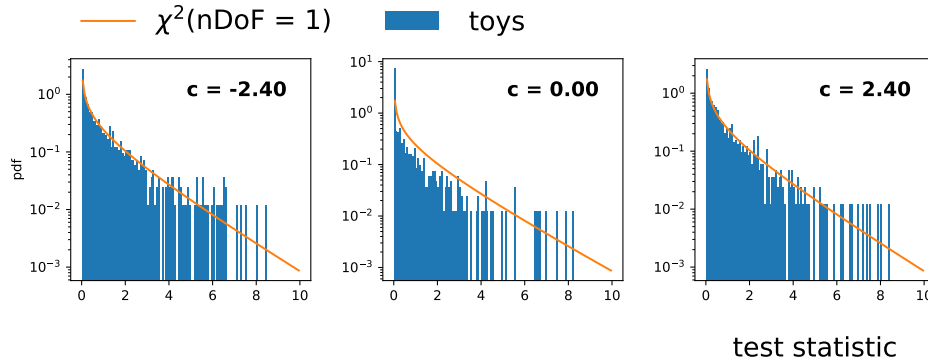


Figure 4-45 Distribution of test statistics for pseudo experiments at multiple values of the T0 wilson coefficient. In the large sample limit where the likelihood approaches a gaussian, the test statistic follows a χ^2 distribution according to Wilkes' theorem. Wilkes' theorem is obeyed at the boundaries obtained by the likelihood ratio scan.

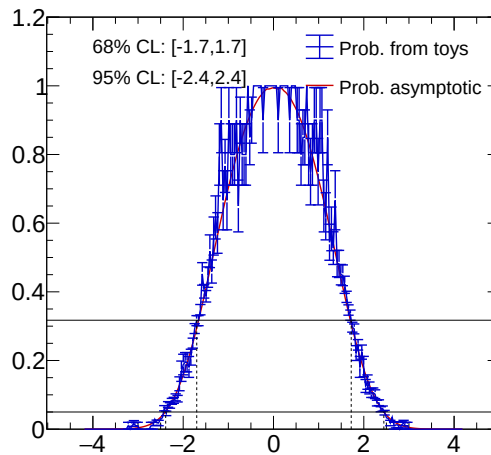


Figure 4-46 Likelihood scan using toys compared to the likelihood scan assuming Wilkes' theorem holds. 200 scan points are sampled and 1000 toys are used at each scan point. The limits from the asymptotic approximation and toys are in agreement.

4.9.4 Unitarization

Operators with mass dimension greater than 4 can lead to interaction probabilities that increase until unitarity is violated and the probability of interaction becomes greater than 1. More physical limits can be obtained by cutting the EFT and interference term beyond a cutoff value while keeping the standard model terms above this value. In line with the ATLAS aQGC task force recommendations, limits are reported with multiple cutoff values

and with no cutoff value using a *clipping scan*. In the *clipping scan* the fit is performed with EFT contributions removed above values of $M_{W\gamma} = .6$ TeV, 1.0 TeV, 1.5 TeV, 2 TeV, 3 TeV and 4 TeV. The resulting limits are compared with the partial-wave unitarity constraints derived in^[104].

4.9.5 Results

Expected and observed limits for dimension-8 operator coefficients, which adjust the couplings of interest, are presented in Tables 4–13 and 4–14 without any clipping applied. Fits to p_{jj}^T and p_l^T provide the highest sensitivity, and consequently, results from these fits are highlighted here.

c	Expected 95% CL Limit	Observed 95% CL Limit
f_{T0}	[-2.4,2.44]	[-1.75,1.8]
f_{T1}	[-1.51,1.58]	[-1.09,1.16]
f_{T2}	[-4.38,4.67]	[-3.14,3.46]
f_{T3}	[-3.3,3.47]	[-2.37,2.55]
f_{T4}	[-2.99,3.04]	[-2.16,2.21]
f_{T5}	[-1.7,1.71]	[-1.24,1.25]
f_{T6}	[-1.45,1.47]	[-1.04,1.06]
f_{T7}	[-3.79,3.87]	[-2.74,2.82]
f_{M0}	[-37.63,37.05]	[-27.08,26.44]
f_{M1}	[-56.65,57.84]	[-40.47,41.6]
f_{M2}	[-14.23,14.15]	[-10.38,10.3]
f_{M3}	[-21.57,21.82]	[-15.55,15.79]
f_{M4}	[-26.01,25.63]	[-18.81,18.46]
f_{M5}	[-20.32,22.06]	[-14.12,16.89]
f_{M7}	[-96.44,94.67]	[-69.43,67.75]

Table 4–13 Expected limits on dimension-8 operators modifying the $WW\gamma\gamma$ coupling when fitting p_{jj}^T .

c	Expected 95% CL Limit	Observed 95% CL Limit
f_{T0}	[-2.52,2.63]	[-2.11,2.23]
f_{T1}	[-1.6,1.71]	[-1.33,1.45]
f_{T2}	[-4.17,4.61]	[-3.43,3.9]
f_{T3}	[-3.44,3.72]	[-2.85,3.15]
f_{T4}	[-2.95,3.04]	[-2.46,2.55]
f_{T5}	[-1.8,1.83]	[-1.51,1.55]
f_{T6}	[-1.42,1.45]	[-1.18,1.22]
f_{T7}	[-3.63,3.76]	[-3.02,3.15]
f_{M0}	[-28.12,27.94]	[-23.86,23.61]
f_{M1}	[-43.4,44.2]	[-36.7,37.69]
f_{M2}	[-9.98,9.96]	[-8.57,8.54]
f_{M3}	[-15.74,15.98]	[-13.35,13.6]
f_{M4}	[-18.22,18.22]	[-15.4,15.41]
f_{M5}	[-16.51,14.23]	[-13.89,12.18]
f_{M7}	[-77.46,76.62]	[-65.87,64.9]

Table 4–14 Expected limits on dimension-8 operators modifying the $WW\gamma\gamma$ coupling when fitting pT_{lep} .

4.10 Results

Results of both observation and differential measurement are shown in this section. Real data are used in this section instead of Monte Carlo samples to have the unblinded results. Expected results are recorded in appendix A.17.

4.10.1 Observed Results

The observed results are presented below, using Sherpa as the default signal hypothesis. Table 4–15 displays the post-fit event yields, along with the yields from the Signal and Control regions in the data.

	SignalRegion	ControlRegion
EWK $W\gamma jj$	776.04 ± 91.00	190.94 ± 40.00
QCD $W\gamma jj$	1628.19 ± 115.71	1896.2 ± 146.56
QCD $Z\gamma jj$	114.78 ± 33.09	147.82 ± 68.62
Top Bkg.	110.11 ± 18.46	189.25 ± 39.07
$j \rightarrow \gamma$	392.34 ± 54.55	412.54 ± 56.48
$e \rightarrow \gamma$	147.58 ± 5.44	172.20 ± 6.12
$j \rightarrow l$	115.72 ± 16.08	113.27 ± 9.86
pileup γ	45.75 ± 0.65	11.18 ± 0.16
EWK $Z\gamma jj$	11.63 ± 1.04	6.65 ± 0.81
Total	3342.12 ± 61.33	3140.04 ± 99.48
Data	3341	3143

Table 4–15 Yields after fit to data in the signal and control region. Sherpa is the signal hypothesis.

The pre-fit and post-fit yields are shown in the signal and control region in Figure 4–47. A large mismodelling in Signal normalization in Sherpa can be seen.

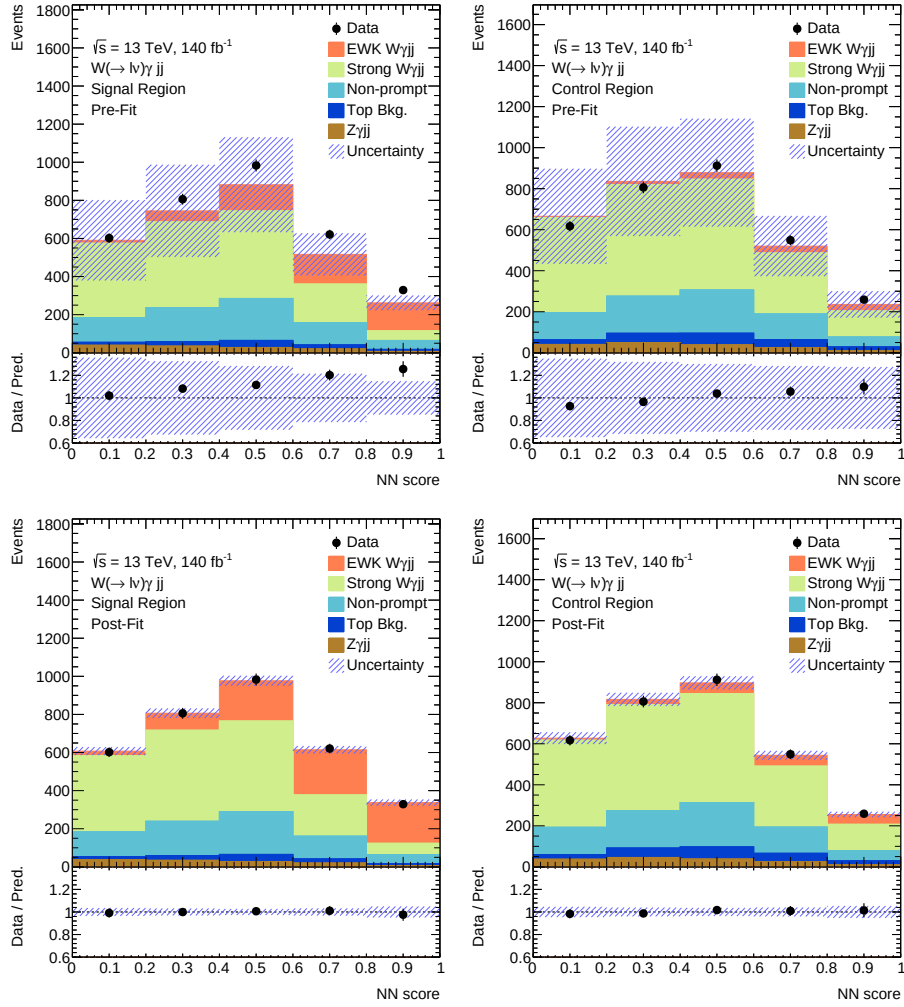


Figure 4–47 Pre-fit and post-fit plots of the NN score under the Sherpa signal hypothesis are shown. These plots incorporate all theoretical and systematic uncertainties on Monte Carlo backgrounds and data-driven estimates as detailed in sections 4.8 and 4.4. The fit is conducted using the complete dataset in the signal region and the control region data.

The fitted norm factors are shown in table 4–16

Parameter	Value
μ_{EW}	$1.51^{+0.19}_{-0.19}$
μ_{QCD}	$1.01^{+0.36}_{-0.36}$

Table 4–16 Electroweak signal strength and QCD normalization after fit to data where sherpa is the signal hypotheses.

The observed (expected) significance is 8.96 (6.26) σ .

4.10.2 Extraction of Fiducial Cross Section

To facilitate comparison with other experiments and for theoretical model integration, it is crucial to unfold the described results to a fiducial cross-section.

4.10.2.1 Fiducial Volume Definition

The definition of the fiducial volume aims to closely mirror the reconstructed signal region to minimize extrapolations to unobserved data regions, while maintaining simplicity for theoretical comparisons and cross-experiment consistency. It also strives for model independence. The specific criteria for the fiducial baseline selection are outlined in appendix A.17.2 and is implemented within a RIVET routine.

4.10.2.2 Fiducial Cross Section Extraction

The fiducial cross section is calculated as

$$\sigma^{fid} = \frac{\mu \cdot N^{exp}}{C \mathcal{L}} \quad (4-41)$$

N^{exp} is the expected event yield in data, μ is the fitted electroweak normalization factor, $\mathcal{L}$ is the integrated luminosity of the Full Run 2 dataset, and C is a correction factor to correct the detector effects

$$C = \frac{N^{reco}}{N^{fid}} \quad (4-42)$$

C is calculated using the MC simulation of our signal samples. N^{reco} and N^{fid} are separately the event yield after the selections used in the analysis on reco and truth level. Electron and muon channels are combined to give the fiducial cross section. The correction factor derived from the Sherpa signal sample is $C = 0.52 \pm 0.02$ for the combined channel, and $C = 0.55 \pm 0.09$ for the electron channel and $C = 0.49 \pm 0.08$ for the muon channel, respectively. The consistency in correction factors across the channels is attributed to different efficiencies in the detector's systems: a combination of low identification efficiency and high trigger efficiency for electrons^{[105], [106]}, and conversely, high identification efficiency and low trigger efficiency for muons^{[107], [108]}.

The uncertainty in the measured fiducial cross section, attributed to a specific source, is

quantified as follows:

$$\Delta\sigma = \sigma_{\text{nominal}} - \frac{(\mu + \Delta\mu) \cdot N_{\text{exp}}}{(C + \Delta C)\mathcal{L}} \quad (4-43)$$

where C represents the nominal correction factor, μ is the normalization factor derived from electroweak processes, ΔC denotes the variation in the correction factor that results from changes in N_{reco} and N_{fid} due to systematic or theoretical uncertainties, and $\Delta\mu$ is the alteration in μ from refitting with a nuisance parameter set to $\hat{\theta} \pm \Delta\hat{\theta}$. This formulation accounts for the correlations between μ , N_{reco} , and N_{fid} in determining the impact of specific uncertainties on $\Delta\mu$.

Note the statistically significant difference in the correction factor between Madgraph and Sherpa. Using the Madgraph signal sample, the correction factor is $C = 0.56 \pm 0.03$. When calculating $\Delta\mu$ related to the uncertainty from the choice of electroweak generator, δC is derived from the difference in C between Madgraph and Sherpa. This effect is symmetrically adjusted consistent with the treatment of the electroweak generator choice uncertainty. The measured (expected) fiducial cross section is reported as $\sigma^{\text{fid}} = 13.2(8.8) \pm 2.5(2.1)$. The contributions of various sources of error to the fiducial cross section are detailed in tables 4–17 and 4–18 for the measured and expected fiducial cross sections, respectively. The measurement is compared with the predictions of Sherpa and Madgraph in Figure 4–48.

Uncertainty Source	Fractional Uncertainty
MC Stats.	0.11
Jets	0.08
Lepton,Photon,Pileup	0.08
EW Wgamma jj Model	0.07
Strong Wgamma jj Model	0.06
Non-prompt Background Model	0.02
Luminosity	0.02
Other Background Model	0.02
E_T^{miss}	0.01

Table 4–17 Fractional uncertainty of various sources of uncertainty to the measured fiducial cross section.

Uncertainty Source	Fractional Uncertainty
MC Stats.	0.15
Strong Wgamma jj Model	0.11
Jets	0.09
EW Wgamma jj Model	0.08
Lepton,Photon,Pileup	0.07
Non-prompt Background Model	0.03
Other Background Model	0.02
Luminosity	0.02
E_T^{miss}	0.01

Table 4–18 Fractional uncertainty of various sources of uncertainty to the expected fiducial cross section.

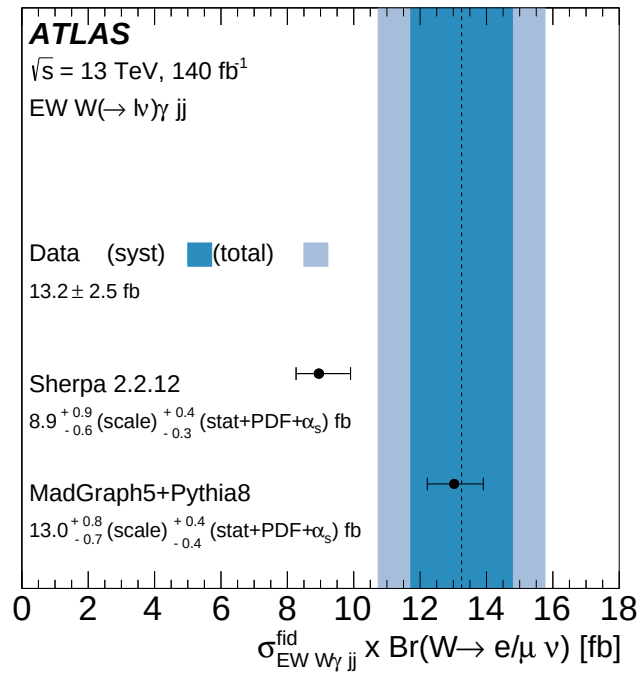


Figure 4–48 The measured fiducial cross section compared with the predictions of Madgraph and Sherpa.

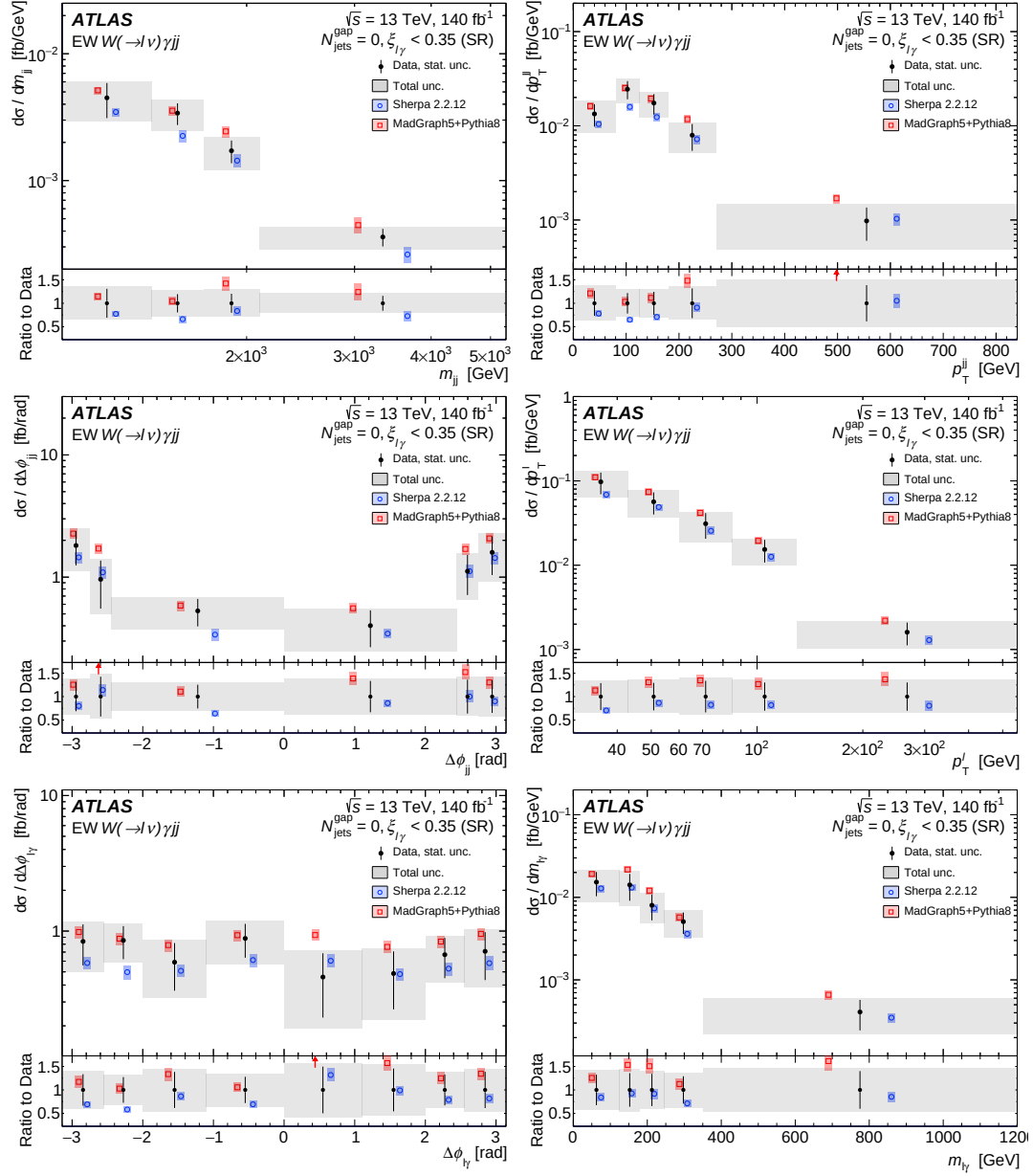


Figure 4-41 EW $W\gamma jj$ unfolded differential cross-section distributions of $m_{jj}, p_T^{jj}, \Delta\phi_{jj}, p_T^l, m_{l\gamma}$ and $\Delta\phi_{l\gamma}$ in the electron and muon combined channel after SR selections extractions and unfolding procedure. Truth predictions are shown for the Madgraph and Sherpa truth Signal samples. The error bars on the predictions are determined from scale, PDF, α_s (for Sherpa), and MC stat uncertainties.^[94]

Chapter 5 Search for Pair Production of Boosted Higgs Bosons with ATLAS Detector

5.1 Introduction

In addition to exploring the electroweak interactions via the $W\gamma jj$ process, this thesis extends its investigation into two other key areas of particle physics. First, a detailed study of the production of Higgs boson pairs through vector boson fusion (VBF) is presented, which not only probes the Higgs sector of the Standard Model but also provides a sensitive test for new physics scenarios, such as modifications to the Higgs self-coupling. The work described in this section is used for illustrating this physics target.

After the discovery of the Higgs boson in 2012, the main focus has changed to investigating the properties of this particle. Then people could compare its properties with the predictions from the SM theory. The study of Higgs boson pair production or di-Higgs(HH) provides us with a probe of both SM and Beyond the Standard Model (BSM) theory^[23-29]. HH production is directly related to the Higgs self-coupling which is the interaction between Higgs boson and Higgs boson itself. And it is also one of the key component of the Electroweak Symmetry Breaking. Therefore, the study of HH production is important to understand the nature of the Higgs boson.

Figure 5–1 is showing the dominant production of HH from the ggF mode of the SM theory. The cross section of these process is calculated at next-next-to-leading order (NNLO) with finite top approximation for a 125 GeV Higgs boson. And the value of the cross section is $\sigma_{ggF HH}^{\text{SM}} = 31.05 \pm 3\%$ (PDF+ α_s) $^{+6\%}_{-23\%}$ (Scale + m_{top}) fb^[30]. The *box* diagram on the left

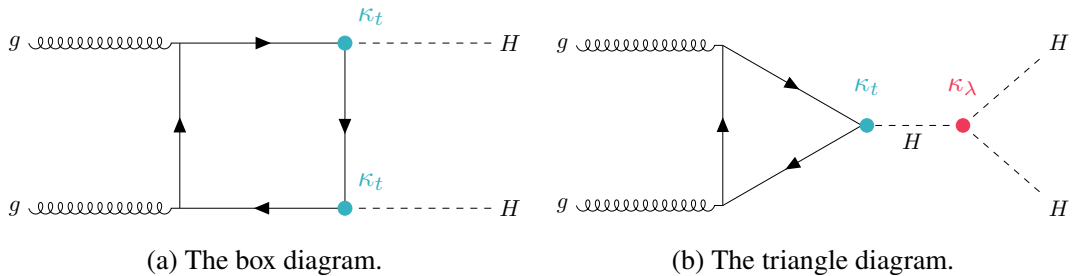


Figure 5–1 The Leading order gluon-gluon fusion di-Higgs production Feynman diagrams.

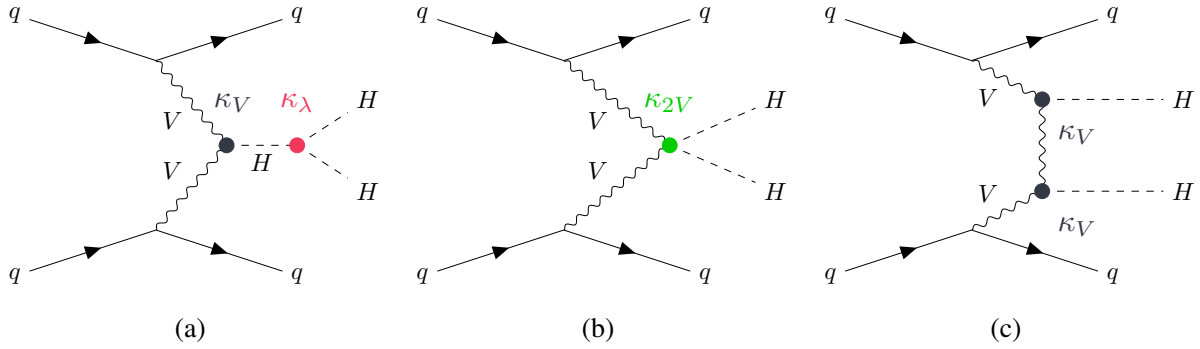


Figure 5-2 The three tree-level vector boson fusion di-Higgs production Feynman diagrams.

depends on the Higgs to Top quark Yukawa coupling and its modifier, κ_t . The *triangle* diagram on the right is dependent on both Higgs to Top Yukawa coupling and trilinear Higgs self-coupling. κ_λ is the modifier and it is the ratio of the modified coupling to its SM value.

The second dominant HH production is the vector boson fusion(VBF), it has a cross-section over an order of magnitude smaller than the ggF mode mentioned above. Its value of cross-section is $\sigma_{VBF\,HH}^{SM} = 1.726 \pm 2.1\%$ (PDF+ α_s) $^{+0.03\%}_{-0.04\%}$ (Scale) fb^[33] at next-to-next-to-next-to-leading order (N3LO) with 125 GeV Higgs boson. It could be used to probe the interaction between HH and two vector bosons. Figure 5-2 is showing the three tree-level VBF HH production diagrams. In the SM theory, the middle one 5-2b and the right one 5-2c cancels each other due to destructive interference. However, if κ_{2V} is deviated from its SM value of one, the diagram in Figure 5-2b begins to dominate, which results in an largely increased cross-section and harder kinematics^[34].

This analysis benefits from the large signal cross-section because of the large branching ratio of the Higgs boson decays in final states. Figure 5-3 is showing the branching ratio of the Higgs boson decay. Apparently, the decay is the most dominant one. We are looking for the decays where each pair of the jets merged into one large- R jet in this analysis. The dominant background against our fully hadronic final stat would be the QCD multijet events which is difficult to model only with MC simulation^[109]. A fully data-driven background estimation is done in this analysis and is described in later sections.

5.1.1 Composite Higgs model

In the Standard Model, the chiral nature of fermions is derived from the irreducible representations of the Lorentz group, while the presence of massless gauge bosons is a con-

$b\bar{b}$	WW^*	gg	$\tau^+\tau^-$	$c\bar{c}$	ZZ^*	$\gamma\gamma$	
33.9%	24.9%	9.5%	7.3%	3.4%	3.1%	0.3%	$b\bar{b}$
	4.6%	3.5%	2.7%	1.2%	1.1%	< 0.1%	WW^*
		0.7%	1.0%	0.5%	0.4%	< 0.1%	gg
			0.4%	0.4%	0.3%	< 0.1%	$\tau^+\tau^-$
				< 0.1%	0.2%	< 0.1%	$c\bar{c}$
					< 0.1%	< 0.1%	ZZ^*
						< 0.1%	$\gamma\gamma$

Figure 5–3 Branching ratios of the di-Higgs at the LHC.

sequence of gauge invariance. The generation of mass for gauge bosons and fermions is attributed to the spontaneous symmetry breaking of gauge invariance. This symmetry breaking is triggered by the Higgs vacuum expectation value (Vev), which is introduced parametrically rather than through any dynamic or fundamental principle. The Higgs sector is notable for containing most of the Standard Model's free parameters, whose stability under radiative corrections raises concerns, leading to the well-known "naturalness" problem. Consequently, the introduction of additional symmetries and/or dynamics is often considered necessary.

One pertinent question in particle physics is why the Higgs boson remains relatively light, given that new physics at higher scales tends to significantly increase its mass. An enduring hypothesis suggests that the Higgs doublet, consisting of four fields, acts as a Nambu-Goldstone mode emanating from the spontaneous breakdown of a larger global symmetry. In this framework, both the Higgs boson and the longitudinal components of the W and Z bosons, denoted W_L and Z_L , are considered Nambu-Goldstone bosons. The classic symmetry in this context is $SO(5)$, which breaks down to the $SO(4)$ symmetry observed in the Higgs sector. Typically, Nambu-Goldstone bosons are massless; however, to accord a small

but non-zero mass to the Higgs, a slight explicit breach of the global symmetry is required. This adjustment renders the Higgs boson not a perfect Nambu-Goldstone mode but rather a pseudo-Nambu-Goldstone boson (pNGB), which is inherently light. This concept is further developed in models such as the holographic Higgs and Little Higgs, which aim to keep the Higgs vacuum expectation value v substantially lower than the global symmetry-breaking scale f , where new strong dynamics are posited to emerge.

The Vector Boson Scattering (VBS) topology presents a prime and distinct setup for probing the proposed new strong dynamics. In this scenario, high-energy quarks emit longitudinal vector bosons that engage with this strong dynamics. It is anticipated that resonances associated with this strong dynamics will manifest. The lightest of these resonances is expected to decay into pseudo-Nambu-Goldstone bosons, which are considerably lighter, such as the longitudinal gauge bosons and the Higgs bosons, drawing an analogy to the $\rho \rightarrow \pi\pi$ decay observed in QCD. In the framework of a simplified model^[36], this lightest resonance is hypothesized to be a scalar η , which decays into the diboson modes $\eta \rightarrow HH, Z_L Z_L$, and $W_L W_L$ exclusively, with the branching ratios following a 1:1:2 proportion.

In the proposed model, the decay width of the η resonance, denoted as Γ_η , is given by the equation $\Gamma_\eta = \frac{a_\eta^2 m_\eta^3}{8\pi f^2}$, where a_η represents the coupling parameter between η and the pseudo-Nambu-Goldstone bosons (pNGBs). For simplicity, it is posited that the unitarization of the scattering of longitudinal vector bosons is facilitated solely through the interplay of Higgs and η exchange, with negligible contributions from heavier resonances. In this model, unitarity is fully preserved when a_η is set to 1, which is the chosen value. The model's free parameters are the resonance mass m_η and the new symmetry-breaking (compositeness) scale f , or equivalently, the mass and width of the resonance. Notably, the fractional width of the resonance, Γ_η/m_η , is calculated to be $4\%(m_\eta/f)^2$.

This model presents two significant advantages over effective field theory (EFT) approaches. Firstly, it provides a direct means for detecting heavy resonances, which is an optimal application for high-energy colliders like the LHC. In contrast, EFT is better suited for characterizing slight deviations in observable values at masses low relative to the collision energy. Secondly, this model inherently preserves unitarity without the need for ad-hoc unitarization methods. This inherent feature obviates the complex unitarization processes often necessary for addressing anomalous couplings and higher-dimensional EFT operators

in descriptions of high-energy scattering.

5.2 Data and Monte Carlo Samples

This analysis is also using the full Run 2 dataset as the previous one. Some of the details would not be repeated here to avoid the overflow of the page. Monte Carlo simulation are used for both modeling signal process and studying background process. However the multijet QCD process is hard to be correctly modeled as we discussed in introduction section. Full simulation modelling of the ATLAS detector is used for all samples.

5.2.1 Non-resonant signal

The POWHEG BOX v2 generator was employed by us to simulate the nominal ggF samples at next-to-leading order (NLO). This included full NLO corrections with a finite top mass, utilizing the PDF4LHC parton distribution function (PDF) set^[110]. The parton showers and hadronization processes were modeled using PYTHIA8 (v.244p3) with the A14 tune. For the normalization, we adopted the SM ggF di-Higgs cross-section, $\sigma_{\text{ggF}} = 31.05 \text{ fb}$, which was calculated at NNLO FTAprox^[111]. This cross-section was further multiplied by the branching ratio for the $4b$ final state, giving $\sigma_{\text{ggF}} \times \mathcal{B}(4b) = 31.05 \text{ fb} \times 0.3392 = 10.532 \text{ fb}$. We assumed a Higgs mass of 125 GeV. There is an alternative ggF sample generated to assess the parton showering uncertainties using POWHEG BOX v2 at the NLO.

VBF signal samples are simulated at leading order using MADGRAPH. The simulation employs the NNPDF3.0NLO PDF set alongside the A14 tune of PYTHIA8. The normalization of these samples is based on the Standard Model (SM) VBF di-Higgs production cross-section, $\sigma_{\text{VBF}} = 1.726 \text{ fb}$, computed at N3LO QCD^[33]. This cross-section is adjusted by the four-b decay branching ratio to yield $\sigma_{\text{VBF}} \times \mathcal{B}(4b) = 1.726 \text{ fb} \times 0.3392 = 0.585 \text{ fb}$. The simulations assume a Higgs boson mass of 125 GeV. For a comprehensive exploration of the κ parameters (κ_λ , κ_{2V} , κ_V), six VBF samples are linearly combined. BSM process cross-sections are initially obtained at LO from the generator and are subsequently scaled to N3LO using the SM k-factor: $\text{N3LO(SM)}/\text{LO(SM)}$ ^[112]. To compensate for the scarcity of events following selections in the boosted regime, four VBF samples are regenerated with a generator-level cut of leading large- R jet truth $p_T > 250 \text{ GeV}$ (TruthJetFilter), replacing the original non-filtered samples. Furthermore, an alternative LO sample is produced to assess

uncertainties related to the parton shower.

5.2.2 Resonant signals

The scalar resonance signal model is simulated at leading order (LO) in α_s using MADGRAPH (v2.9.9). Hadronization and parton showering processes are handled by PYTHIA8 (v.306), using the A14 tune alongside EVTGEN (v.1.7.0), and the nominal parton distribution function (PDF) is NNPDF 3.0 NLO. This is implemented as a two-Higgs-doublet model (2HDM) where a new neutral scalar, produced via vector boson fusion (VBF), is forced to decay into a pair of Standard Model (SM) Higgs bosons. The heavy scalar is assumed to have a width significantly smaller than the detector resolution, set at 40 MeV. Other 2HDM particles are not included in this calculation. A range of resonance masses, from 1.0 TeV to 5.0 TeV, is considered in this boosted analysis. Additionally, resonant signal samples using the spin-0 Radion model with broader widths have been generated. Broad width samples for the 1.0 TeV and 2.0 TeV mass hypotheses are set to 20% of the true mass value, with an additional sample for the 2.0 TeV signal at the HRC-recommended width of 28 GeV.

In summary, the following mass points are generated:

- 2HDM: [1, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.8, 2, 2.5, 3, 4, 5] TeV
- Broad: [1, 2] TeV

Additional samples utilizing the Composite Higgs model^[36] were generated at leading order in α_s using MADGRAPH¹. Hadronization and parton showering processes were conducted using the A14 tune of PYTHIA8 along with EVTGEN, and the nominal PDF employed was NNPDF 3.0 NLO. The mass points are summarized as:

Narrow width, 2% of m_X [1, 1.5, 2] TeV

Broad width, 20% of m_X [1, 1.2, 1.5, 1.8, 2] TeV

But we have found one bug in the generation of the 1 TeV sample, so this sample would not be used in the analysis. Methodologies would be discussed in later sections. To assess parton shower uncertainties in the resonant analysis, additional 2HDM samples were generated using HERWIG (v.7.2.2) for selected mass points. These parton showering uncertainties derived from the 2HDM samples are also employed in the interpretation of the Composite Higgs model.

¹ <https://its.cern.ch/jira/browse/ATLMCPROD-10470>

5.2.3 Background samples

As we discussed in sections above, the dominant background for this analysis is the multi-jet QCD process. And since it is difficult to have a good modeling of this process, fully data-driven method would be adopted here. And the background samples are simulated for $t\bar{t}$ and di-jet QCD process only for selection and kinematic region optimizations at the very early stage of this work. The $t\bar{t}$ samples are generated using POWHEG combined with the A14 tune of PYTHIA 8 (v8.230) and EVTGEN (v1.6.0). The matrix elements are calculated employing the NNPDF3.0_{NLO} PDF set. For analysis, two distinct sets of samples are utilized to represent different final states with HT filters: one set for the non-all hadronic final state (DSID = 407342 – 407344) and another for the all hadronic final state (DSID = 410428, 410429, 410444). Additionally, the di-jet QCD Monte Carlo simulations are performed by PYTHIA 8 (v2.44p3) with EVTGEN (v1.7.0) using the A14 NNPDF2.3_{LO} tune. These are segmented by p_T , with slices JZ2–4 designed to include at least two γ -jets at the truth level (via a truth b -jet filter) utilized (DSID = 800285–800287).

5.3 Event Selection

We mentioned in the previous section that we are focusing on a regime where both of the b jets are merged into large R jets. And the Xbb taggers are used to recognize those large R jets for the analysis.

5.3.1 Large Radius Jets

Anti- k_t jets with a radius parameter of $R = 1.0$, commonly referred to as “large- R ” or “fat” jets, are employed to effectively capture the decay of a boosted $\rightarrow$. In such scenarios, the two high-energy b -jets from the final state typically merge into one jet with a greater radius. These jets are reconstructed using the anti- k_t algorithm, which clusters the jet constituents iteratively, starting from the hardest and closest ones. The jet constituents consist of *locally calibrated* calorimeter clusters^[113].

Due to their large area, large- R jets are prone to incorporating energy from pile-up and underlying events. To mitigate this issue, the jets are trimmed by re-clustering the $R = 1.0$ jet with the k_t algorithm into sub-jets of $R = 0.2$, discarding any sub-jets where the p_T is below 5% of the large- R jet’s p_T .

In Monte Carlo (MC) simulations, these trimmed jets are calibrated using the `EtaJES_JMS` sequence, applying settings from `JES_MC16recommendation_FatJet_Trimmed_JMS_comb_17Oct`. For data samples, the calibration is executed through the `EtaJES_JMS_Insitu_InsituCombinedMass` sequence with settings from `JES_MC16recommendation_FatJet_Trimmed_JMS_comb_March2017`.

The mass of these large- R jets is determined through the *combined mass* method^[78], which enhances mass resolution across the jet p_T range compared to solely using calorimeter-based or track-assisted mass calculations. This method calculates the calorimeter-based mass, m_{calo} , and the track-assisted mass, m_{TA} , as follows:

$$m_{\text{calo}} = \sqrt{\left(\sum_{i \in \text{Jet}} E_i\right)^2 - \left(\sum_{i \in \text{Jet}} \vec{p}_i\right)^2}; \quad m_{\text{TA}} = \frac{p_T^{\text{calo}}}{p_T^{\text{track}}} \cdot m_{\text{track}} \quad (5-1)$$

where E_i and $\vec{p}_i$ represent the energy and momentum of each calorimeter cell cluster within the jet, and m_{track} , p_T^{track} , and p_T^{calo} denote the mass and p_T computed using tracking data¹, and the calorimeter-based p_T , respectively.

The combined mass is computed as follows:

$$m_{\text{comb}} = w \cdot m_{\text{calo}} + (1 - w) \cdot m_{\text{TA}} \quad (5-2)$$

Here, w is a weight derived for each large- R jet, based on the resolution from the calibrated track and calorimeter mass components. As these components are only minimally correlated, the combined mass is a straightforward linear combination of them.

Operational parameters for large- R jets stipulate that they must have $200 < p_T < 3000$ GeV, a mass between $50 < m < 600$ GeV, and an absolute rapidity of $|\eta| < 2$, tighter than the 40 GeV threshold used in triggers, in accordance with Jet/ETMiss guidelines.

5.3.2 b-tagging

Large R jets are discussed above, but we still need to find those jets with special tactics. The double b -tagging algorithm^[114] enhances the selection of boosted Higgs bosons by leveraging advanced b -tagging techniques applied to VR track-jets. It assigns probabilities for b -, c -, and light-flavor identities to the top three subjets. These probabilities, together with the large- R jet's p_T and η , are input into a neural network designed to differentiate between

¹ p_T^{track} is the transverse momentum sum of all tracks linked to the large- R jet, and m_{track} their aggregate mass.

Higgs signals and backgrounds from multijet and top events. The neural network output is then transformed into a discriminant D_{Xbb} , which classifies $R = 1.0$ jets as follows:

$$D_{\text{Xbb}} = \ln \left(\frac{P_{\text{Higgs}}}{f_{\text{top}} \cdot p_{\text{top}} + (1 - f_{\text{top}}) \cdot p_{\text{multijet}}} \right) \quad (5-3)$$

In this formulation, f_{top} is the predefined fraction of the top background, currently set at 0.25. The $X \rightarrow bb$ tagger, utilizing this approach, exhibits superior performance in discriminating against top and multijet backgrounds compared to other large- R jet -tagging algorithms such as DL1r utilized by ATLAS. Within our analysis framework, the working point (WP) for D_{Xbb} is established above 2.44 to maintain a 60% detection efficiency for $\rightarrow$ jets. This threshold achieves a QCD background rejection rate of 80.6 and a top background rejection of 28.1.

Studies have been done to compare two approaches on jet tagging for object reconstruction. The first approach is to tag two VR trk jets with DL1r tagger, and the second approach is to tag the large- R jets with directly the Xbb tagger.

Figure 5–4 presents a comparison of the $X \rightarrow bb$ tagger's efficiency against that of the DL1r, specifically evaluated on ghost-associated VR track jets. This comparison is mapped as a function of the p_{T} of the leading large- R jet and the invariant mass of the HH system, which comprises the two leading large- R jets, for the HH VBF signal where $\kappa_{2V} = 0$. The DL1r algorithm exhibits a decrease in efficiency with increasing p_{T} , particularly evident when tagging highly collimated objects within a single jet. This reduction in efficiency is influential in the observed bias in the mass $m(HH)$ calculations.

5.3.3 Small Radius Jets

Small- R jets are constructed using the anti- k_t algorithm with a distance parameter of $R = 0.4$ ^[115], specifically to identify two jets characteristic of the VBF production mode. These jets are formed from particle-flow (PFlow) objects, which enhance jet resolution at lower p_{T} . This enhancement takes advantage of the precise tracking resolution to more accurately estimate the energy of lower p_{T} clusters^[116]. Adjustments to the jet energy and direction include corrections for pile-up background, fluctuations related to the jet's origin, its inherent stochastic nature, and systematic discrepancies between the data and MC simulations^[117]. The configuration file employed for applying the Jet Energy Scale (JES) calibration is:

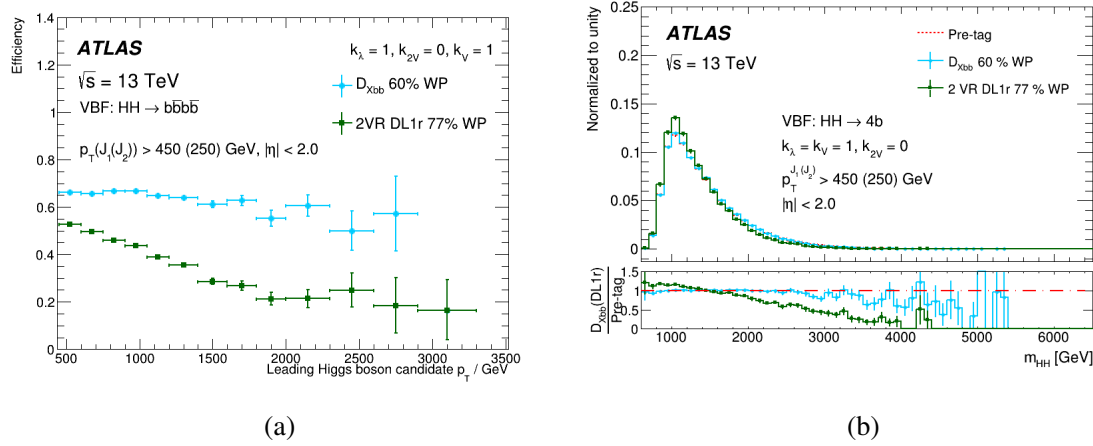


Figure 5–4 Efficiency of double-tagging as a function of the transverse momentum of the leading large- R jet (left) and the invariant mass distribution of the HH system from the two leading large- R jets before and after double-tagging (right). Efficiency comparisons are made between the $X \rightarrow b\bar{b}$ tagger and the DL1r algorithm, evaluated on VR track jets, for jets from $\rightarrow$ decay in VBF HH production with $\kappa_{2V} = 0$.^[32]

JES_MC16Recommendation_Consolidated_PFlow_Apr2019_Rel21.config

Furthermore, to mitigate the effects of pile-up contamination, jets with $p_T < 60$ GeV and $|\eta| < 2.4$ must satisfy a Jet Vertex Tagger (JVT) threshold. The selected default, tight working point of JVT shows a 96% efficiency rate for identifying hard scatter jets^[118-119]. For this analysis, PFlow jets with $|\eta| < 4.5$ and p_T as low as 20 GeV are utilized.

5.3.4 Event selection

Our targets aim at both resonant and non-resonant search and the same set of selections are used in this analysis for both of them. A workflow of event selections are shown in Figure 5–5. All of the selections are optimized with MC signal samples and background samples to have optimal significance for the target which are $\kappa_{2V} = 0$ and resonant signals. At the same time, the statistics of the left events should be enough for later BDT (pBDT) trainings.

5.3.4.1 Triggers

Both data and simulated events must satisfy the lowest un-prescaled large- R jet trigger conditions. The specific triggers applied are HLT_j360_a10_lcw_sub_L1J100,

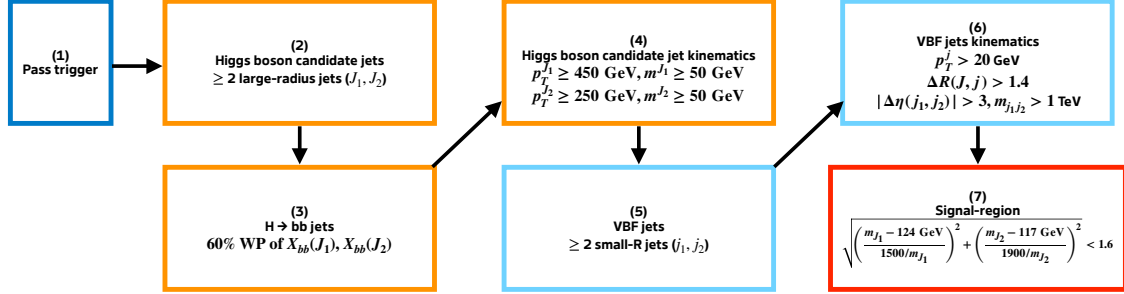


Figure 5–5 Cut flow chart for the boosted analysis.

HLT_j420_a10_lcw_L1J100, HLT_j420_a10t_lcw_jes_40smcINF_L1J100, and HLT_j420_a10t_lcw_jes_35smcINF_L1J100, corresponding to data collected in the years 2015, 2016, 2017, and 2018, respectively. Each of these triggers demands an E_T threshold for single large- R jets. Additionally, the triggers for the years 2017 and 2018 incorporate supplementary requirements of 40 GeV and 35 GeV on the mass of the large- R jets to qualify for the trigger.

5.3.4.2 Higgs candidates

The boosted regime is defined where each Higgs decay is collimated and should be clustered into one single large- R jet. The final state of interest consists of two Higgs so each event falling into our region should be having at least two large- R jets to form the Higgs candidates. The top two p_T jets are selected if there are more than two large- R jets. We further require the two Higgs candidates to pass the X_{bb} tagger mentioned in last section at a working point (WP) of 60%. In order to maintain the efficiency for the triggers, the leading and sub-leading jets should have a p_T greater than 450 GeV and 250 GeV separately. And those jets should have an invariant mass which is greater than 50 GeV. We have studied different WPs for the X_{bb} tagger but all of other choice would result in worse limits than the 60%.

5.3.4.3 VBF jets

The VBF jets are selected from those small- R jets left and satisfy $p_T^j > 20$ GeV and $\Delta R(J, j) > 1.4$, J here referees to large- R jet (Higgs candidates) and j referees to the small- R jets. Similarly, the top two leading small- R jets are selected according to their p_T order and then required to pass the following selections:

- $|\Delta\eta(j, j)| > 3$
- $m_{jj} > 1$ TeV

Optimization of these selections are done with MC samples and the statistics left is enough for the BDT (pBDT) trainings afterwards.

5.3.4.4 Signal Regions

In this analysis, we use a $m_{H1}-m_{H2}$ plane for the region definitions. And the previous resolved analysis^[120] has defined a SR in the formula here:

$$X = \sqrt{\left(\frac{m_1 - 124 \text{ GeV}}{0.1 m_1}\right)^2 + \left(\frac{m_2 - 117 \text{ GeV}}{0.1 m_2}\right)^2}. \quad (5-4)$$

However, due to different kinematic distribution of the final state, this formulation needs to be re-optimized. The function of these variables is similar to the equation of ellips, except that the radius is a function of Higgs candidate masses to allow harsher cuts for higher Higgs masses where the jet resolution is better than before.

$$X_1 = \sqrt{\left(\frac{m_{H1} - 124 \text{ GeV}}{a_1/m_{H1}}\right)^2 + \left(\frac{m_{H2} - 117 \text{ GeV}}{a_2/m_{H2}}\right)^2} < r \quad (5-5)$$

$$X_2 = \sqrt{\left(\frac{m_{H1} - 124 \text{ GeV}}{2 \cdot a_1/(m_{H1} + m_{H2})}\right)^2 + \left(\frac{m_{H2} - 117 \text{ GeV}}{a_2/m_{H2}}\right)^2} < r \quad (5-6)$$

$$X_3 = \sqrt{\left(\frac{m_{H1} - 124 \text{ GeV}}{a_1/m_{H1}}\right)^2 + \left(\frac{m_{H2} - 117 \text{ GeV}}{2 \cdot a_2/(m_{H1} + m_{H2})}\right)^2} < r \quad (5-7)$$

The optimization of this formula is processed by doing a grid scan on r from 1.4 to 2, with a step of 0.2; a_1, a_2 from 1300 to 2000, with a step of 100. The chosen of r is used for a closure of the boundary. The significance $Z_A = \sqrt{2((s+b) \ln(1 + \frac{s}{b}) - s)}$ is checked and the maximum Z_A is used. But for our boosted regime, the SM VBF sample could not be used

for the optimization due to its low statistics. So we use the sample of signal hypothesis $\kappa_{2V} = 0$ and dijet+ $t\bar{t}$ MC background. 5–6 shows the optimized (with highest Z_A) SR in the (m_{H_1}, m_{H_2}) mass plan with the three forms and the old X definition (in black).

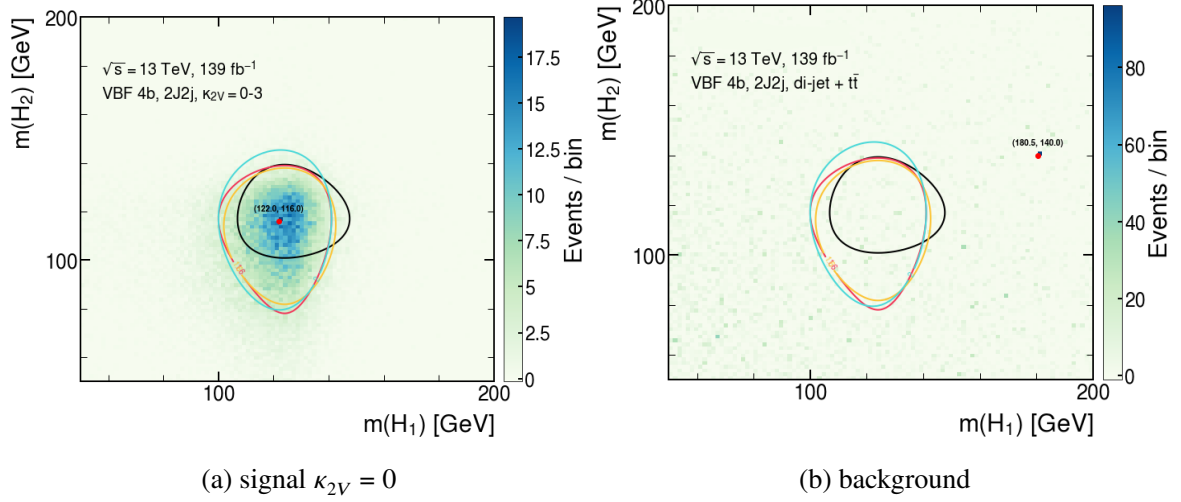


Figure 5–6 The (m_{H_1}, m_{H_2}) mass plane is presented for both the signal with $\kappa_{2V} = 0$ and the combined dijet + $t\bar{t}$ MC background. The black curve represents the original X definition, while the red, yellow, and blue curves correspond to optimized forms X_1 5–5, X_2 5–6, and X_3 5–7, respectively. Note that this optimization was conducted without applying the $X \rightarrow b\bar{b}$ efficiency scale factors and used a different large- R jet ordering scheme than the p_T -based ordering employed in the final analysis. However, these updates are unlikely to significantly affect the selection of the signal region.^[32]

Finally, the SR is defined to be as the form of the equation 5–8

$$X = \sqrt{\left(\frac{m_1 - 124 \text{ GeV}}{1500/m_1}\right)^2 + \left(\frac{m_2 - 117 \text{ GeV}}{1900/m_2}\right)^2} < 1.6. \quad (5-8)$$

and the significance from $\kappa_{2V} = 0$ and dijet+ $t\bar{t}$ MC background study gives 3.704 at maximum.

5.3.4.5 Validation and control regions

The validation region (VR) is defined using Equation 5–9 and excluding the SR ($X > 1.6$):

$$VR = \sqrt{\left(\frac{m_1 - 124 \text{ GeV}}{0.1 \ln(m_1)}\right)^2 + \left(\frac{m_2 - 117 \text{ GeV}}{0.1 \ln(m_2)}\right)^2} < 100. \quad (5-9)$$

While the control region (CR) is defined as:

$$CR = \sqrt{\left(\frac{m_1 - 124 \text{ GeV}}{0.1 \ln(m_1)}\right)^2 + \left(\frac{m_2 - 117 \text{ GeV}}{0.1 \ln(m_2)}\right)^2} > 100 \text{ \& } < 170 \quad (5-10)$$

The validation region (VR) and control region (CR) are less stringent compared to the previous resolved analysis to gather more statistics. Their shapes differ from the signal region (SR) to avoid the low mass region, which sees a higher prevalence of QCD background events. Additionally, merely expanding the SR radius beyond 1.6 does not ensure the closure of the curve or create a connected region, making it impossible to directly apply the X formula for defining VR and CR. Figure 5–7 illustrates the SR, VR, and CR regions using data. Analogous mass planes for the signal samples, including SM VBF, $\kappa_{2V} = 0$, and the resonant $m_X = 1.0 \text{ TeV}$ (2HDM), are shown in 5–8.

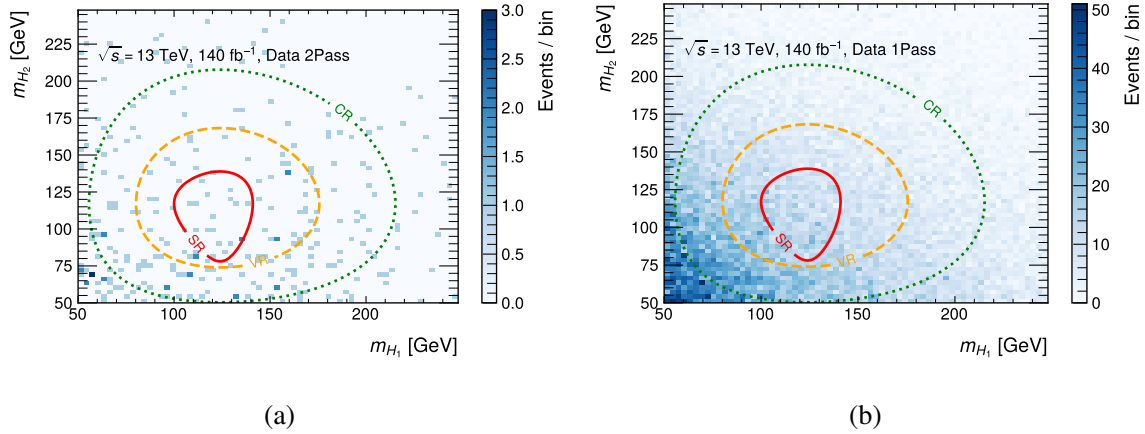


Figure 5–7 Mass plane with X contours by using data in the (a) 0F and (b) 1F regions. VR and CR definitions are displayed as well. These plot were updated after unblinding the analysis and already utilise the p_T -based ordering.^[32]

5.4 Background Estimation

We have defined exclusive regions for the background estimation and study of interesting events. There are four regions in total based on orthogonal Xbb tagging working points from control regions:

- SR, 0F: Both Higgs jets pass 60% Xbb tagger WP in the SR;

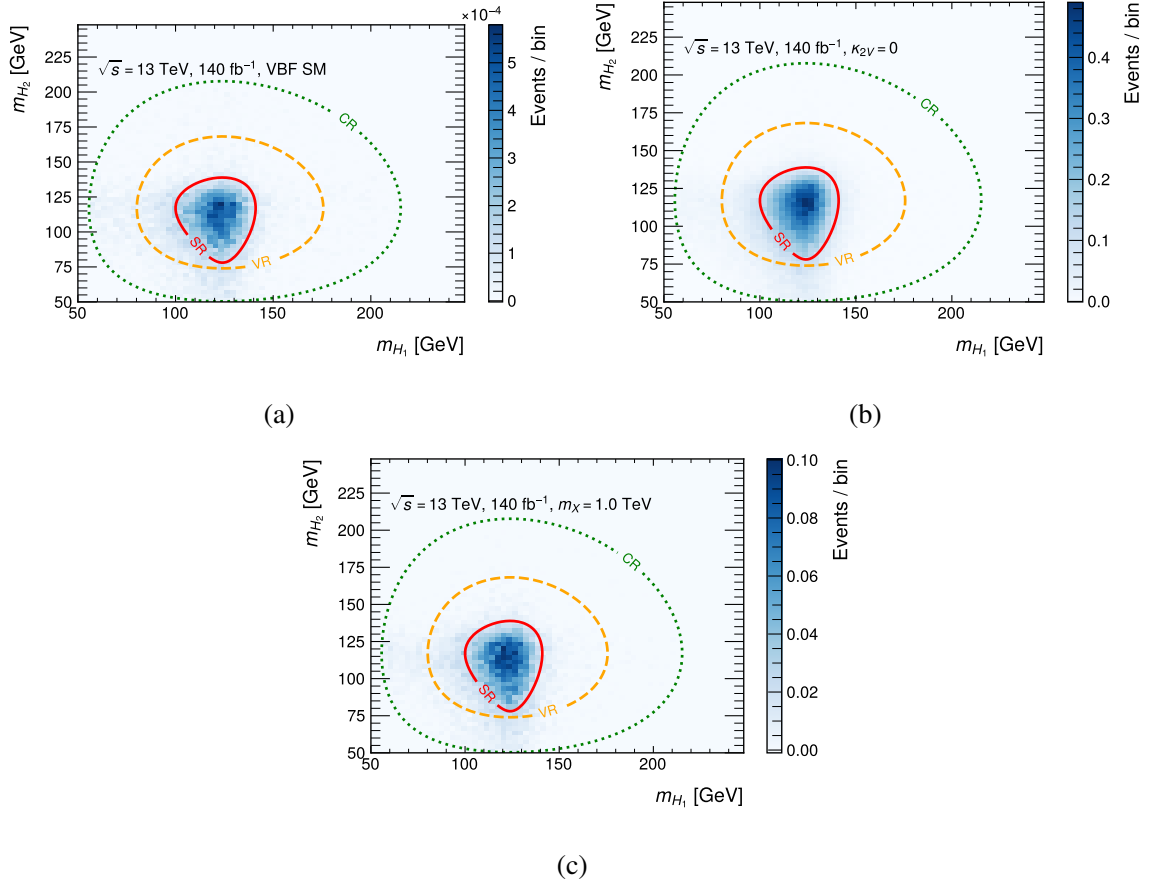


Figure 5–8 Mass plane with X contours by using the signal samples SM VBF (a), $\kappa_{2V} = 0$ (b), and the resonant $m_X = 1.0$ TeV (c) in the 0F region. VR and CR definitions are displayed as well. These plot were updated after unblinding the analysis and already utilise the p_T -based ordering.^[32]

- SR, 1F: One Higgs passing the 60% WP the other failing the 60% Xbb tagger WP in SR.
- CR, 0F: Both Higgs jets pass 60% Xbb tagger WP in the CR;
- CR, 1F: Only one Higgs jet pass 60% Xbb tagger WP in the CR.

We have already discussed the definition of SR and CR in the section above.

We assume that the ratio between 0F and 1F in CR is the same as the ration of 0F and 1F in SR with a ABCD method (or matrix method). So that the relation could be expressed as the following:

$$P(\text{SR}, 0\text{F}) = P(\text{SR}, 1\text{F}) \cdot \frac{P(\text{CR}, 0\text{F})}{P(\text{CR}, 1\text{F})},$$

where P is the distribution of events in the corresponding regions. Generally, this can be

accomplished in different ways:

- **Background Estimation with Neural Networks:** Estimation could be performed by learning density ratios in regions (CR 1F to 0F) using neural network classifiers and applying these to SR 1F to predict background in SR 0F. Those ratio could be functions of several different kinematic variables as described in Ref.^[121-122]. A reweighting study with NN is tested in this analysis, and in order to validate the performance, a validation region (VR) is also used. The distribution of events in CR before and after reweighting versus the kinematic variables are shown in figure 5–9.
- **Bin-by-bin ratio factor:** One could also calculate such ratio factors from CR 1F to 0F and then we can have background estimations when we apply this factor into SR 1F.

There is no obvious evidence that the shapes in 1F and 0F are different according to our studies.

Due to the low statistics following extensive preselection cuts and the similarity in kinematic distributions across different Xbb b -tagging regions, an inclusive normalization factor is derived from 1F and applied to 0F. Consequently, the shape of the distribution in SR, 0F is assumed to mirror that of SR, 1F. The derived normalisation factor is estimated to be:

$$\frac{N(\text{CR}, 0\text{F})}{N(\text{CR}, 1\text{F})} = 0.0081 \pm 0.0008.$$

where N is the total yields in that region.

The validity of the background estimation method described earlier may be questioned if there is significant signal leakage into the Validation Regions (VR) and Control Regions (CR), a scenario conceivable in the broad width context of the resonant analysis. However, investigations have confirmed that the impact of such leakage on the background estimation is negligible. This finding substantiates the reliability of the current background estimation approach for all search scenarios outlined in this analysis.

5.5 Multivariate Discriminants

5.5.1 Non resonant signal optimization

The classification method employed is XGBoost^[123], which is optimized for the non-resonant VBF signals after applying selection criteria. The kinematic variables listed in Ta-

ble 5–1, representing HH as the combination of two Higgs candidates, are used as inputs. The Boosted Decision Tree (BDT) is trained specifically in the signal region (SR), which is defined by the Higgs masses. To ensure the BDT’s response remains consistent across the validation and control regions (VR/CR) compared to the SR, the Higgs masses are excluded from the inputs. The analysis includes comparisons between VBF Monte Carlo (MC) simulations with κ_{2V} variations, standard model (SM) gluon-gluon fusion (ggF) MC, and a data-driven background estimate.

$H1, H2$ (large- R jet)	p_T, η
HH	p_T, η, m
VBF jet 1, jet 2	p_T, η, E

Table 5–1 Kinematic variables used as input features in the XGBoost training.

In the training process, $\kappa_{2V} = 0$ VBF MC is identified as the signal, while standard model (SM) ggF, VBF MC, and SR 1F data-driven samples are considered as backgrounds. This selection is aimed at excluding $\kappa_{2V} = 0$, which is of particular interest in the analysis and serves as a reasonable proxy for other Beyond Standard Model (BSM) signals, thereby improving constraints on κ_{2V} . Additionally, due to the softer p_T^H , the event selection efficiency is too low for the SM signal, rendering it difficult to constrain the upper limit of the SM HH production cross-section (XS). When this analysis is combined with the resolved analysis^[120], the contribution to the SM HH upper limit from the boosted channel is negligible. For the training/validation phase, 80% of events selected by `event number (%5 < 4)` are utilized, with the remainder allocated for statistical studies (test). Three background components of the training and validation samples are scaled to equal event numbers, and the total signal and background are balanced by ensuring equal total weights to accommodate different sample sizes.

A grid search of a 5-fold cross-validation method is employed on the training and validation samples to avoid overfitting and to optimize the hyper-parameters `num_boost_round` and `max_depth`, within the ranges of $[1, 150]$ and $[1, 12]$ respectively, and with `eta = 0.1`. The hyper-parameters are defined as follows:

num_boost_round Number of boosting iterations.

max_depth Maximum depth of a tree. Increasing this value will make the model more

complex and more likely to overfit. 0 indicates no limit on depth. The `exact` tree method requires a non-zero value.

eta Step size shrinkage used in updates to prevent overfitting. After each boosting step, we can directly get the weights of new features, and `eta` shrinks the feature weights to make the boosting process more conservative. Range: [0, 1].

The evaluation matrix is log loss¹. After training, the optimized `num_boost_round` is 161 and `max_depth` is 2. Variable “importances” are ranked in the Figure 5–10. “Importance” is defined by the average gain across all splits where a variable is used. p_T of Higgs candidates contribute most in discriminating the signal/background.

The fitted XGBoost model is then applied to test samples. Figure 5–11 illustrates the BDT response distributions between VBF MC with κ_{2V} variations, SM ggF MC, and data-driven background. The binning of the BDT distribution has been optimized for statistical studies. The black curve with a gray band (representing statistical error) depicts the data-driven background. The blue curve represents the SM ggF, while other colored curves indicate different κ_{2V} VBF MC scenarios. Notably, great discrimination is observed between VBF MC and other components, except for $\kappa_{2V} = 1$.

Due to the similarity in kinematic distributions between SM VBF and the background, the specialized XGBoost model trained with $\kappa_{2V} = 0$ VBF signal and SM VBF background does not fully separate it from the data-driven distribution. Figure 5–12(a) presents the log loss values calculated from BSM κ_{2V} VBF signal and total background components. Figure 5–12(b) displays the ROC curves and AUC values² calculated from BSM κ_{2V} VBF signal and total background components, although AUC is not utilized as the evaluation matrix in the training.

Different training strategies were tested, such as mixing SM HH signal and $\kappa_{2V} = 0$ VBF as training signal targets, or retaining all ϕ variables for better discrimination. However, the sensitivities to constrain κ_{2V} from these strategies either diminished or did not show significant improvement. To maintain a consistent set of variables used in the resonant analysis for clearer interpretation, the following non-resonant results are based on the optimization presented here.

¹ https://scikit-learn.org/stable/modules/generated/sklearn.metrics.log_loss.html

² https://en.wikipedia.org/wiki/Receiver_operating_characteristic

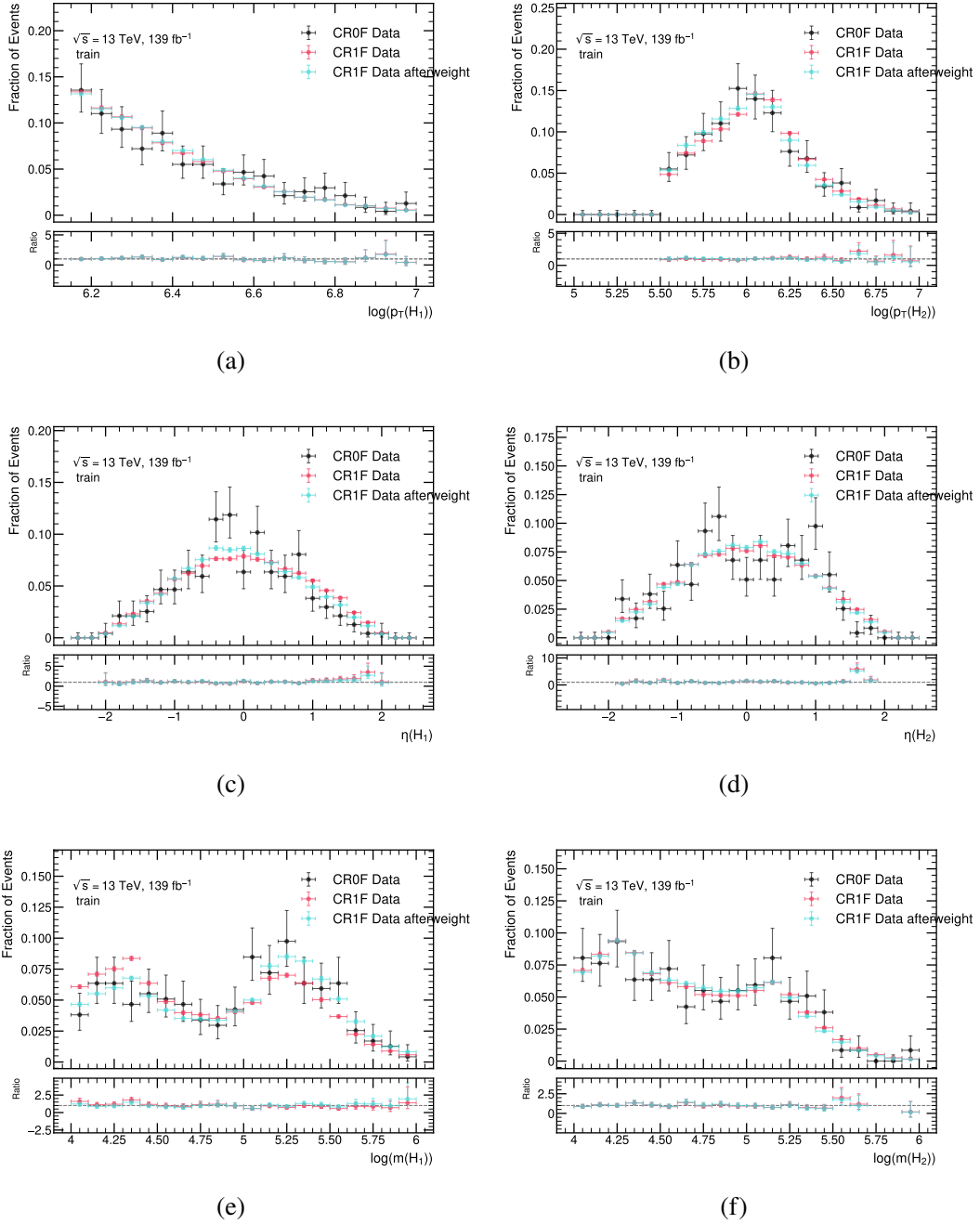


Figure 5-9 Comparison of the 1F (source) before and after kinematic reweighting and the 0F (target) kinematic variable distributions for events in the CR. The error bars indicate the statistical uncertainty in the data. Note that this plot utilizes a different large- R jet ordering scheme than the p_T -based ordering used by the final analysis, which is expected to differ by a few %.^[32]

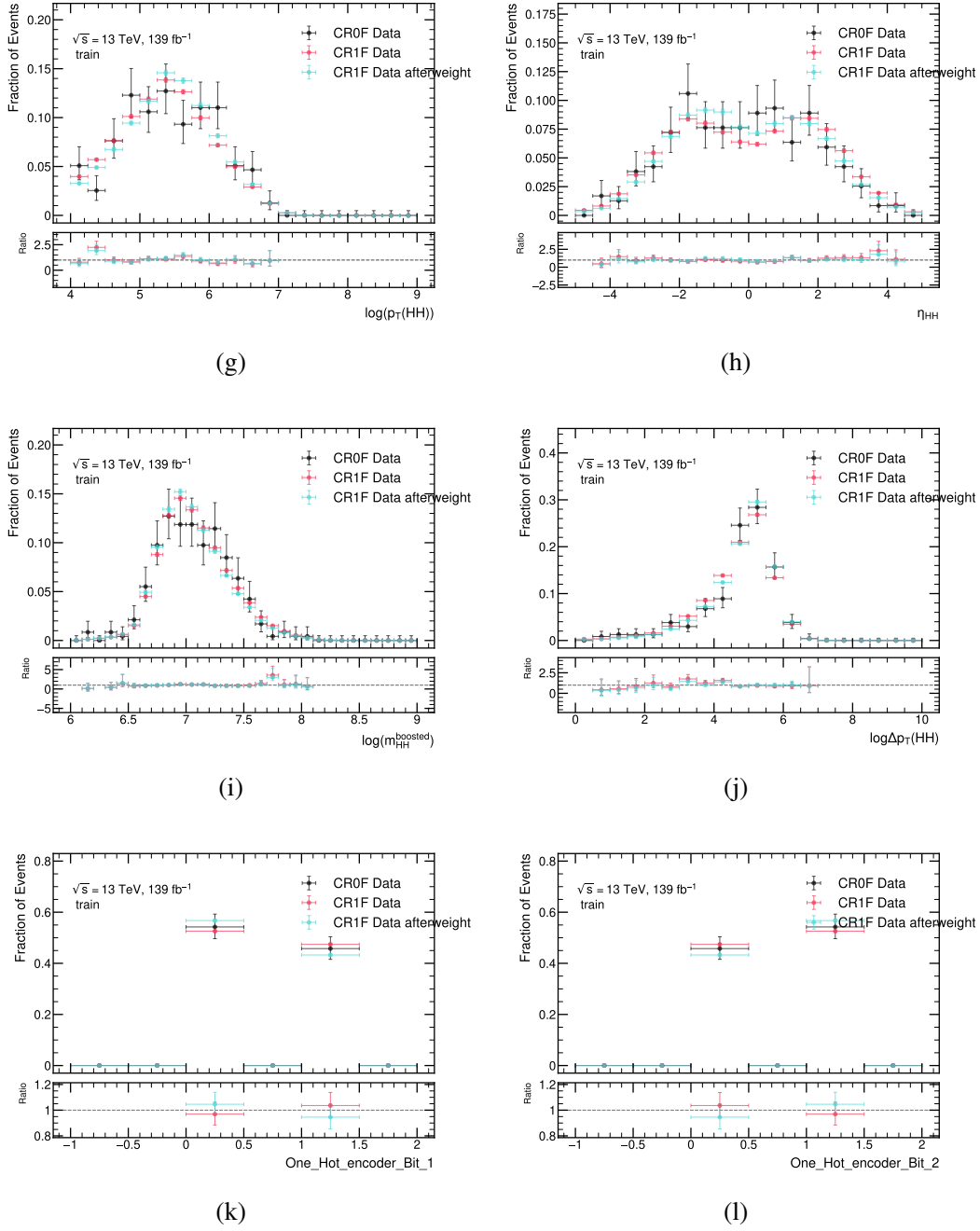


Figure 5–9 Comparison of the 1F (source) before and after kinematic reweighting and the 0F (target) kinematic variable distributions for events in the CR. The error bars indicate the statistical uncertainty in the data. Note that this plot utilizes a different large- R jet ordering scheme than the p_T -based ordering used by the final analysis, which is expected to differ by a few σ .^[32]

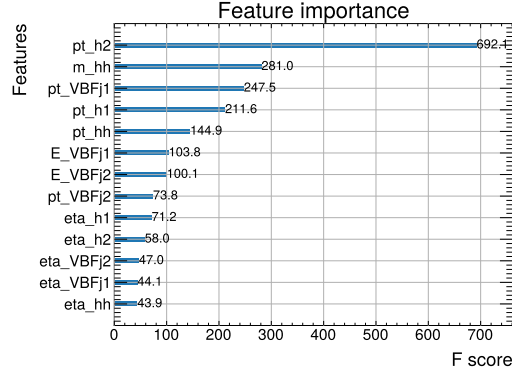


Figure 5–10 Rank of kinematic variable “importances” in the training. “Importance” is defined by the average gain across all splits where a variable is used.^[32]

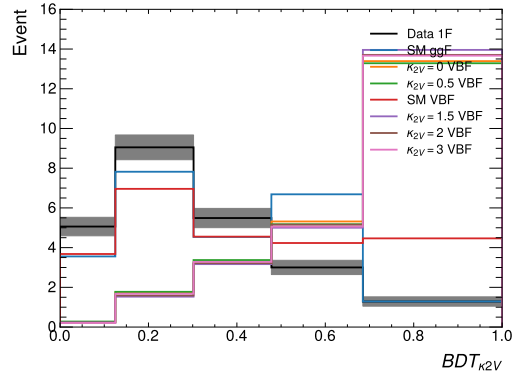


Figure 5–11 BDT response distributions among VBF MC with κ_{2V} variations, SM ggF MC, and data-driven background for all test samples. To facilitate direct comparison, all distributions are normalized to the number of events in the data-driven background. This normalization ensures that the relative differences in shape between the various MC predictions and the data-driven background are clearly visible, providing insight into the discrimination power of the BDT across different signal and background scenarios.^[32]

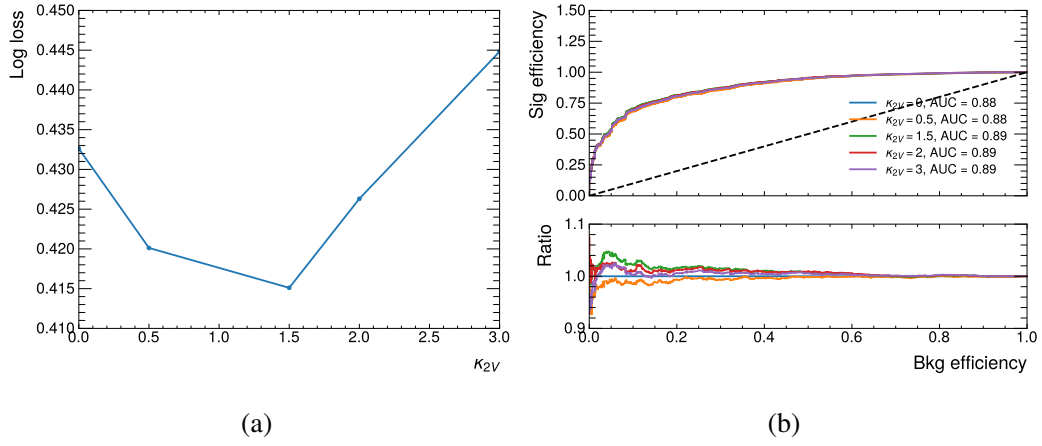


Figure 5–12 (a) Log loss values calculated from BSM κ_{2V} VBF signal and total background components. (b) ROC curves and AUC values calculated from BSM κ_{2V} VBF signal and total background components. The bottom pad shows the ratio of ROC values of signals over that of $\kappa_{2V} = 0$ signal.^[32]

5.5.2 Resonant optimization

A parameterized version of the XGBoost classifier, denoted as pBDT, is utilized for optimizing the resonant VBF signal. Drawing inspiration from parameterized neural networks^[124] and previous implementations in ATLAS analyses^[125], this approach integrates resonant signal samples of varying hypothesized truth masses for the heavy Higgs boson into a single signal category. Each event within the signal is tagged with a parameteric variable m_X , representing the truth mass of the hypothesized signal. Background events, lacking a true mass, are assigned a random m_X value sampled from the signal distributions. The pBDT is trained on an equal number of events from each signal hypothesis, with background events scaled to match the combined size of the signal datasets, leveraging the SR 1F data-driven background estimation method.

The architecture of pBDT incorporates m_X alongside kinematic variables $\vec{x}$, enabling the model to bifurcate its decision trees based on the truth mass. Consequently, the pBDT model functions parametrically with respect to m_X . During application, this model discriminates between background and signal for any specific truth mass by aligning the m_X values of all events to that mass. A conceptual diagram of this approach is presented in Figure 5–13.

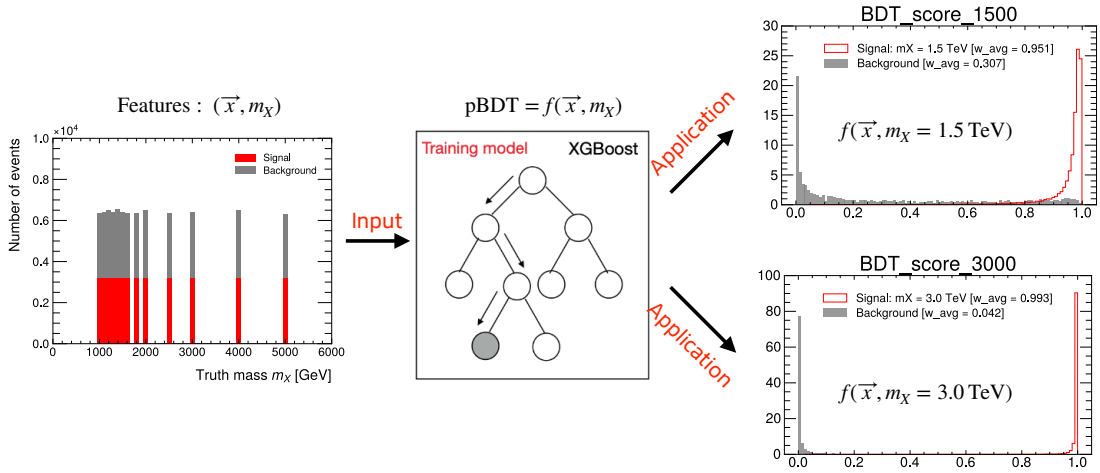


Figure 5–13 Procedure for the pBDT training and application.^[32]

The reconstructed kinematic variables used as input features together with the truth mass

$H1, H2$ (large- R jet)	p_T, η
HH	p_T, η, m
VBF jet 1, jet 2	p_T, η, E

Table 5–2 Kinematic variables used for the training of the pBDT. They are used as input features together with the truth mass.

for the pBDT training are shown in Table 5–2.

In order to have enough statistics for the pBDT training, we decided to loose the pre-selections for the events. Specifically, the WP requirement for the Xbb tagger is changed to 70%. Moreover, we removed the cuts applied on $\Delta\eta(j, j)$ and m_{jj} of VBF jets. A balance of training data is ensured by requiring same amount of background events for each mass point. After training and validating the model, the Xbb tagger WP is switched back to 60% together with the cuts on VBF jets.

A comprehensive grid search was conducted to refine the parameterization of the pBDT training further. The hyperparameters varied during this search included *Number of Trees*, *Max Depth*, and *Learning Rate*. For each hyperparameter combination, the AUC (Area Under the ROC Curve) for the testing set was computed alongside the absolute discrepancy between the training and testing AUCs, utilizing an 80% – 20% train-test split for each sample. The primary objective was to identify parameter settings that minimize the difference between the training and testing AUCs while maintaining a high testing AUC, indicating a well-generalized model. The grid search evaluated the following values:

- Number of Trees: 100, 200, 300, 400, 500, 600, 800;
- Max Depth: 4, 6;
- Learning Rate: 0.01, 0.03, 0.05;

resulting in a total of 42 distinct combinations.

For all tested models, the objective function for the pBDT was set to `binary:logistic`, which is commonly employed in binary classification tasks. This function outputs a probability between 0 and 1, where values closer to 1 indicate a higher likelihood that an event is of the signal type.

The efficacy of various hyperparameter configurations on the pBDT performance is depicted in Figure 5–14. This illustration shows that multiple parameter sets achieve a desirable

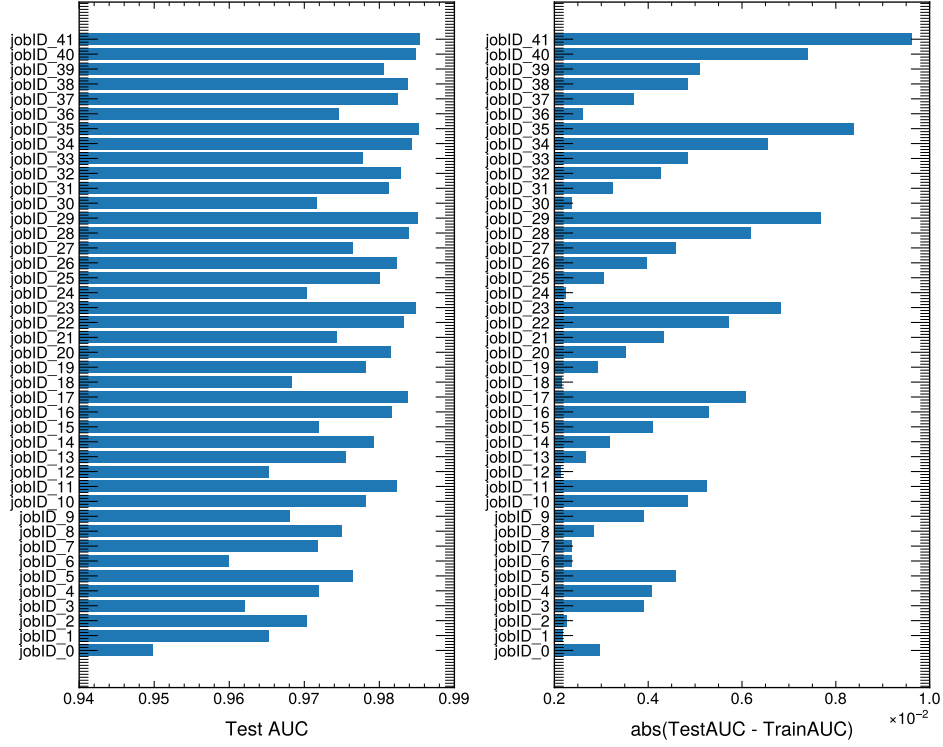


Figure 5–14 Left plot: test AUC for several combinations of hyperparameters, indexed by job IDs. Right plot: Absolute value of the difference between test AUC and train AUC for each pBDT setup.

equilibrium between high test AUC and minimal variance between the training and testing AUCs. The optimal configuration for the final model setup was determined to be $[600, 4, 0.03]$, corresponding to job ID number 31 in Figure 5–14.

The responses of the pBDT on both training and testing datasets were analyzed to determine the presence of overfitting using the final model setup. To quantify the similarity between the distributions of the pBDT scores, the p-value from the Kolmogorov-Smirnov test was utilized¹. According to this test, the null hypothesis that two distributions are identical should be rejected if the p-value is less than 0.05. The comparative results are illustrated in Figure 5–15, where no p-value fell below the 0.05 threshold. This indicates that there is no significant overfitting in the pBDT model.

Figure 5–16 presents the ROC curves for all considered mass hypotheses in this analysis. It is apparent that the discrimination performance enhances as the signal mass increases. This improvement is attributed to the altered kinematic variable distributions at higher mass

¹ https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.ks_2samp.html

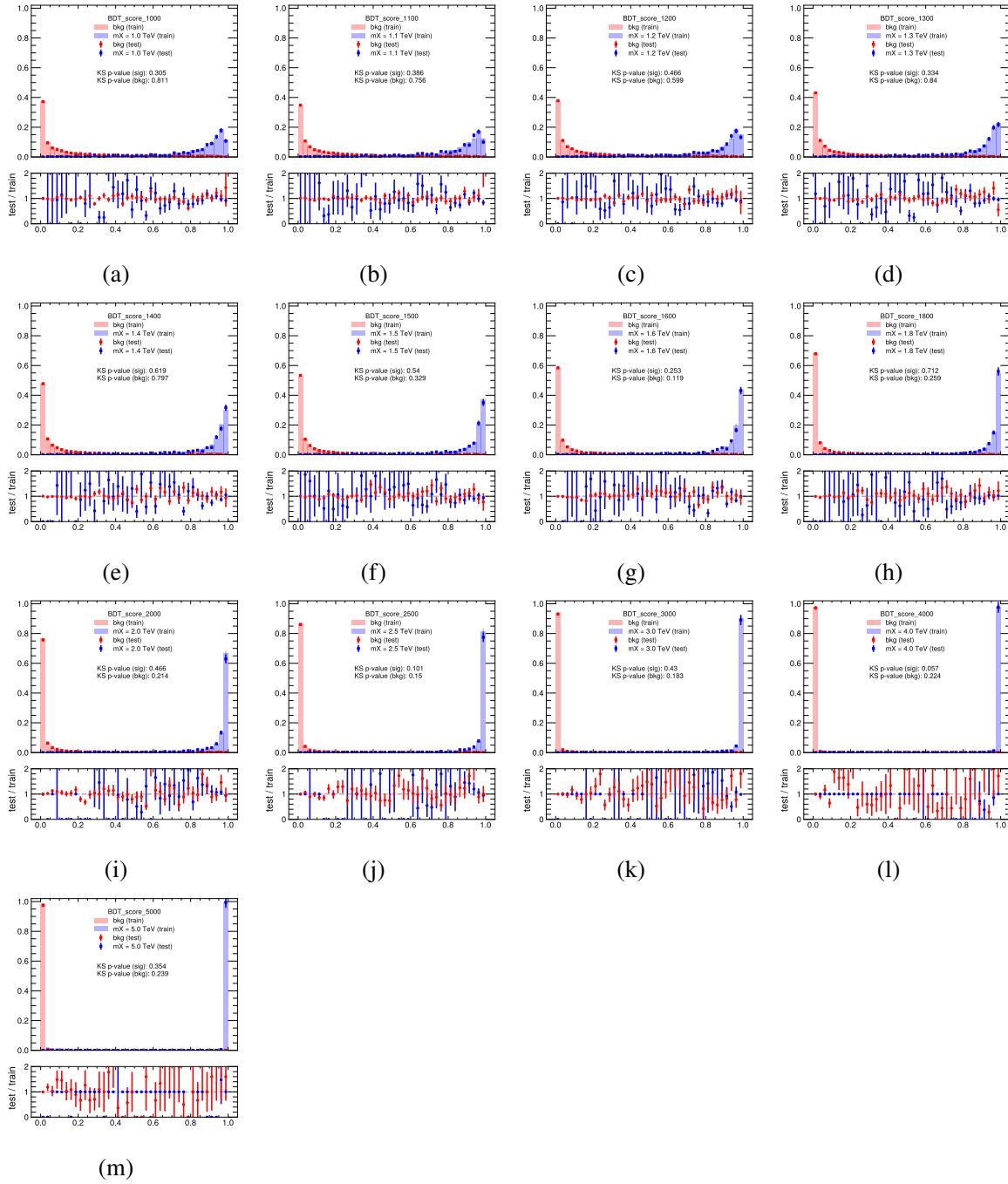


Figure 5–15 Comparison of the pBDT response between training and testing samples in the assumption of different mass hypotheses. Only the precuts have been applied to these datasets. Note that these plots utilize a different large- R jet ordering scheme than the p_T -based ordering used by the final analysis, which is expected to differ by a few %.^[32]

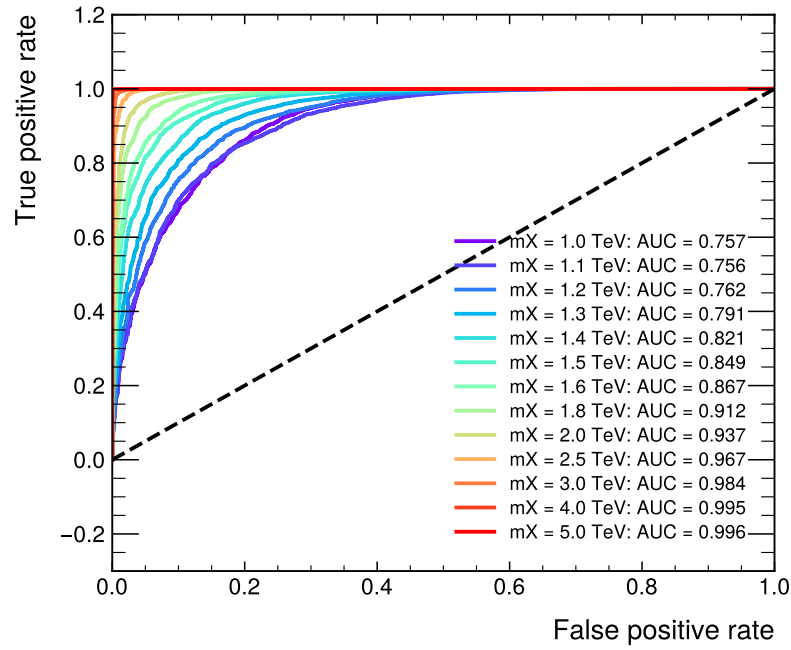


Figure 5–16 ROC curves after training with all cuts being applied in the full datasets.^[32]

points. Notably, the transverse momentum of the Higgs boson becomes more pronounced in higher mass signal samples.

Figure 5–17 displays the pBDT distributions for each mass hypothesis, with the boosted baseline signal region (SR) cuts applied. The cross-section for each signal sample is normalized to match the total background cross-section. The binning for each mass hypothesis has been tailored to optimize statistical analysis. The error bars incorporate both background normalization and shape systematic uncertainties.

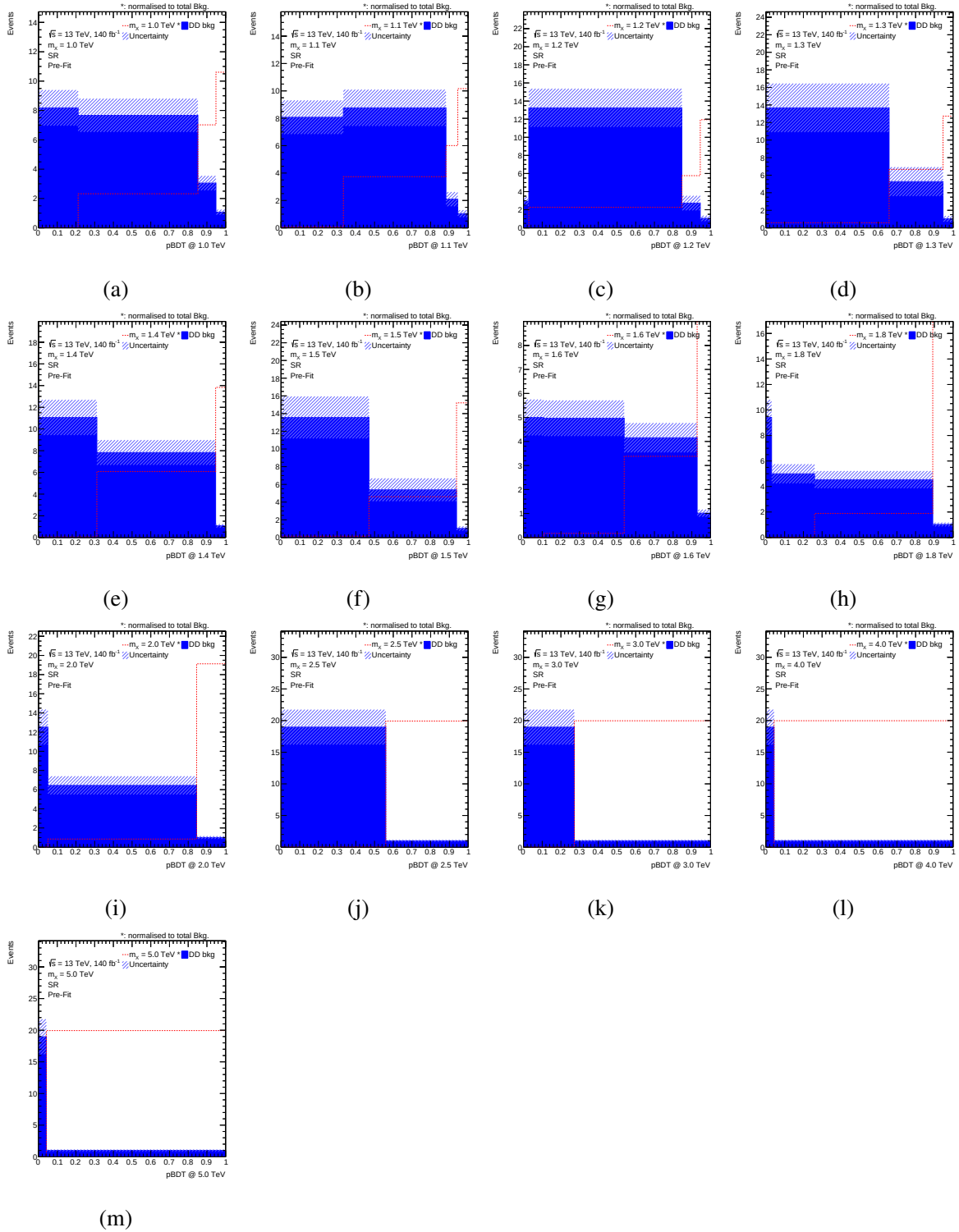


Figure 5–17 The pBDT distributions for each signal sample, following the application of the boosted baseline SR selection, are depicted in the histograms. These background histograms account for normalization and shape systematic uncertainties. The signal samples have been normalized to the total background cross-section. It is important to note that these plots employ a different *large* – *R* jet ordering scheme from the p_T -based ordering used in the final analysis, with expected differences of a few percent.^[32]

5.6 Systematic Uncertainties

In this section, we will be discussing uncertainties which have influences over this analysis. Those could be divided into uncertainties affecting MC samples and also uncertainties affecting the data-driven background.

5.6.1 Luminosity uncertainty

The uncertainty associated with the combined integrated luminosity for the years 2015 to 2018 is 0.83%, derived from primary luminosity measurements made using the LUCID-2 detector as referenced in^[126]. This uncertainty impacts the normalization of the signal prediction, though its effect on the analysis is minimal.

5.6.2 Large-R jet resolution and scale uncertainties

The calibration and uncertainty quantification of large-R jets involve multiple methods designed to correct and verify the jet energy scale, jet energy resolution and jet mass scale from ATLAS data and simulation discrepancies.

The jet energy scale calibration utilizes the balance of large-R jets with well-defined objects such as photons, $Z \rightarrow ee$, $Z \rightarrow \mu\mu$ or calibrated jets to correct the discrepancies in the central p_T region. Additionally, "dijet eta-intercalibration" helps to even out responses across the detector, aiding in the extension of the η range. The uncertainties from JES arises primarily from detector effects, selection criteria, available statistics and modeling inaccuracies. Other factors such as jet flavor composition and topology difference also contribute to the uncertainty which could not be corrected by in-situ calibrations.

The jet energy resolution employs the di-jet balance asymmetry, which is adequate for covering the kinematically supported regime for large-R jets. It incorporates nominal data/MC differences to the overall uncertainties. It covers the uncertainties from detector effects, selection criteria, statistics and modelings. Those uncertainties are also propagated through JES calculations with the entire set represented in smearing adjustments in both Monte Carlo and pseudo-data. Notably, the treatment addresses substantial anti-correlations observed between jets in different detector regions.

The jet mass scale is derived from Forward Folding method applied to W boson and top quark mass peaks in semi-leptonic $t\bar{t}$ events. The R_{trk} method, comparing calorimeter-only to

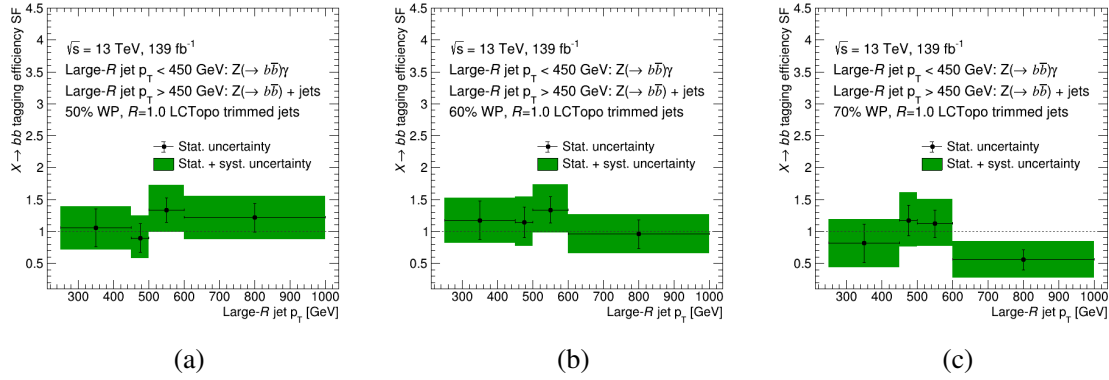


Figure 5–18 Signal efficiency scale factors for $X \rightarrow bb$ tagger at 50%, 60% and 70% efficiency working points. The analysis uses the 60% WP only, others are shown for illustration.^[32]

track-only quantities in data versus simulation, supports this calibration. The uncertainty of this term stems from the Forward Folding and R_{trk} techniques, interpolation between mass bins and variations between QCD and hadronic-decay jet mass responses.

Moreover, a flat 20% jet mass resolution uncertainty is maintained as a conservative measure for the fat jet mass. Each of these calibration endeavors is supported by respective configuration files and schemes specifying nuisance parameters to account for systematic variations.

5.6.3 Xbb tagging uncertainties

The $X \rightarrow bb$ tagger algorithm is trained with MC samples and there could be difference between MC and data distributions. A calibration therefore has been designed and utilized here. The signal efficiency is calibrated using $Z(\rightarrow \gamma) + \text{jets}$ and $Z(\rightarrow \gamma) + \gamma$ events. And one data-to-MC efficiency scale factor as a function of the large- R jet transverse momentum is extracted. The scale factors are shown in Figure 5–18b for the 60% efficiency working point. The uncertainties includes statistical and systematics uncertainties on these factors. The other WPs are also shown in the same picture separately for 50% and 70% WPs. Performance of the calibration is stable generally.

The dominance of the $X \rightarrow bb$ uncertainty affects both resonant and non-resonant signal events due to error magnitudes of approximately 30% across the entire p_T spectrum. The requirement for tagging and selecting two large- R jets amplifies the impact, modifying BDT responses by +70% and –50%. Figure 5–19 illustrates this uncertainty for $\kappa_{2V} = 0$ signal

events. Since the $Z \rightarrow bb$ calibration is separately performed within distinct p_T bins, and considering that the primary uncertainty sources (spurious signal and statistical uncertainty) are uncorrelated, it is feasible to treat the impacts in four p_T bins as independent, aiding in mitigating the overall effect on the analysis.

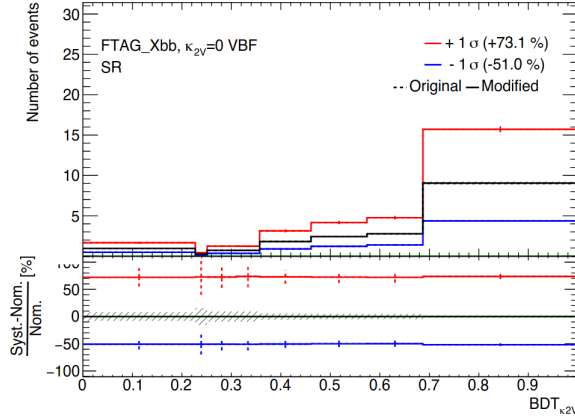


Figure 5-19 Up/down $X \rightarrow bb$ uncertainties in the $\kappa_{2V} = 0$ VBF events. Note that this figure utilizes an older large- R jet ordering scheme, which is expected to differ from the analysis’ p_T -based ordering by a few %. Additionally, an older BDT score binning scheme is used compared with the final analysis binning choice.^[32]

5.6.4 Small- R jet resolution and scale uncertainties

The JETUNCERTAINTIES tool calculates the Jet Energy Scale (JES) and Jet Energy Resolution (JER) uncertainties, referenced in^[127]. JES uncertainties are assessed through several approaches: dijet η -intercalibration, +jet, +jet, and multi-jet balance, with the high- p_T uncertainties determined via single-particle methods. JER uncertainties are estimated using the noise term, evaluated in zero bias data with random cones, and dijet asymmetry. The configuration file `JetUncertainties/CalibArea-08/rel21/Summer2019/R4_CategoryReduct` containing approximately 30 NPs for JES and 13 NPs for JER, is utilized. This configuration is recommended for analyses that intend to combine results with other searches, and thus, it has been adopted by all di-Higgs group analyses participating in the di-Higgs and related combinations. Uncertainties for VBF jets are specifically labelled as `JES_*` and `JER_*` in the analysis.

5.6.5 Theoretical uncertainties

5.6.5.1 Uncertainty on HH cross sections

The uncertainties in the HH cross-section calculation is included in the limits on the non-resonant signal strength, but excluded when evaluating the limits on cross sections. At $\sqrt{s} = 13$ TeV and $m_H = 125$ GeV, the uncertainties for different production modes are detailed in Ref.^[128]. For the gluon-gluon fusion (ggF) process, the PDF and α_S uncertainties amount to $\pm 3.0\%$, while the combined scale and top quark mass (m_{top}) uncertainties are $^{+6\%}_{-23\%}$. For vector boson fusion (VBF), the scale uncertainty is $^{+0.03\%}_{-0.04\%}$ and the PDF + α_S uncertainties are $\pm 2.1\%$. These uncertainties are applied exclusively to the non-resonant signal.

5.6.5.2 Theoretical uncertainty on efficiency and acceptance

Uncertainties from α_S and PDF are evaluated using alternative weights in the nominal samples, as described in Ref.^[129]. The α_S uncertainty is calculated using the same PDF set with different α_S values. Half the difference between the NNPDF30_nlo_as_0119 and NNPDF30_nlo_as_0117 variations is taken as the uncertainty and symmetrized about the nominal. The PDF uncertainty is the standard deviation of the 100 variations of the NNPDF30_nlo_as_0118. These uncertainties are combined quadratically and applied similarly to both resonant and non-resonant analyses. The PDF + α_S uncertainty is less than 1% for $\kappa_{VV} = 0$ VBF and resonant samples, and thus is neglected.

Renormalization and factorization scale uncertainties due to missing higher-order corrections are evaluated using the 7-point scale variations, combined by taking an envelope of all variations, as per Ref.^[129].

5.6.5.3 $H \rightarrow b\bar{b}$ BR uncertainty

They include uncertainties in the $H \rightarrow b\bar{b}$ branching ratio (BR)^[130] (with $m_H = 125$ GeV). The total uncertainty of the $H \rightarrow b\bar{b}$ BR is derived by linearly adding the total parametric uncertainty (PU) and the total theoretical uncertainty (THU)^[131], considering the Higgs decay to two b -quarks. Specifically, $\Delta BR = 2 \times (\Delta BR(THU) + \sqrt{\Delta BR(PU_{m_q})^2 + \Delta BR(PU_{\alpha_S})^2}) = ^{+3.4\%}_{-3.5\%}$. This uncertainty is applied to both non-resonant and resonant signals.

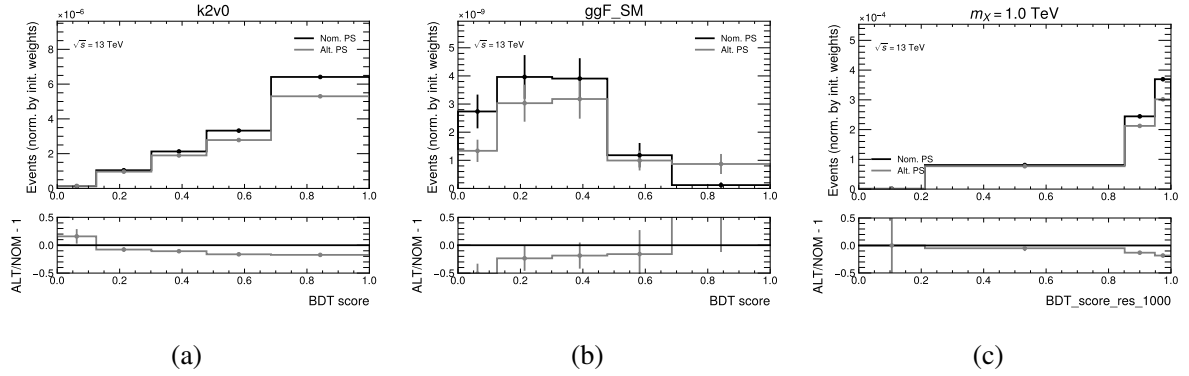


Figure 5–20 (p)BDT distributions using the nominal and alternative parton shower samples for $\kappa_{2V} = 0$, ggF SM and $m_X = 1.0$ TeV. All histograms are normalised to the integrated luminosity times the state-of-art cross sections. For the resonant samples, the cross section is set to be 1 fb.^[32]

5.6.5.4 Parton Shower

Parton shower uncertainties are evaluated by comparing samples generated with both PYTHIA 8 and HERWIG 7. This uncertainty is added to both non-resonant and resonant signals. For non-resonant studies, the results of $\kappa_{2V} = 0$ samples are used for all VBF samples, while for ggF SM, the estimation is done separately. In the resonant analysis, samples using the alternative parton shower are available for a few mass points, necessitating interpolation to obtain the corresponding systematic uncertainty for each mass point. Figure 5–20 presents the (p)BDT distributions for $\kappa_{2V} = 0$, ggF SM, and $m_X = 1.0$ TeV (2HDM), for both nominal and alternative parton showers. Each sample is normalized to the integrated luminosity times the state-of-the-art cross section. For the 2HDM samples, the cross section is set to 1 fb.

5.6.6 Reweighting uncertainties

The reweighting uncertainty on ggF (from SM to other κ_λ variations) is neglected and has been validated in previous analyses^[109]. The non-closure of reweighted VBF distributions (from SM to other κ_λ , κ_{VV} , and κ_V variations) are compared to the available simulated samples that are not used as the basis. The difference between the “combined” (reweighted) and “validation” (simulated) distributions agrees with statistical uncertainties. Assigning a reweighting uncertainty may double count the statistical uncertainty. Therefore, the reweighting uncertainty is neglected in VBF.

5.6.7 Background uncertainties

5.6.7.1 Normalization uncertainty

The nominal normalization factor of the background is derived in the CR: $\frac{N(\text{CR},0F)}{N(\text{CR},1F)} = 0.0081 \pm 0.0008$. The alternative normalization factor is estimated in the VR: $\frac{N(\text{VR},0F)}{N(\text{VR},1F)} = 0.0091 \pm 0.0012$. The normalization uncertainty is extracted by comparing these two factors and is estimated to be 12.3%.

For the resonant analysis, the resolved SR veto is not applied, slightly changing the normalization factor. The normalization uncertainty for the resonant analysis is estimated to be 14.4%.

5.6.7.2 Shape uncertainties

The nominal shape of the background is derived from the SR, 1F. To estimate the possible deviation of the discriminating variable distributions between SR, 1F and SR, 0F, the uncertainty can be extracted in the VR. This assumes that in different m_H phase spaces (SR, VR), the transition from 1F to 0F is the same.

For the non-resonant study, the BDT response is used as the discriminating variable. The distribution of BDT score in SR,1F and VR,1F are compared and similarity is found therefore the assumption is more reliable. And the BDT distribution of the VR,1F and VR,0F is also compared to extract the uncertainty on the shape. The ratio pad from Figure 5–21 both on the left and right shows the uncertainties. But obviously there is huge statistical fluctuations in these uncertainties. In order to mitigate the effects of limited statistics, a smoothing need to be done, otherwise the shape uncertainty NP would be over-constrained.

One 2-bin smoothing method is applied here to stabilize the distributions of BDT scores and to reduce the statistical error in each bin. In Figure fig:5:6:BDT2BinUnc, VR data events in the first 3 bins and last 2 bins are merged respectively. The first bin is referred to as the background-like bin and the second bin is referred to as one signal-like bin. Shape uncertainty could be therefore extracted from the ratio panels and is propagated to the SR. The uncertainty is symmetrized in the statistical model as shown in Figure fig:5:6:BDT2BinUnc. The black curve is the nominal background BDT distribution in SR, slashed band representing the statistical errors.

As for the resonant analysis, the pBDT response is used as the discriminating variable.

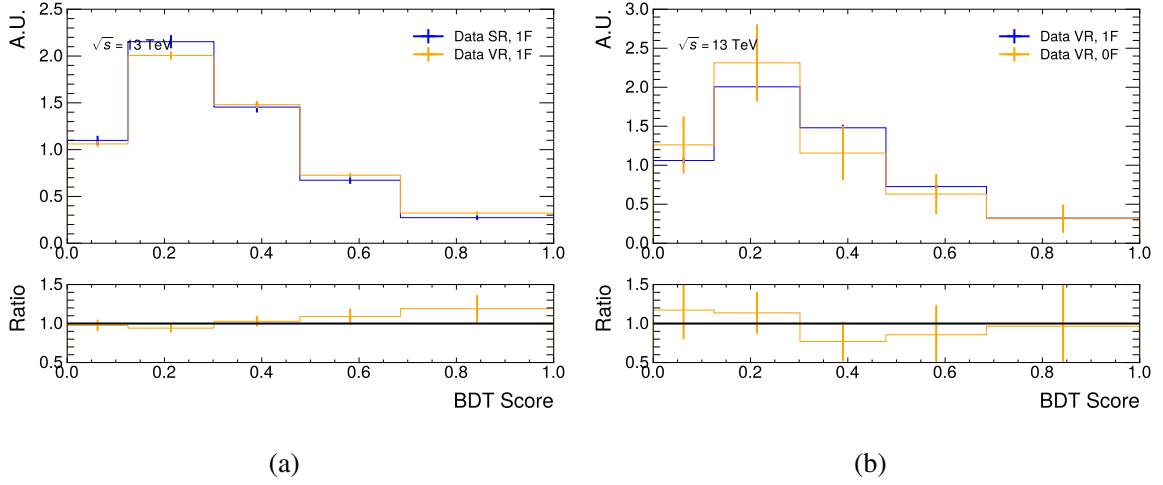


Figure 5-21 (a) Shape comparison of BDT response in SR, 1F and VR, 1F to confirm similar distributions so that the assumption of the same transition from 1F to 0F between SR and VR is more reliable. The black curve with gray band (statistical errors) is the BDT distribution in the SR, 1F and the blue curve is the distribution in the VR, 1F. (b) Shape comparison of BDT response in VR, 1F and VR, 0F to extract the shape uncertainty. The blue curve is the distribution in the VR, 1F and the orange curve is the response in VR, 0F.^[32]

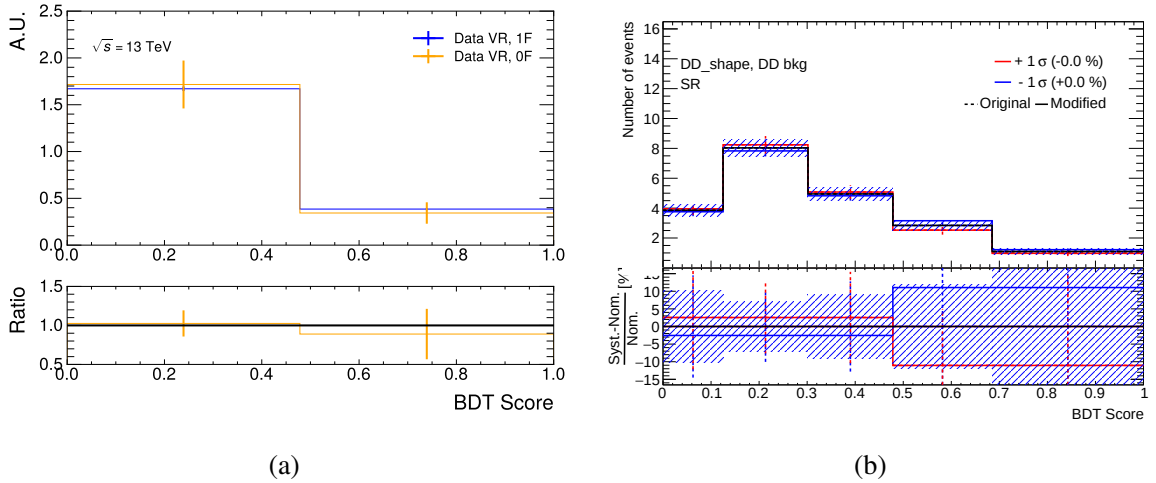


Figure 5-22 (a) VR data events in the first 3 bins and last 2 bins of the BDT are merged respectively. The blue curve is the distribution in the VR, 1F and the orange curve is the response in VR, 0F. The shape uncertainty is estimated from the ratio pad. (b) Background nominal and shape variation distributions in the SR, 1F. The black curve is the nominal BDT distribution, with slashed band representing the statistical errors. Red and blue curves show the upper and lower variations of the shape uncertainty. By construction, the relative uncertainties in the first 3 bins and the last 2 bins are the same respectively.^[32]

We have compared the pBDT distribution in SR,1F and VR,1F for every signal mass points. The similarity in the distributions are found to be good in all cases and the assumption that we can use this method to extract the shape uncertainty is reasonable. And the comparison between shapes of pBDT in VR,1F and VR,0F is also done to extract the shape uncertainty. And the result in Figure 5–23 shows that most of the differences are statistical fluctuations. Therefore, we need to use the similar 2 bin smoothing techniques to mitigate the statistical errors as we did in the non-resonant analysis. However, the binnings for every mass points are different and one needs to decide the cut point where to split these signal like bin and background like bin. In this analysis, we decided to define the cut point when the integral from left to right reaches 50% of the total events. And the uncertainty is propagated to the SR and symmetrized in the statistical model. Figure 5–24 is showing the uncertainties for all mass points.

5.6.8 Summary of systematics

Table 5–3 summarizes the systematics used in the analysis.

Table 5–3 Systematics considered in the analysis and the effects on the fitting variable (normalization or shape effects).

Sytematics	Type	Signal	Background
General			
LUMI	Norm	✓	
PRW	Norm & Shape	✓	
Boosted jets			
JES	Norm & Shape	✓	
JER	Norm & Shape	✓	
JMS	Norm & Shape	✓	
JMR	Norm & Shape	✓	
Resolved jets			
JES	Norm & Shape	✓	
JER	Norm & Shape	✓	
b-tagging			
Xbb	Norm & Shape	✓	
Theory			
Scale	Norm & Shape	✓	
PDF	Norm & Shape	✓	
BR_bb	Norm	✓	
PS	Norm & Shape	✓	
Bkg	Norm & Shape		✓
MC (data-driven) statistical errors		✓	✓

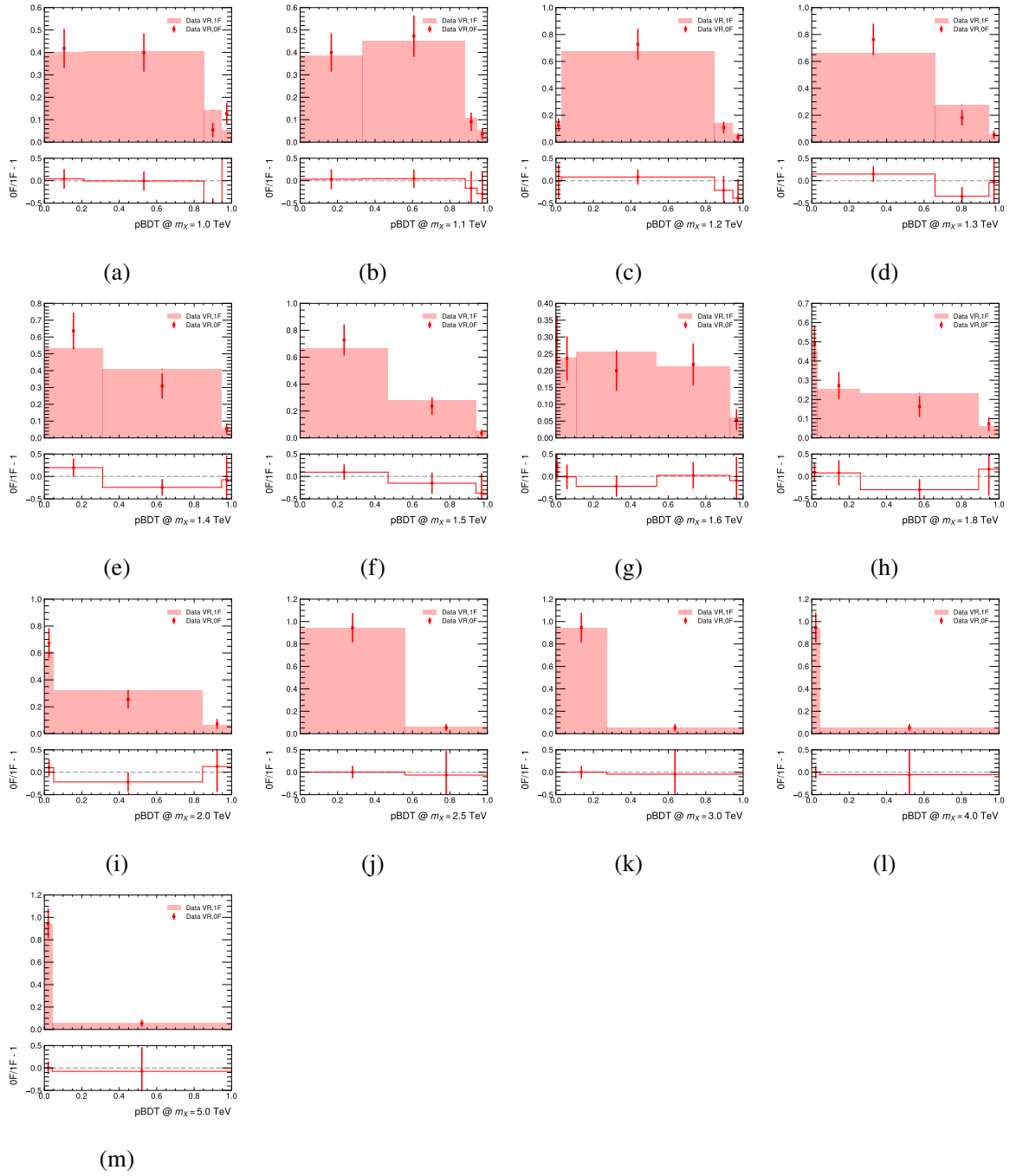


Figure 5-23 Shape comparison of pBDT response in VR, 1F and VR, 0F for the different mass hypotheses.^[32]

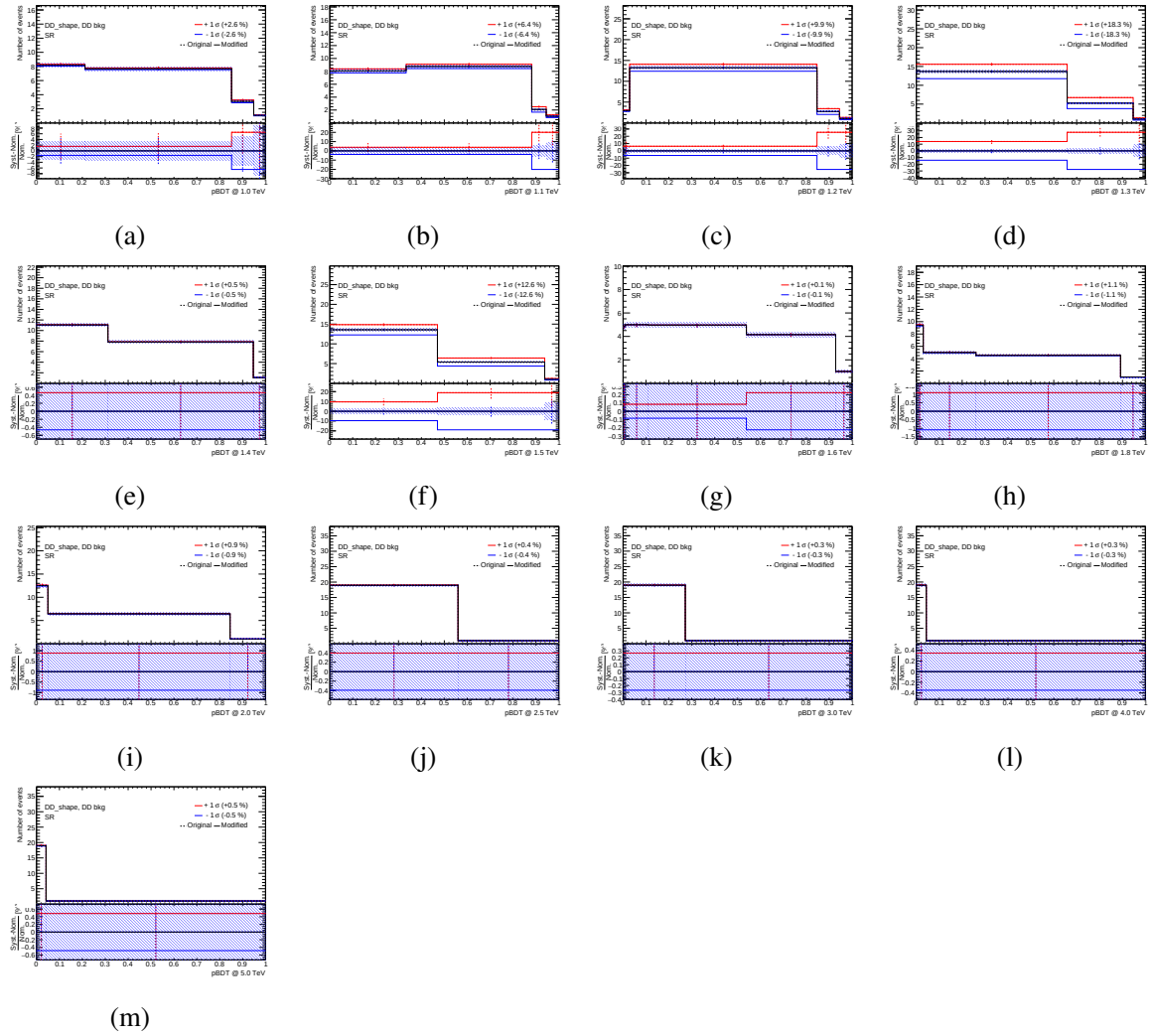


Figure 5-24 Background nominal and shape variation distributions in the SR, 1F. The black curve is the nominal pBDT distribution, with band representing the statistical error.^[32]

5.7 Results

In the nominal study, the signal extraction fit is performed using the BDT (pBDT in the resonant case) response as an observable, and the maximum binned likelihood fit is performed. Another strong candidate due to its relatively good separation power among other kinematic variables is m_{HH} , which was used in the previous analysis.

The frequentist exclusion limits are based on a hypothesis testing procedure using a profile likelihood test statistic and are performed using the standard asymptotic formulas^[132]. Histograms of the discriminant with their systematic variations are used in the profile likelihood fit. The likelihood describing the agreement between data and prediction can be summarized as follows:

$$\mathcal{L}(\mu, \theta) = \prod_{c \in \text{categories}} \prod_{b \in \text{bins}} \text{Pois}(n_{c,b} | \lambda_{c,b}(\hat{\mu}, \hat{\theta})) \cdot \prod_{s \in \text{systematics}} \text{Gaus}(\hat{\theta}_s | \theta_s).$$

Here, μ is the parameter of interest (POI), also known as the signal strength, where $\mu = 0$ corresponds to the background-only model and $\mu = 1$ corresponds to the background and predicted signal. θ_s are the nuisance parameters (NPs) that parametrize the known systematic effects in the analysis, and θ is the ensemble of all NPs. Interpolation and extrapolation of θ_s are necessary for the likelihood evaluation; a 6th-order polynomial interpolation and a linear extrapolation are used as defaulted in HISTFACTORY^[133]. The θ also alter the Poisson expectation $\lambda_{r,b}(\hat{\mu}, \hat{\theta})$ and need to be determined, but are of minor interest.

Following the Neyman-Pearson lemma, a profile likelihood ratio test statistic is used in hypothesis testing and is constructed as follows:

$$\tilde{\lambda}(\mu) = \begin{cases} \frac{\mathcal{L}(\mu, \hat{\theta}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\theta})} & \hat{\mu} \geq 0, \\ \frac{\mathcal{L}(\mu, \hat{\theta}(\mu))}{\mathcal{L}(0, \hat{\theta}(0))} & \hat{\mu} < 0. \end{cases}$$

Note, this has no explicit dependence on the NPs. $\hat{\theta}(\mu)$ denotes the maximum likelihood estimates of the NPs for a given value μ , while $\hat{\mu}$ and $\hat{\theta}$ are the maximum likelihood estimates (best fit values). The tilde ($\sim$) on λ is placed to emphasize the boundary at $\mu = 0$ for the differing definition for the $\hat{\mu} < 0$ case. The test statistic, $\tilde{q}_\mu$, considered for limit setting is defined as follows:

$$\tilde{q}_\mu = \begin{cases} -2 \ln \tilde{\lambda}(\mu) & \hat{\mu} \leq \mu \\ 0 & \hat{\mu} > \mu \end{cases} = \begin{cases} -2 \ln \frac{\mathcal{L}(\mu, \hat{\theta}(\mu))}{\mathcal{L}(0, \hat{\theta}(0))} & \hat{\mu} \leq 0, \\ -2 \ln \frac{\mathcal{L}(\mu, \hat{\theta}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\theta})} & 0 \leq \hat{\mu} \leq \mu, \\ 0 & \hat{\mu} > \mu. \end{cases}$$

The distributions of the test statistics, $f(\tilde{q}_\mu)$, for a given μ hypothesis are given by the asymptotic formulas^[132,134]. Then, the p -value can be calculated as follows:

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

$$p_0 = 1 - \int_{\tilde{q}_{\mu, \text{obs}}}^{\infty} f(\tilde{q}_\mu | \mu = 0, \theta(\mu = 0)) d\tilde{q}_\mu.$$

The 95 % confidence level CL_s exclusion limit, μ_{up} , is obtained by solving:

$$p'_\mu = \frac{p_\mu}{1 - p_0} \leq 5 \%.$$

The one and two standard deviation error bands on the limits are estimated using the following formula with some fine-tuning (the known `betterBand` option).

$$\mu_{\text{up}+N} = \mu_{\text{up}} \left(\Phi^{-1}(1 - 0.05\Phi(\pm N)) \pm N \right),$$

Here, Φ^{-1} is the quantile function (inverse of the cumulative distribution) of a standard Gaussian distribution.

To account for uncertainties coming from limited statistics, a Poisson constraint is applied in each bin. A pruning threshold of 1 % is set on MC statistical and systematic errors to stabilize the fitting. The `TRExFitter`¹ is used to build up the statistical model.

5.7.1 Binning optimization

Binning for each of these distributions are optimized using a "Transformation D" method of `TRExFitter`. The binning has been constructed downwards starting from score equals to 1.0 and going to 0.0. It has been imposed that each bin should have at least one full data-driven background event count. And the first bin (bkg-like) would be merged to the second one if it has a width lower than 0.01. Finally, we have decided the binning of the non-resonant study to be [0.0, 0.125, 0.302, 0.478, 0.685, 1.0]. And the binnings for the resonant study is presented in table 5–4.

¹ <https://gitlab.cern.ch/TRExStats/TRExFitter>

Mass points [TeV]	z_s	z_b	Exact binning
1.0	2	2	[0.0, 0.211667, 0.851667, 0.948333, 1.0]
1.1	3	1	[0.0, 0.333333, 0.881667, 0.945, 1.0]
1.2	3	1	[0.0, 0.028333, 0.846667, 0.945, 1.0]
1.3	3	0	[0.0, 0.658333, 0.946667, 1.0]
1.4	2	1	[0.0, 0.311667, 0.946667, 1.0]
1.5	2	2	[0.0, 0.47, 0.938333, 1.0]
1.6	1	4	[0.0, 0.01, 0.108333, 0.538333, 0.928333, 1.0]
1.8	1	4	[0.0, 0.03, 0.26, 0.891667, 1.0]
2.0	1	3	[0.0, 0.05, 0.845, 1.0]
2.5	1	1	[0.0, 0.56, 1.0]
3.0	1	1	[0.0, 0.271667, 1.0]
4.0	1	1	[0.0, 0.043333, 1.0]
5.0	1	1	[0.0, 0.041667, 1.0]

Table 5–4 pBDT binnings per signal hypothesis obtained with the “Transformation D” algorithm from **TRExFitter**. z_s and z_b stand for the hyper-parameters that state the expected relative contributions of signal and background at each bin. Their values are chosen to be the ones that give the best significance for each case. The first bin has been merged to the second one in case it had a width lower than 0.01.

5.7.2 Unblinded non-resonant results

Figure 5–25 shows the post-fit BDT distributions of SM ggF, VBF, and data-driven background compared to the data. In this figure, ggF is fixed to the SM, and the data agrees with the total sample distribution. We estimate the upper limit of $\mu_{SM\ VBF}$ to be less than 551 (672 expected) at 95% CL. The expected error band in the 1σ (2σ) interval is [484, 1075] ([361, 1829]). The observed limit is compatible with the expected limit within 1σ , and no excess above the background is observed.

We find that $\kappa_{2V} = 1.01^{+0.24}_{-0.23}$ (1.0 ± 0.4 expected) at 68% CL. The 95% CL for κ_{2V} is estimated to be [0.52, 1.52] ([0.32, 1.71] expected). Our analysis excludes $\kappa_{2V} < 0$ with 3.4σ (2.9σ expected) significance. The observed results are better than the expected results due to a deficit of data in the most sensitive BDT bin. Figure 5–26 shows the observed and expected $t_\mu = -2 \ln \Lambda$ distributions as a function of κ_{2V} .

In Figure 5–27, we present the 95% CL upper limits of $\sigma(VBF\ HH)$ as a function of κ_{2V} . The observed results align with the expected results. By comparing to the theoretical

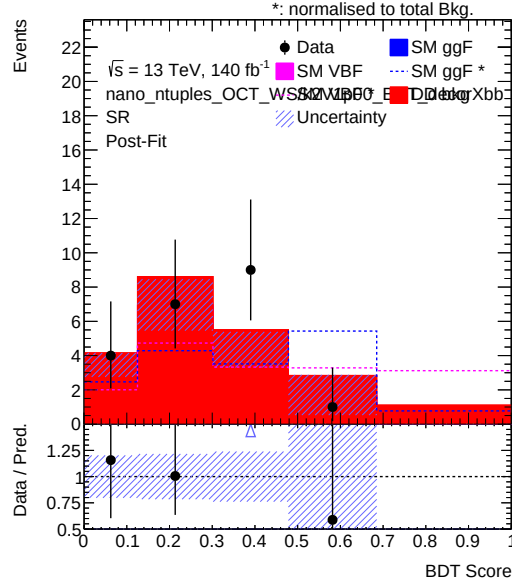


Figure 5–25 Post-fit BDT distributions of SM ggF, VBF, and data-driven background compared to the data. ggF is fixed to the SM. Black points represent the data. The red band shows the data-driven background. The blue band represents ggF, and the pink band represents VBF. The dashed blue and pink lines are ggF and VBF events normalized to the data-driven background, respectively. The slashes indicate the post-fit uncertainties. The ratio pad compares the data and the post-fit total sample distributions. The data agrees with the total sample.^[32]

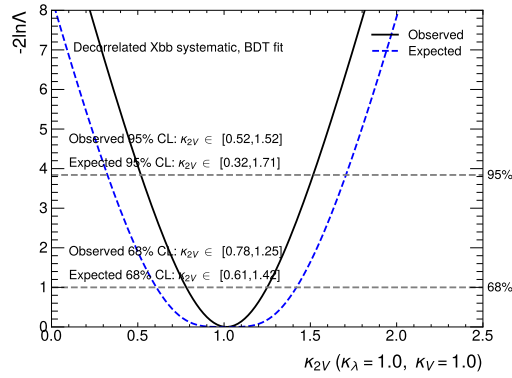


Figure 5–26 Observed and expected $t_\mu = -2 \ln \Lambda$ distributions as a function of κ_{2V} . The solid line represents the observed result, and the blue dashed line represents the expected result. The 68% and 95% CL for κ_{2V} can be extracted when $t_\mu = 1$ and 3.84, respectively.^[32]

predictions, the limit of κ_{2V} can also be extracted. In this approach, the 95% CL for κ_{2V} is [0.46, 1.57] ([0.33, 1.70] expected). This limit differs slightly from the likelihood approach, as the CL_{s+b} limit is obtained in the likelihood approach, while the CL_s limit is obtained in the cross-section approach. The hypotheses differ as well; in the likelihood approach, the SM VBF is assumed, while in the cross-section approach, no VBF signal is assumed. Despite the small SM VBF in the analysis, the VBF cross-section theory uncertainties are included in the likelihood approach but are removed in the cross-section approach.

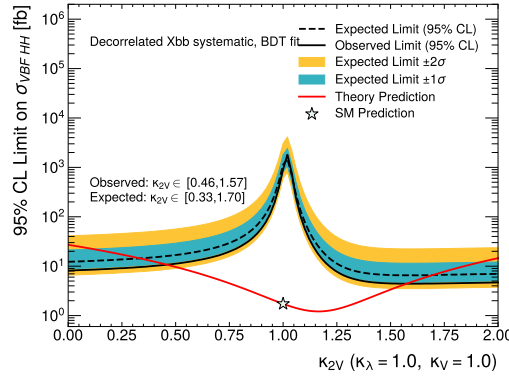


Figure 5–27 95% CL upper limits of $\sigma(\text{VBF } HH)$ as a function of κ_{2V} . The solid black line represents the observed limit, and the dashed black line represents the expected limit. The cyan and yellow bands represent the 1σ and 2σ errors of the expected limits. The red curve represents the theory VBF cross-sections as a function of κ_{2V} . The star indicates the SM VBF cross-section.

By intersection, the limits of κ_{2V} can be extracted.^[32]

5.7.3 Unblinded resonant results

For the resonant result, the signal and background are compared to the observed data and likelihood scan is done for every mass point. The result post-fit distribution is shown in Figure 5–28.

A plot containing fit results for each mass point is presented in Figure 5–29, and the corresponding numbers are conveniently displayed in Table 5–5. The total uncertainty has been split between statistical and systematic components. For all mass hypotheses, the statistical uncertainties are the dominant ones.

Upper limits for the cross-sections are set at the 95% confidence level (CL) using both the asymptotic approximation and toy methods. The corresponding plots are displayed in Figure 5–30, and detailed numerical comparisons between the two methods are provided in

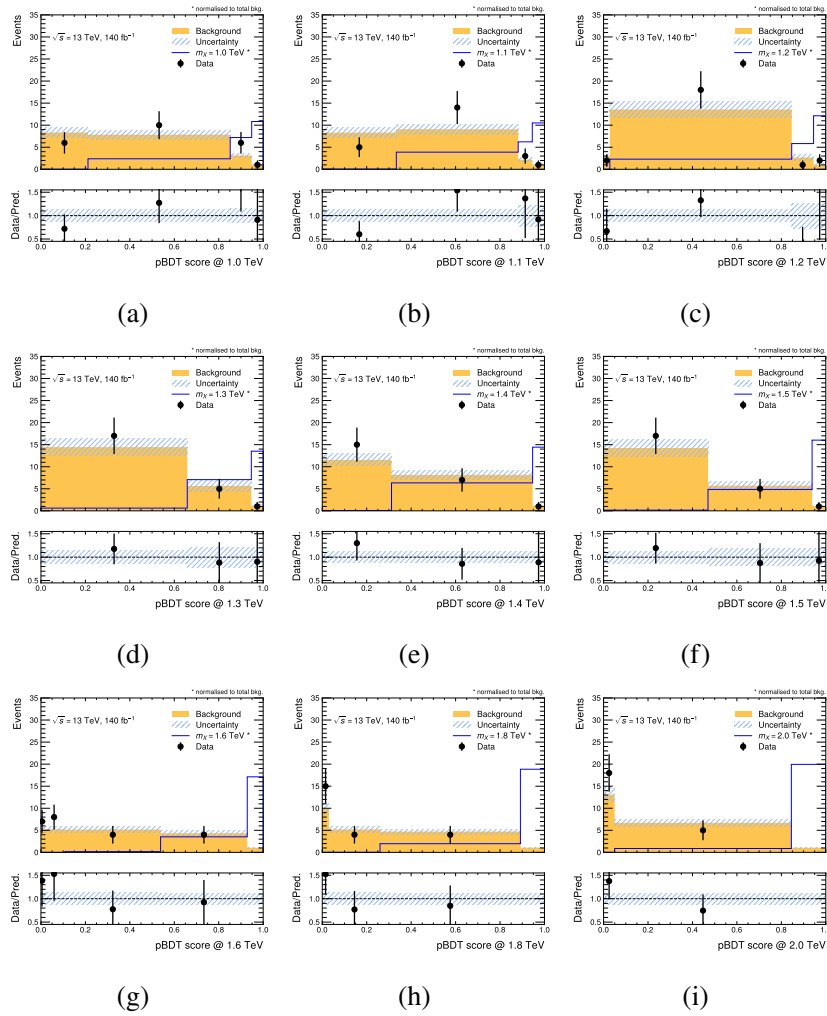


Figure 5-28 Post-fit plots. Due to the deficit of data events in the signal-like pBDT bin for high masses, the fit should be constrained to positive values of μ_{VBF} .^[32]

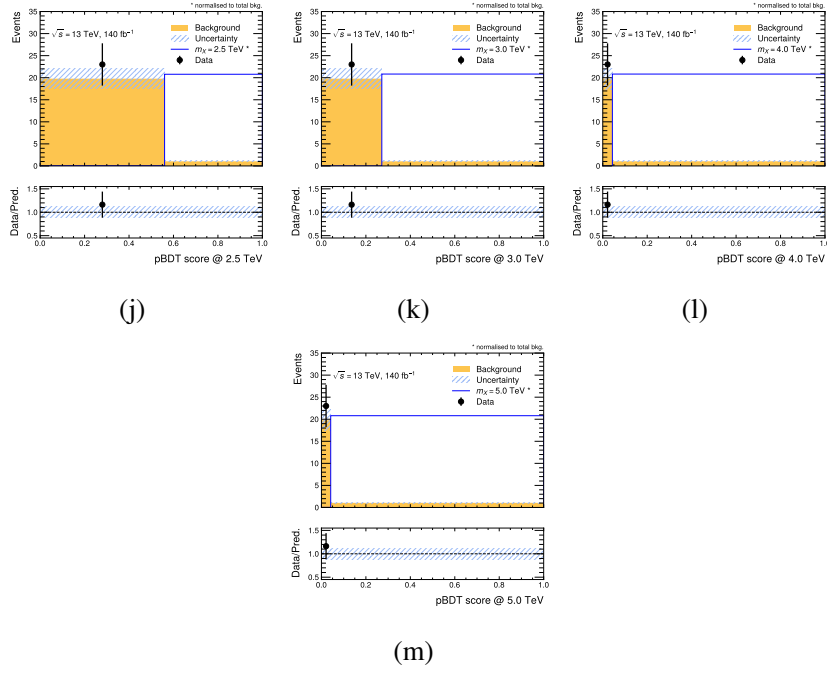


Figure 5-28 Post-fit plots. Due to the deficit of data events in the signal-like pBDT bin for high masses, the fit should be constrained to positive values of μ_{VBF} .^[32]

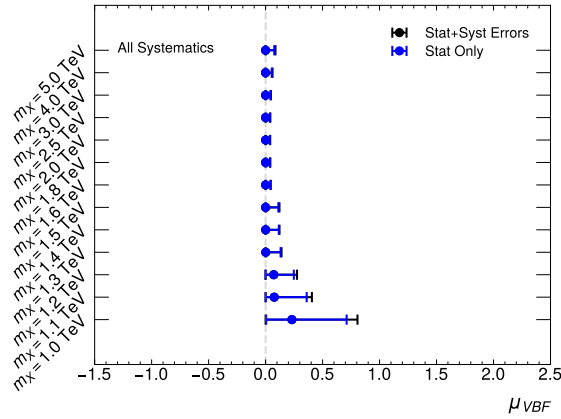


Figure 5-29 Fit result for each mass hypothesis. The error bars were split according to their statistical or systematic nature. Lower errors are bouded at zero due to the constraint $\mu_{VBF} > 0$.^[32]

Table 5–5 Fit result for each mass hypothesis. The error bars were split according to their statistical or systematic nature. Lower errors are bouded at zero due to the constraint $\mu_{VBF} > 0$.

Mass point [TeV]	$\hat{\mu}_{VBF}$	Upper error
1.0	0.231	0.575(0.480(stat) + 0.317(syst))
1.1	0.076	0.33(0.284(stat) + 0.168(syst))
1.2	0.072	0.204(0.176(stat) + 0.104(syst))
1.3	0.001	0.139(0.130(stat) + 0.048(syst))
1.4	0.001	0.121(0.115(stat) + 0.038(syst))
1.5	0.000	0.122(0.112(stat) + 0.048(syst))
1.6	0.000	0.045(0.043(stat) + 0.015(syst))
1.8	0.000	0.041(0.039(stat) + 0.015(syst))
2.0	0.000	0.04(0.037(stat) + 0.015(syst))
2.5	0.000	0.042(0.038(stat) + 0.017(syst))
3.0	0.000	0.047(0.042(stat) + 0.021(syst))
4.0	0.000	0.061(0.054(stat) + 0.029(syst))
5.0	0.000	0.087(0.076(stat) + 0.042(syst))

Table 5–6. For all mass hypotheses, the differences between the asymptotic and toy results are less than 20%. The difference between the expected and observed limits becomes relatively constant for masses above 1.6 TeV due to the lack of data events in the signal-like bin.

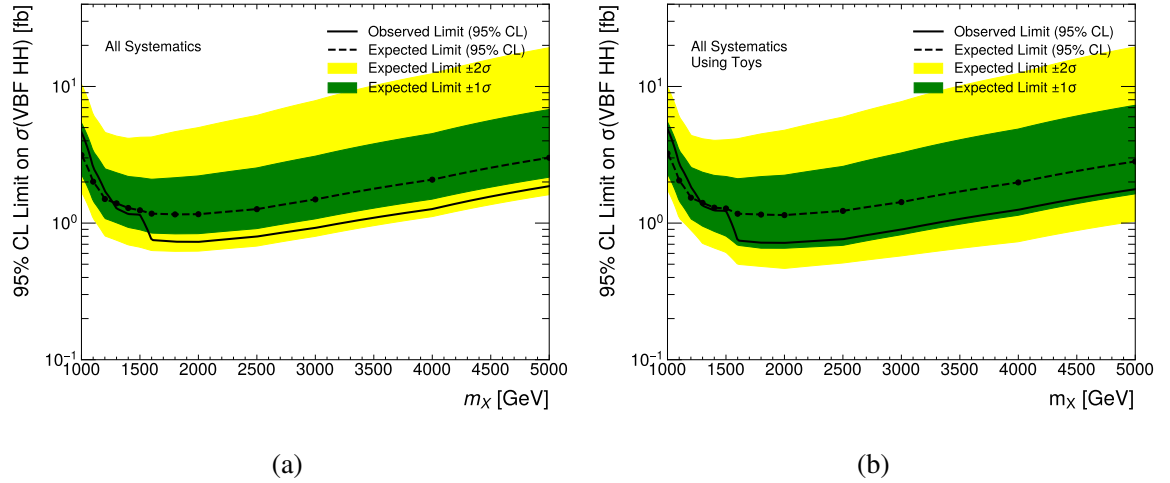


Figure 5–30 Unblinded results for the 95% CL limits on the cross-sections of 2HDM signals using (a) the asymptotic limit and (b) toys.

Table 5–6 Unblinded results for the 95% CL limits on the cross-sections of 2HDM signals using asymptotic approximation and toys. For each mass point a total of 100k toys have been generated. Results are all expressed in fb.^[32]

Mass [TeV]	Exp. Asymp.	Exp. Toys	$\frac{\text{Toys} - \text{Asymp.}}{\text{Asymp.}} [\%]$	Obs. Asymp.	Obs. Toys	$\frac{\text{Toys} - \text{Asymp.}}{\text{Asymp.}} [\%]$
1.0	3.148	3.235	2.763	4.634	4.902	5.784
1.1	2.01	2.051	2.055	2.543	2.7	6.142
1.2	1.501	1.535	2.271	1.715	1.841	7.342
1.3	1.395	1.406	0.781	1.279	1.339	4.702
1.4	1.29	1.298	0.573	1.165	1.237	6.194
1.5	1.241	1.28	3.155	1.152	1.229	6.691
1.6	1.173	1.171	-0.167	0.752	0.746	-0.831
1.8	1.158	1.154	-0.267	0.731	0.719	-1.583
2.0	1.161	1.144	-1.499	0.729	0.716	-1.704
3.0	1.49	1.424	-4.461	0.922	0.896	-2.826
4.0	2.079	1.984	-4.551	1.267	1.251	-1.258
5.0	3.008	2.825	-6.063	1.863	1.77	-4.975

Results for the Composite Higgs model

In this subsection, we present the results obtained for the Composite Higgs model in the broad width scenario. The available samples are for $m_X \in [1.2, 1.5, 1.8, 2.0]$ TeV. In all cases, the width of the heavy spin-0 particle is set to 20% of the mass. Although a sample at $m_X = 1.0$ TeV was initially produced, an issue in the job options was discovered that severely affects the analysis for this mass point. Therefore, the results are restricted to $m_X \geq 1.2$ TeV.

The pulls and impact on the signal strength for the scenario where $m_X = 1.2$ TeV are presented in Figure 5–31. In the broad width hypothesis, the nuisance parameters related to background modeling have a greater impact on the signal strength. This is expected due to the higher presence of signal in the background-like bins of the pBDT response distribution, as shown in the post-fit plot in Figure 5–32 for $m_X = 1.2$ TeV. However, it has been verified that the data-driven background modeling used in this analysis remains valid in the broad width case.

As observed in the 2HDM NW model, the asymptotic limits are similar to those obtained via pseudo-experiments. This has been confirmed in the broad-width case, as shown in Table 5–7, indicating that the upper limits on the cross-section are based on the asymptotic limits. The upper limits of the signal cross-section at 95% CL using the asymptotic

approximation are presented in Figure 5–33. There is not enough sensitivity to exclude the Composite Higgs model in the mass range between 1.2 TeV and 2.0 TeV if assuming the width is 20% of the mass.

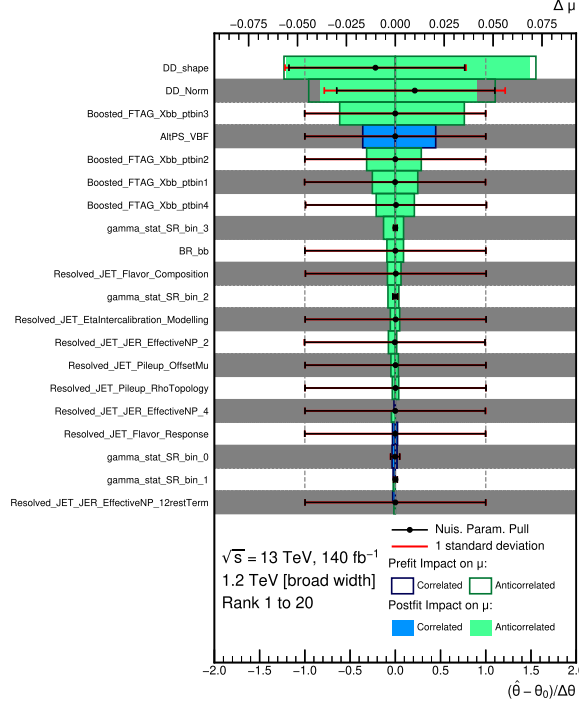


Figure 5–31 Pulls of dominant systematics in the unblinded resonant analysis for the CH model for $m_X = 1.2$ TeV in the broad width scenario. The blue band represents the positive correlation between the uncertainty and the POI, while the green represents the negative correlation.^[32]

Table 5–7 Unblinded results for the 95% CL limits on the cross-sections for the CH model in the broad width scenario using asymptotic approximation and toys. For each mass point a total of 100k toys have been generated. Results are all expressed in fb.^[32]

Mass [TeV]	Exp. Asymp.	Exp. Toys	$\frac{\text{Toys} - \text{Asymp.}}{\text{Asymp.}} [\%]$	Obs. Asymp.	Obs. Toys	$\frac{\text{Toys} - \text{Asymp.}}{\text{Asymp.}} [\%]$
1.2	2.13	2.17	1.93	2.51	2.62	4.25
1.5	1.64	1.68	2.10	1.52	1.59	4.35
1.8	1.38	1.38	-0.23	0.86	0.83	-4.06
2.0	1.32	1.32	-0.44	0.81	0.80	-1.50

So far, we have described the analysis optimization and results for the HH non-resonant and resonant analysis in 4b final states. The observed(expected) limit on the SM VBF HH

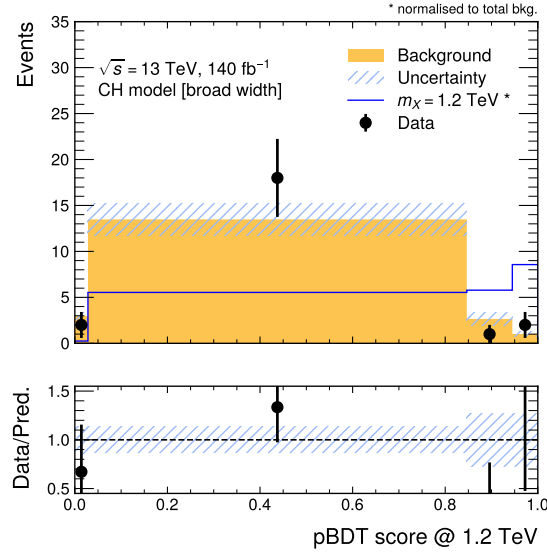


Figure 5–32 Post-fit in the resonant analysis. The signal model here is the CH model with $m_X = 1.2 \text{ TeV}$ and width equals to $20\% m_X$. In the broad width scenario the signal models have larger presence in the bkg-like bins of the pBDT, reducing thus the sensitivity of the analysis.^[32]

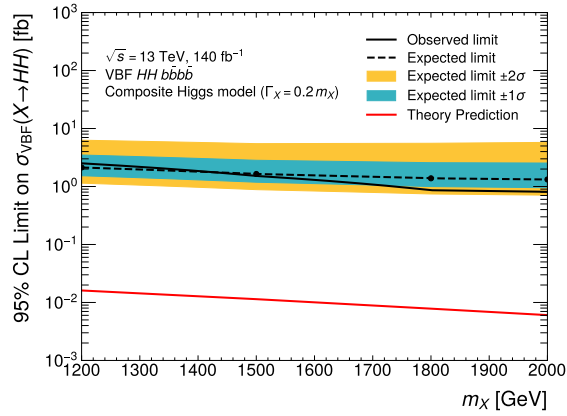


Figure 5–33 Unblinded results for the 95% CL limits on the cross-sections in the CH model with broad width scenario using the asymptotic limit. The theory curve shows that the CH model in this mass range can not be excluded with the current upper limits.

signal strength is 551 (672), observed constraints on κ_{2V} are [0.52, 1.52] ([0.32, 1.71]). The significance for excluding $\kappa_{2V} = 0$ is 3.4σ (2.9σ expected). The 95% CL intervals of κ_λ and κ_{2V} are estimated to be [-3, 11] ([-5, 11] expected) and [0.55, 1.49] ([0.37, 1.67] expected). The significance for excluding $\kappa_{2V} = 0$ is 3.8σ (3.3σ expected) by combining with the resolved analysis.

Chapter 6 Probe of Electroweak Phase Transition with Future Lepton Collider

6.1 Introduction

Finally, the potential for new physics searches in future lepton colliders is examined, particularly in the context of exotic Higgs decays. These three studies (together with VBS $W\gamma jj$, boosted VBF HH4b), while focusing on distinct physical processes, all serve the overarching goal of rigorously testing the Standard Model and exploring possible extensions through electroweak interactions, Higgs physics, and future experimental facilities. This section will be briefly introducing the work done in future lepton collider to fully cover the topics of this dissertation.

In the year of 2012, Higgs boson was discovered in LHC, particle physics has then entered a new era. Precise measurements of the Higgs' properties are the main target of physicists in the field of high-energy physics in the next ten years. Higgs boson's properties can affect the process of ElectroWeak Phase Transition (EWPT). Therefore, the emergence of particle of the Higgs boson signals a gateway to a deeper understanding of nature.

The Circular Electron Positron Collider (CEPC) is an electron-positron collider which is under pre-research that will be operating at around $\sqrt{s} = 240$ GeV in the future. It is designed to produce Higgs bosons at million level, providing great opportunities for Higgs boson studies. At CEPC, the Higgs boson will be produced in association with a Z boson through electron-positron annihilation. This setup offers unique advantages over studies at the Large Hadron Collider (LHC). The cleaner environment at CEPC provides high ratios when talking about signal over background processes, which is essential to precise measurements of the Higgs boson and probabilities of discovering the physics Beyond Standard Model (BSM). This work will not only emphasis the important role of Higgs boson factory for precision study, but also increase the BSM aspects of the physics motivation for the CEPC project.

A critical question at the intersection of high-energy physics and cosmology is investigating the thermal history of ElectroWeak Symmetry Breaking (EWSB) in the early universe. Certain types of EWSB could potentially resolve numerous mysteries, including the matter-

antimatter asymmetry^[135]. Non-perturbative lattice simulations indicate that within the Standard Model (SM), our universe experienced a smooth crossover phase transition^[136-139]. This type of EWSB is less intriguing for us because phenomena like electroweak baryogenesis^[135,140] and the stochastic gravitational wave background^[141] are associated with a strong first-order electroweak phase transition (SFOEWPT). The gravitational waves from such a transition could be detected by future space-based experiments like LISA^[142].

An SFOEWPT is anticipated in Beyond Standard Model (BSM) scenarios, where the Higgs field interacts with a gauge singlet—either real^[143] or complex^[144]—or with electroweak multiplets^[145], among others. New particles involved in such transitions must have a significant interaction with the SM Higgs boson and their masses should not be excessively heavy compared to the electroweak temperature scale^[146]. In my work listed in this dissertation, I explore the cases where a lighter BSM real singlet particle is produced with a mass less than half that of the SM Higgs particle. This new particle, denoted as s , couples with the SM Higgs h and could facilitate an SFOEWPT. Theoretical analyses of this BSM model gives conclusion that a lower bound on the exotic Higgs decay branching ratio could be derived as a function of the new scalar's mass^[147]. I will outline the model in the next section, and one can refer to^[148] for a complementary study on exotic Higgs decays as signatures of an SFOEWPT.

The potential energy involving the exotic scalar field S and the Higgs field from the SM, H , can be written as^[147,149]

$$V = -\mu^2|H|^2 + \lambda|H|^4 + \frac{1}{2}a_1|H|^2S + \frac{1}{2}a_2|H|^2S^2 \quad (6-1)$$

$$+ b_1S + \frac{1}{2}b_2S^2 + \frac{1}{3}b_3S^3 + \frac{1}{4}b_4S^4. \quad (6-2)$$

After electroweak symmetry breaking (EWSB), one can parametrize the two scalar fields as follows:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h \end{pmatrix}, \quad S = v_s + s, \quad (6-3)$$

Here, $v = 246$ GeV represents the vacuum expectation value (VEV) for the Higgs field at zero temperature, and v_s is the VEV for the singlet field. To proceed, one can either add a

tadpole term in the potential and set $v_s = 0$ or remove the tadpole term while keeping v_s . In this study, the former approach was chosen.

The mass eigenstates of the field could be derived by the mixing of two scalar fields h and s

$$\begin{aligned} h_1 &= h \cos \theta + s \sin \theta \\ h_2 &= -h \sin \theta + s \cos \theta, \end{aligned} \quad (6-4)$$

we take h_1 to be singlet-like particle with mass m_1 , h_2 to be SM-like Higgs particle with $m_2 = 125$ GeV. In order to observe a visible decay of the SM-like Higgs h_2 , I require the mixing angle $\cos \theta \neq 0$. Constrained by experimental limits, $|\cos \theta|$ cannot be too large, and the electroweak phase transition (EWPT) region with successful tunneling is insensitive to the precise value. Here I take $\cos \theta = 0.01$, and this value is large enough for the singlet-like particle h_1 to decay promptly^[147]. The trilinear scalar interactions in terms of mass eigenstates read

$$V \supset \frac{1}{6} \lambda_{111} h_1^3 + \frac{1}{2} \lambda_{211} h_2 h_1^2 + \frac{1}{2} \lambda_{221} h_2^2 h_1 + \frac{1}{6} \lambda_{222} h_2^3, \quad (6-5)$$

where λ_{211} governs the exotic Higgs decay. This cubic coupling's value is

$$\lambda_{211} = 2s^2 c b_3 + \frac{a_1}{2} c (c^2 - 2s^2) + (2c^2 - s^2) s v a_2 - 6\lambda s c^2 v. \quad (6-6)$$

where $s \equiv \sin \theta$ and $c \equiv \cos \theta$.

The total width of the singlet-like scalar particle and SM-like Higgs boson are

$$\begin{aligned} \Gamma(h_1) &= \cos^2 \theta \Gamma(h_2) \\ \Gamma(h_2) &= \sin^2 \theta \Gamma^{\text{SM}}|_{m_2} + \Gamma(h_2 \rightarrow h_1 h_1), \end{aligned} \quad (6-7)$$

where the exotic decay partial width is

$$\Gamma(h_2 \rightarrow h_1 h_1) = \frac{1}{32\pi^2 m_2} \lambda_{211}^2 \sqrt{1 - \frac{4m_1^2}{m_2^2}}. \quad (6-8)$$

As shown in Ref.^[147], only m_1 , $\cos \theta$, a_2 , b_3 , and b_4 are free parameters in this model. I take $m_1 \in [5, 60]$ GeV to enable the occurrence of the exotic Higgs decay and the value of $\cos \theta$ is chosen to be 0.01 to fit the experimental constraint. The decay enables the tests for the small mixing angle $\cos \theta$, which can be detected up to $\mathcal{O}(0.01)$ in future colliders^[147,150].

Under a given scalar mass m_1 and $\cos \theta$, the study scans over $a_2, b_3/v \in [10^{-4}, 1]$, and $b_4 \in [10^{-5}, 1]$ in the numerical simulation. The parameter region that satisfies a SFOEWPT has been worked out^[147], whose results I have reproduced for this study.

The search for such similar models could be performed in several experiments in the field of high-energy physics, including the ongoing LHC and potential future lepton colliders^[147-148]. Among these experiments, future e^+e^- colliders could have better sensitivity to probe the new scalar masses down to at least ~ 10 GeV during an SFOEWPT scenario^[147-148,151]. Under such promising scenarios, I propose to perform a detailed study of this exotic Higgs decay search with the simulation conducted from CEPC collaboration.

6.2 CEPC Detector

The Circular Electron Positron Collider (CEPC) is a proposed facility aimed at producing Z and Higgs bosons^[152-153]. The main ring of CEPC spans a circumference of 100 km, nearly four times the length of the LHC. As a Z boson factory, CEPC will generate approximately one tera of Z bosons at a center-of-mass energy (E_{cm} or $\sqrt{s}$) of 91.2 GeV. Furthermore, as a Higgs boson factory, it is designed to produce one million Higgs bosons at E_{cm} of 240 GeV.

Beyond the baseline operating scheme, E_{cm} of CEPC could be upgraded to 360 GeV. This upgrade would enable detailed studies of the top quark and Higgs boson. The cleaner collision environment of CEPC, compared to the hadronic collisions in the LHC, is anticipated to significantly enhance the precision in measuring the properties of the Higgs boson, surpassing the capabilities of the High Luminosity LHC (HL-LHC) by an order of magnitude^[154].

6.2.1 Tracking system

The tracking system of the CEPC consists of two primary components. The vertex detector gives high spatial resolution because it is used for precise vertex reconstruction. The main tracker, essential for the CEPC physics program, is optimized to achieve high tracking efficiency and resolution.

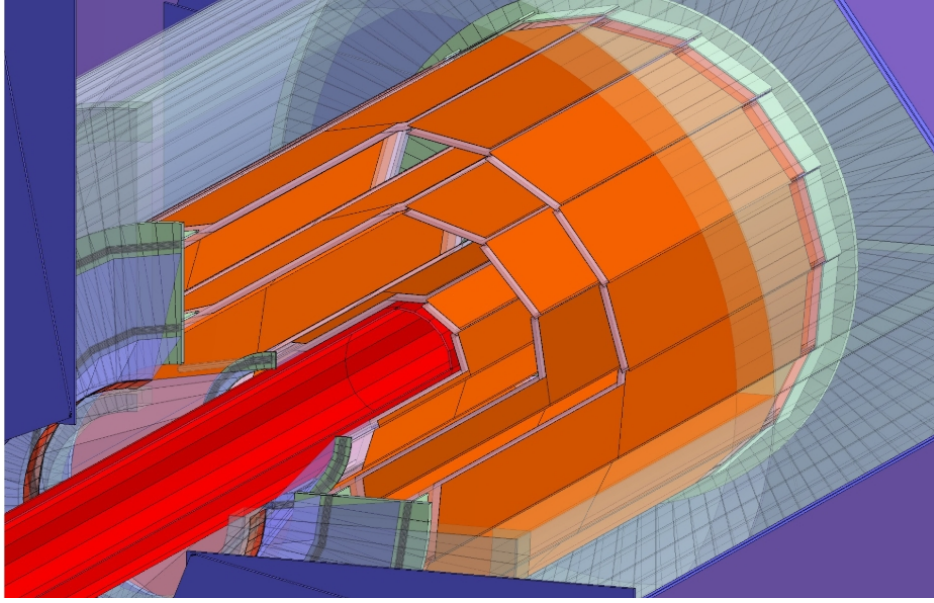


Figure 6-1 Schematic view of the pixel detector. Two layers of silicon pixel sensors are mounted on both sides of each of the three ladders to provide six space points. Only the silicon sensor sensitive region (in orange) is depicted. The vertex detector surrounds the beam pipe (red).

6.2.1.1 Vertex detector

The reconstruction of short-lived particles could be hard because of the limited distance before its decay, the reconstruction needs the information of track parameters of charged particles near the Interaction Point(IP). Therefore, the identification of quarks and τ leptons is of vital importance for this physics program.

The baseline design of the CEPC vertex detector comprises six concentric cylindrical layers of high spatial resolution silicon pixel sensors, positioned between 16 and 60 mm from the beam line 6-1. These layers provide six precise space-points for charged particles traversing the detector. The primary mechanical structure, known as a ladder, supports sensors on both sides, resulting in three sets of ladders for the vertex detector. Each detector layer, including its supporting material, has a material budget of approximately $0.15\% X_0$.

Extensive simulation studies indicate that this configuration, with its single-point resolutions, meets the required impact parameter resolution.

The fundamental concept of the CEPC vertex detector, encompassing the detector layout, the material budget per layer, and the pixel sensor specifications necessary for the impact parameter resolution, is incorporated into the baseline detector simulation.

6.2.2 Time projection chamber and silicon tracker

The Time Projection Chamber (TPC) is the default choice for the outer tracker in the CEPC baseline detector concept. Its high density of space points offers exceptional pattern recognition capability. To enhance track momentum resolution, the TPC is supplemented by an envelope of silicon detectors. These silicon detectors also serve to monitor potential field distortions in the TPC and assist with alignment.

6.2.2.1 Time projection chamber

The CEPC TPC 6–2 comprises a field cage constructed from advanced composite materials, and two self-contained readout end-plates that incorporate gas amplification, readout electronics, supply voltage, and cooling. The TPC features a cylindrical drift volume with an inner radius of 0.3 m, an outer radius of 1.8 m, and a total length of 4.7 m. A central cathode plane is maintained at a potential of 50 kV, while the two anodes at the end-plates are at ground potential. The cylindrical walls of the volume form the field cage, ensuring a highly homogeneous electric field of 300 V/cm between the electrodes. The drift volume is filled with a gas mixture of $Ar/CF_4/iC_4H_{10}$ in the ratio of 95%/3%/2%. Ionization electrons released by charged particle tracks drift along the electric field to the anodes, where they are amplified in an electron avalanche and read out using a Micro-Pattern Gas Detector (MPGD).

The CEPC TPC provides 220 space point measurements per track with a single-point resolution of $100\mu m$ in $r - \phi$. Besides position information, the TPC measures the ionization energy loss (dE/dx) on each readout pad. This measurement, combined with the momentum measurement in the magnetic field, facilitates particle identification.

6.2.2.2 Silicon tracker

The silicon tracker, TPC and the vertex detector, constitute the complete tracking system of the CEPC baseline detector concept. With a sufficiently low material budget to minimize the multiple-scattering effect, the silicon tracker provides additional high-precision hit points along the trajectories of charged particles, significantly enhancing tracking efficiency and precision.

The silicon tracker in the baseline design comprises four components: the Silicon Inner Tracker (SIT), the Silicon External Tracker (SET), the Forward Tracking Detector (FTD),

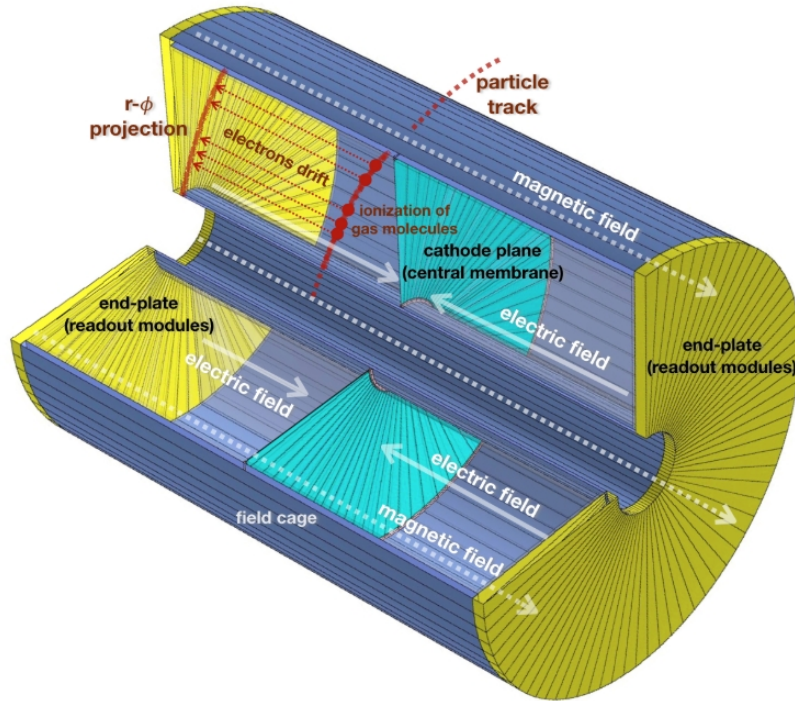


Figure 6–2 Sketch plot of the TPC detector. The TPC is a cylindrical gas detector with an axial electric field formed between the end-plates (yellow) and a central cathode plane/membrane (light blue). The cylindrical walls of the volume form the electric field cage (dark blue). Gas ionization electrons due to charged particles drift to the end-plates where they are collected by readout modules (yellow).

and the Endcap Tracking Detector (ETD). The overall layout is illustrated in Figure 6–3, and the main parameters are summarized in Table 6–1.

6.2.3 Calorimeter

Calorimeter is necessary for a whole detector system which is used for collecting energies of particles like electrons, photons and hadronic jets. Two distinct approaches are considered: particle-flow and dual-readout calorimeters. The baseline configuration used in our analysis adopts the particle-flow approach.

The CEPC particle-flow calorimetry system consists of two separate sampling calorimeters: the Electromagnetic Calorimeter (ECAL) and the Hadronic Calorimeter (HCAL). These are installed inside the bore of the solenoid to minimize the amount of inactive material in front of the calorimetry system and to ensure reliable association of tracks with energy de-

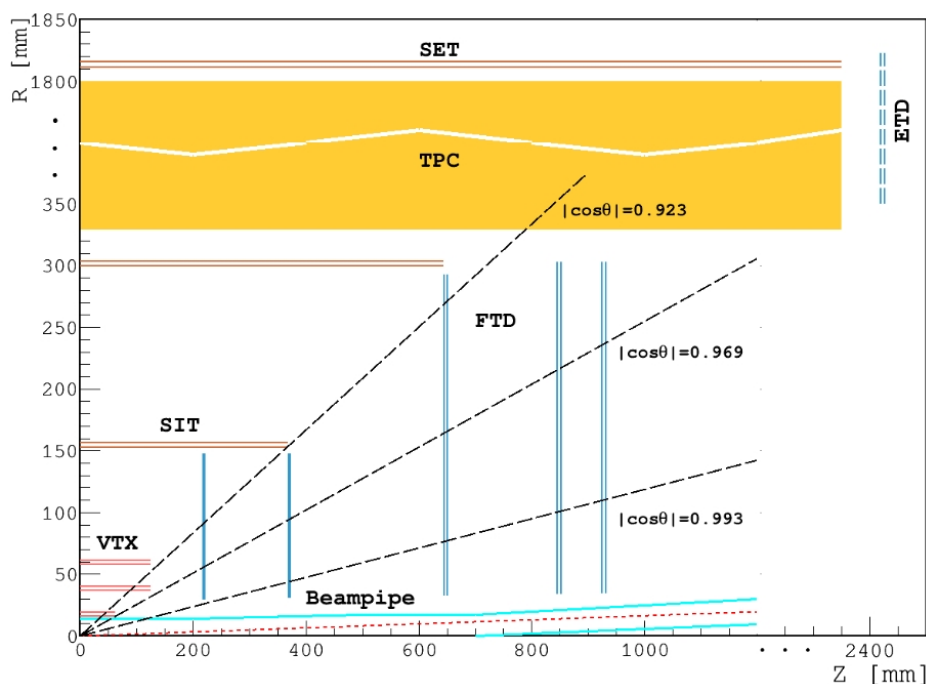


Figure 6–3 Preliminary layout of the tracking system of the CEPC baseline detector concept. The TPC is embedded within the Silicon Tracker. Colored lines indicate the positions of the silicon detector layers: red lines for the Vertex Detector (VTX) layers; orange lines for the Silicon Inner Tracker (SIT) and Silicon External Tracker (SET) components of the silicon tracker; gray-blue lines for the Forward Tracking Detector (FTD) and Endcap Tracking Detector (ETD) components of the silicon tracker. The cyan lines represent the beam pipe, and the dashed red line shows the beam line position with a beam crossing angle of 16.5 mrad.

posits. Both ECAL and HCAL are organized into a cylindrical barrel section and two disk-like endcap sections.

6.2.3.1 Particle flow oriented electromagnetic calorimeter(ECAL)

The particle flow paradigm significantly impacts the design of the ECAL. With its excellent pattern recognition capabilities, the ECAL is expected to identify photons and electrons from the collected hit points in the detector, reconstruct detailed properties of the EM-showers, and distinguish electromagnetic showers from hadronic ones. The ECAL is composed of 30 layers in the longitudinal direction, split into two sections with different absorber layer thicknesses to optimize energy resolution. The initial segment includes 20 layers of tungsten plates, each with a thickness of 0.6 times the radiation length (X_0), or 2.1 mm, totaling 12 radiation lengths. The subsequent segment comprises 10 layers of tungsten plates,

Detector		Radius R [mm]		$\pm z$ [mm]	Material budget [X_0]
SIT	Layer 1	153		371.3	0.65%
	Layer 2	300		664.9	0.65%
SET	Layer 3	1811		2350	0.65%
		R_{in}	R_{out}		
SIT	Disk 1	39	151.9	220	0.50%
	Disk 2	49.6	151.9	371.3	0.50%
	Disk 3	70.1	298.9	644.9	0.65%
	Disk 4	79.3	309	846	0.65%
	Disk 5	92.7	309	1057.5	0.65%
ETD	Disk	419.3	1822.7	2420	0.65%

Table 6–1 Main parameters of the CEPC silicon tracker. Silicon pixel sensors are planned for the two inner disks of the FTD whereas silicon microstrip sensors are envisioned for the rest. The column labelled $\pm z$ shows the length of the SIT and SET layers, and the z position of the FTD and ETD disks.

each 1.2 times the radiation length (X_0), or 4.2 mm thick, also summing up to 12 radiation lengths. The ECAL initiates with a sensitive layer, featuring 0.5 mm thick silicon sensors. The granularity of these sensitive layers is dictated by the size of the silicon sensors, which is $10 \times 10 \text{ mm}^2$ for all layers. Both longitudinal sections are mounted on a carbon fiber base plate that is 20 mm thick.

The ECAL barrel section comprises 8 staves, each made up of 5 trapezoidal modules as illustrated in Figure 6–4. Each barrel module consists of 5 columns. The modules and columns are aligned along the beam line and are arranged in odd numbers and symmetric positions to prevent any pointing-like dead zones in the azimuthal plane perpendicular to the beam direction at the IP. The column size is set at 186 mm, based on mechanical constraints and cost efficiency, accommodating exactly two 6-inch wafers or one and a half 8-inch wafers. Taking into account the column size, module walls, and additional allowances, the total length of the barrel along the beam direction is 4700 mm.

There is typically a 100 mm gap between the sides of the barrel and the front faces of the endcaps. The exact size of this gap will be determined by the service requirements for the ECAL, HCAL, and tracker systems, which include power and DAQ cabling, cooling pipes, patch panels, and other necessary infrastructure.

The endcap sections are structured into 4 quadrants, each comprising 2 modules: one

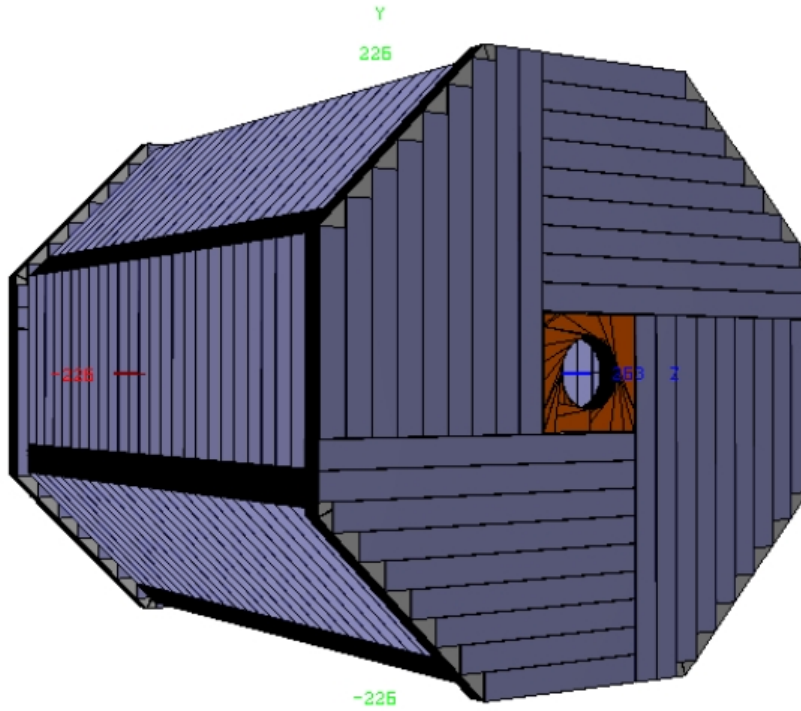


Figure 6–4 Schematic of the CEPC ECAL layout in its baseline design. The ECAL is organized into one cylindrical barrel and two disk-like endcap sections, with 30 layers in each section. The barrel section is arranged into 8 staves, each consisting of 5 trapezoidal modules. Each of the two endcap sections is made of four quadrants, each consisting of 2 modules. The ECAL barrel overall radius is 2028 mm in the X-Y plane, and the two endcaps are located at ± 2635 mm.

containing 4 columns and the other containing 3 columns. The ECAL ring sets the endcap's inner radius at 400 mm. With a configuration of 7 columns, the outer radius of the endcap measures 2088 mm. To accommodate the electromagnetic showers hitting the overlap area, a 32 mm buffer is maintained between the outer radii of the barrel and the endcaps. This configuration sets the barrel section's inner radius to 1843 mm. Overall, including all the barrel and endcap sections, a total of 256 ECAL columns are required.

6.2.3.2 Particle flow oriented hadronic calorimeter(HCAL)

The HCAL system, designed as a sampling calorimeter, uses steel as the absorber material and scintillator tiles or gaseous devices with embedded electronics as the active medium. The choice of steel offers the advantage of self-support without needing auxiliary structures that could create dead regions. The favorable ratio of hadronic interaction length ($\lambda_I = 17$ cm) to

electromagnetic radiation length ($X_0 = 1.8$ cm) allows for fine longitudinal sampling in terms of X_0 , with a manageable number of layers in λ_I . This ensures the detector volume and the number of readout channels remain small, which is beneficial for both capturing substantial electromagnetic energy within hadronic showers and resolving the shower substructure for particle separation.

As shown in Figure 6–5, the barrel section consists of 5 independent, self-supporting wheels along the beam axis. Each wheel is divided into 8 identical modules, mirroring the segmentation of the ECAL barrel. A module contains 40 stainless steel absorber plates with independent readout cassettes inserted between them. The absorber plates include a total of 20 mm of stainless steel: 10 mm from the welded structure and 10 mm from the mechanical support of the detector layer. Each wheel is independently supported by two rails on the inner wall of the cryostat of the magnet coil. Cables and cooling pipes are routed outside the HCAL, in the space between the outer side of the barrel HCAL and the inner side of the cryostat.

The active detector elements in the HCAL feature finely segmented readout pads, available in sizes of 1×1 cm² or 3×3 cm², throughout the entire HCAL volume. Each readout pad is individually read, resulting in a readout channel density of approximately $4 \times 10^{4-5}/\text{m}^3$. For an HCAL with a volume of about 100 m³, this corresponds to a total of $4 \times 10^{6-7}$ channels, presenting a significant challenge for the HCAL system. However, simulations suggest that even for calorimeters with cell sizes as small as 1×1 cm², simple hit counting can provide accurate energy measurements for hadrons. Consequently, the readout system can be simplified to record merely 'hit' or 'no hit' based on a single threshold (equivalent to a '1-bit' ADC). A hadron calorimeter employing this simplified readout approach is termed a Digital Hadron Calorimeter (DHCAL). In a DHCAL, each readout channel registers a 'hit' rather than measuring energy deposition as in traditional HCAL systems. Gas detectors, such as RPC or GEM, are excellent candidates for the active elements in a DHCAL. Alternatively, the Analog Hadron Calorimeter (AHCAL) uses scintillator tiles coupled with SiPMs as the active sensors.

There are other facilities, such as muon detector systems and magnetic systems, but these are not crucial to our analysis in this section and will therefore be excluded from detailed description.

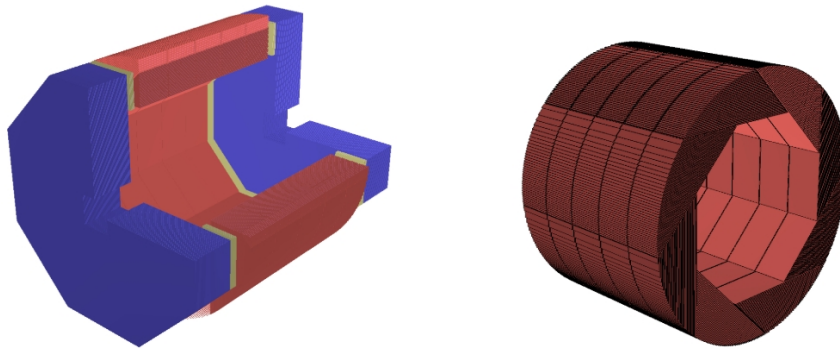


Figure 6–5 The baseline design of the CEPC HCAL is depicted schematically, with a cylindrical barrel (in red) extending radially from 2058 mm to 3144 mm, and two endcaps (in blue) positioned between 2650 mm and 3736 mm in $|z|$. An isometric view of the barrel HCAL is shown on the right.

6.3 Signal and Background Modeling

MADGRAPH5_aMC@NLO^[155] and WHIZARD^[156] Monte Carlo event generators are utilized in this analysis to simulate both signal and background processes. The singlet-like exotic Higgs signal model discussed in introduction section is implemented using FEYN-RULES^[157] and subsequently imported into MADGRAPH5_aMC@NLO. Signal events are generated at leading order (LO) using MADGRAPH5_aMC@NLO, with parton showering and hadronization modeled by PYTHIA8^[158]. Signal samples are produced for various mass points ranging from 15 GeV to 60 GeV in 5 GeV increments. Other Standard Model (SM) background events are generated using WHIZARD, with PYTHIA8 facilitating parton showering and hadronization. All samples used in the analysis are generated for non-polarized electron-positron collisions at $\sqrt{s} = 240$ GeV. Detector simulation is carried out by Mokka^[159], a Geant4^[160] based software, with digitization and reconstruction of simulated hits performed by ArborPFA^[161]. All backgrounds are modeled using samples simulated by CEPC.

6.4 Object Reconstruction

Charged leptons, such as electrons and muons, are identified using the Lepton Identification in Calorimeter with High Granularity (LICH) algorithm. LICH is a multivariate lepton identification technique designed for future detectors employing high-granularity calorimeters. Electrons and muons are identified with efficiencies of 99.7% and 99.9%, respectively,

with misidentification rates below 0.07%. Lepton isolation is also applied in the analysis, requiring $E_{\text{cone}} < 4E_\ell + 12.2$ GeV, where E_ℓ represents the lepton energy and E_{cone} denotes the energy within a cone of $\cos \theta_{\text{cone}} > 0.98$ around the lepton. Jets are reconstructed from particle flow objects (PFO) using the LCFIPlus software package, which integrates vertex finding and flavor tagging with jet reconstruction. The LCFIPlus package also provides flavor tagging information for each jet. Prior to jet reconstruction, leptons are removed from ArborPFO. Jets are clustered by grouping particles based on their momentum and spatial distribution using the Durham algorithm. For this analysis, an exclusive clustering was performed, requiring exactly four jets in the final state.

6.5 Event Selection

We aim to retain events featuring four b -jets originating from a singlet-like exotic scalar and two same-flavor opposite-sign leptons resulting from the Z -boson decay. Event selection is conducted in two stages: an initial loose pre-selection phase followed by a more sophisticated multivariate approach. This approach classifies signal and background events using a Boosted Decision Tree (BDT).

6.5.1 Pre-selection

At the pre-selection stage, a set of loose criteria is applied to remove as many background events as possible. Since the analysis examines both electron and muon final states, each event must contain two same-flavor isolated leptons with opposite charges (e^+e^- or $\mu^+\mu^-$). Each electron and muon must have energy greater than 20 GeV. Additionally, the two leptons must satisfy $|\cos \theta_{e^+e^-}| < 0.71$ or $|\cos \theta_{\mu^+\mu^-}| < 0.81$. To exclude most background events with lepton pair production, we require the angle between the two isolated tracks corresponding to the leptons to satisfy $\cos \phi_{e^+e^-} > -0.93$ and $\cos \phi_{\mu^+\mu^-} > -0.93$. To further reduce backgrounds, the invariant mass of the lepton system ($M_{\ell\bar{\ell}}$) must fall within the Z -mass window of 77.5 – 104.5 GeV. In signal-like events, the recoil mass should be around the Higgs boson mass. Therefore, to further suppress non-Higgs backgrounds, the recoil mass of the di-lepton system ($M_{\ell\bar{\ell}}^{\text{recoil}}$) is required to be in the range of $M_{\ell\bar{\ell}}^{\text{recoil}} \in [124, 140]$ GeV, where the recoil mass is defined in Eq. 6–9. The selection criteria are summarized in Table 6–2.

$$M_{\ell\bar{\ell}}^{\text{recoil}} = \sqrt{(\sqrt{s} - E_{\ell} - E_{\bar{\ell}})^2 - (\vec{P}_{\ell} + \vec{P}_{\bar{\ell}}) \cdot (\vec{P}_{\ell} + \vec{P}_{\bar{\ell}})} \quad (6-9)$$

Table 6–2 List of criteria applied in the pre-selection.

Variable	Selection Criteria
Lepton p_T	$p_T^{\text{lep}} > 20 \text{ GeV}$
Lepton angle	$ \cos \theta_{e^+e^- (\mu^+\mu^-)} < 0.71 (0.81)$
Track angle	$\cos \phi > -0.74$
Dilepton mass	$M_{\ell\bar{\ell}} \in [77.5, 104.5] \text{ GeV}$
Recoil mass	$M_{\text{recoil}}^{\ell\bar{\ell}} \in [124, 140] \text{ GeV}$

After selecting events with two leptons and four jets, the singlet-like exotic scalar is reconstructed by combining the jets. The reconstruction process involves evaluating all possible combinations of jet pairs and selecting the pair with the smallest mass difference. The reconstructed signal mass distributions are illustrated in Figure 6–6. As the mass increases, the distribution becomes wider.

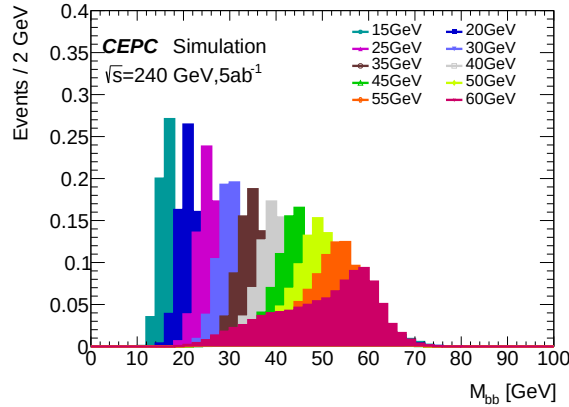


Figure 6–6 Reconstructed invariant mass distributions (M_{bb}) of the di- b -jet system after pairing the jets. Histograms in different colors correspond to different signal samples with masses ranging from 15 GeV to 60 GeV.

The background contributions are categorized into three groups: Higgs processes with $b\bar{b}$ final state ($\ell\ell H b\bar{b}$), other Higgs processes ($\ell\ell H$), and non-Higgs processes. Given that

the $H \rightarrow b\bar{b}$ process alone constitutes a significant background, it is treated as a separate category, while all other Higgs decay modes are grouped together.

6.5.2 Flavor tagging

Flavor tagging significantly enhances background suppression and improves the reconstruction of M_s . We utilized the flavor tagging toolkit in LCFIPLUS, which employs a multivariate approach. The training for the b -tagging algorithm is performed using gradient-boosted decision trees, leveraging variables such as jet kinematics, track impact parameters, and secondary vertex parameters. The b -tagging model provides a b -likeness value for each jet, representing the probability that a jet is a b -jet, with values ranging from 0 to 1. The b -likeness (L_b) values of the individual jets are used to compute a combined b -likeness or b -jet efficiency (f_b), defined as

$$f_b = \frac{L_{b1}L_{b2}L_{b3}L_{b4}}{L_{b1}L_{b2}L_{b3}L_{b4} + (1 - L_{b1})(1 - L_{b2})(1 - L_{b3})(1 - L_{b4})} . \quad (6-10)$$

We further define the b -jet inefficiency factor as

$$b_{\text{ineff}} = \log(1 - f_b) . \quad (6-11)$$

In this analysis, b_{ineff} is used to enhance the rejection of non- b -jet backgrounds. The signal process features four b quarks in the final states, thus the likelihood of such events being missed by the b -tagging tool is lower compared to other processes.

6.5.3 Gradient-boosted decision tree

After pre-selections, this analysis employs a multivariate approach by training a Boosted Decision Tree (BDT) to enhance signal sensitivity. The BDT is implemented using the LIGHTGBM^[162] Python package and trained to classify signal events from standard model background events. Specifically, we utilize gradient-boosted decision trees for our study. While many commonly used tools rely on depth-wise tree growth, LIGHTGBM grows trees leaf-wise. The leaf-wise growth algorithm can lead to faster convergence compared to depth-wise growth; however, without appropriate parameters, leaf-wise growth might cause overfitting.

To maximize the sensitivity of signal samples at each mass point, 10 models are trained

with different signal samples with m_S ranging from 15 GeV to 60 GeV, with a separate model trained for each mass point. The model hyperparameters are optimized using the Optuna^[163] hyperparameter optimization framework. The best configuration for each model is different, and these configurations are summarized in Table. A total of 100 trials are conducted to tune the hyperparameters for each model, achieving an area under the curve (AUC) of approximately 0.99 for every BDT.

The BDTs are trained using 24 input variables, which are briefly described in Table 6–3. Kinematic variables such as the p_T of the leading and subleading leptons, the recoil mass of the dilepton system, the energy of each jet, the invariant mass of the four-jet system, and the recoil mass of the four-jet system are utilized for BDT training. The mass of the di-bjet system reconstructs the mass of the singlet-like exotic scalar. Since there are two s particles in the process, the average of the two reconstructed masses (M_{bb}) is used for BDT training. Additionally, the difference between the reconstructed masses of the two s particles (M_{diff}^{ss}) is included as a training variable.

Beyond the kinematic observables, the number of particles used to reconstruct the four jets of an event (N_{particle}^{4j}) is crucial for suppressing fake jets. Only jet constituent particles with energy greater than 0.4 GeV are considered. Selected distances between pairs of the top 7 jet constituents ranked by transverse momentum are also used. Furthermore, we incorporate the boosted angle and opening angle between the reconstructed s particles along with the helicity angle of the two jets. The helicity angle of the first and third jets ($|\cos \theta_{j0,j2}^{\text{Helicity}}|$) is used since the other two jets have the same value. The BDT also employs the b_{ineff} to enhance the model's ability to distinguish between signal and background.

Figure 6–7 illustrates four variables with significant signal-to-background discrimination power used in the BDT training.

6.6 Uncertainty Estimation

The primary source of systematic uncertainty arises from the event yields of fixed backgrounds. To estimate uncertainties from background modeling, we vary the event yields of the primary $\ell\ell Hbb$ background by $\pm 5\%$ while other background processes are varied by $\pm 100\%$ ^[164]. The systematic uncertainties from luminosity^[165] and lepton identification^[164] are considered small and are thus ignored in this analysis.

Table 6–3 Variables used for the BDT training. Helicity angle of the first jet and the third jet is used because the other two jets have the same value.

Variable	Description
p_T^{l1}, p_T^{l2}	Lepton p_T
$M_{\ell\bar{\ell}}^{\text{recoil}}$	Recoil mass of the di-lepton system
$E^{j0}, E^{j1}, E^{j2}, E^{j3}$	Energy of each reconstructed jet
M^{4j}	Invariant mass of the four-jet system
M_{4j}^{recoil}	Recoil mass of the four-jet system
M_{bb}	Average mass of the two reconstructed s candidates
M_{diff}^{ss}	Difference between the two reconstructed s particles
N_{particle}^{4j}	Number of particles inside the four jets
$y_{12}, y_{23}, y_{34}, y_{45}, y_{56}, y_{67}$	Distance between jet constituents
$\cos \theta_{\text{boost}}^{s1}, \cos \theta_{\text{boost}}^{s2}$	Boosted angle between two jets from each s candidate
$\cos \theta_s^{\text{open}}$	Opening angle between the reconstructed s particles
$ \cos \theta_{j0}^{\text{Helicity}} , \cos \theta_{j2}^{\text{Helicity}} $	Helicity of the first and the third jets
b_{ineff}	b -jet inefficiency

Additionally, the analysis depends on flavor tagging; hence, the corresponding uncertainties are taken into account. We follow the method from Ref.^[166], where the uncertainty was estimated to be 0.78% using the $ZZ \rightarrow q\bar{q} + \mu^+\mu^-$ control sample. However, considering that this analysis involves more jets, we adopt a more conservative approach by assigning a 1% flat uncertainty as the flavor tagging uncertainty.

Jet energy resolution (JER) is also a critical factor in this analysis. The jets in our signal process are soft, and the CEPC detector is expected to perform worse in reconstructing these soft jets. We estimated this uncertainty for the low-energy signal-like jets by calculating the energy difference between a truth jet and a reconstructed jet using the $e^+e^-k_t$ -algorithm from the FastJet package^[167]. An additional correction factor is added to account for the difference between the two jet clustering packages, FastJet and LCFIPlus. The LCFIPlus jet clustering

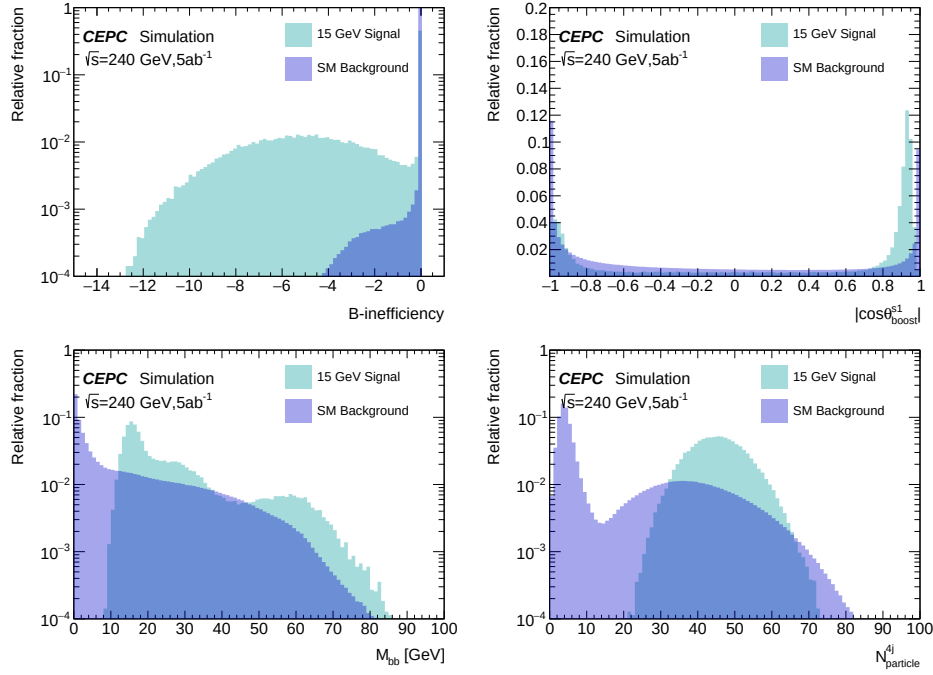


Figure 6-7 Signal and background distributions of four (out of 24) variables used for the BDT training. The signal histogram is from 15 GeV singlet MC samples.

algorithm reads vertex detector information from the particle-flow objects (PFO) in CEPC simulation. The total uncertainty is estimated by combining these two independent factors:

$$\text{JER} = \sqrt{\sigma_{\text{FastJet-TruthJet}}^2 + \sigma_{\text{FastJet-LCFIPlus}}^2}, \quad (6-12)$$

where σ is the jet resolution uncertainty. The estimated JER uncertainty is shown in Figure 6-8 as a function of truth jet energy.

Among the three different sources of uncertainties, the jet energy resolution uncertainty tends to be negligible after the statistical fit. The post-fit flavor tagging uncertainty is approximately 1%. The background modeling uncertainty due to limited yields of the Higgs process is around 4% post-fit. The contribution from non-Higgs processes is between 2-5% above $M_s = 20$ GeV, whereas it is around 10% at $M_s = 15$ GeV. For non-Higgs processes, the range is between 10-30%.

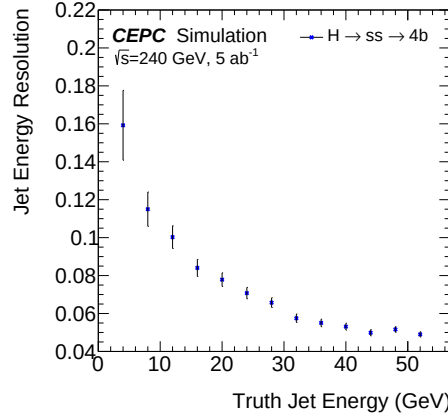


Figure 6–8 The jet energy resolution (Eq. 6–12) as a function of truth jet energy. The error bars represent statistical errors.

6.7 Results

In this analysis, we utilized the raw output of the BDT classifier as the primary discriminant. The BDT score is significantly higher for signal events compared to background events, as illustrated in Figure 6–9. The error band in Figure 6–9 includes both systematic and statistical uncertainties, as discussed in Sec 6.6.

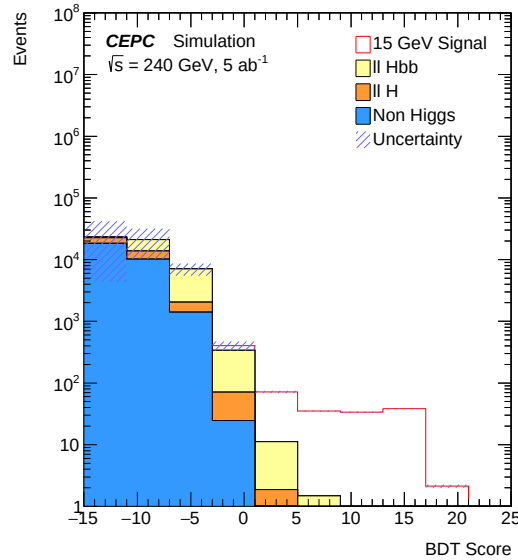


Figure 6–9 BDT score distribution for the combined electron and muon channel, along with an uncertainty band that includes both statistical and systematic uncertainties. The signal scores are shown in red histogram. All the histograms are scaled to 5 ab^{-1} luminosity.

The BDT score distribution bins are utilized to define a test statistic based on the profile likelihood ratio. This test statistic is employed to determine an expected upper limit on the signal cross-section multiplied by the branching ratio ($\sigma_{ZH} \times B(H \rightarrow ss)$) at the 95% confidence level (CL) using the CL_s method^[168-170]. The fit accounts for both systematic uncertainties and statistical uncertainty. Systematic uncertainties are integrated into the likelihood function via nuisance parameters, with Gaussian, log-normal, or Poisson priors applied to these parameters.

Figure 6–10 and Table 6–4 present the ratio of the 95% CL upper limit on ($\sigma_{ZH} \times B(H \rightarrow ss)$) to the Standard Model (SM) production cross-section (σ_{SM}) as a function of the singlet mass, M_s . The expected limit curve is nearly flat, allowing us to probe the singlet scalar with a mass as low as 15 GeV. However, due to limited signal simulations, our results do not extend below 15 GeV.

For comparison, the upper limits of existing results from ATLAS and CMS using various channels, as well as projections for the future High Luminosity LHC (HL-LHC), are also shown. The HL-LHC limit can reach up to 0.1 with the full dataset, while the CEPC can push the limit to approximately 0.002 using a cut-and-count analysis. Although a cut-based approach was studied and optimized using the “ $n - 1$ ” method, it was deemed unnecessary to develop selections based on 10 signal samples. Instead, we decided to use 10 BDT classifiers to handle the 10 signal samples. The BDT has demonstrated superior performance in variables such as b_{ineff} , thereby improving the limits further by a factor ranging from 2 ~ 4 depending on the signal masses.

The CEPC is expected to achieve unprecedented sensitivity in the search for scalar particles from Higgs decay compared to the HL-LHC. A similar study was conducted and submitted as a Snowmass white paper^[171]. This paper performs a comprehensive study of jet energy resolution, which is crucial for this analysis since the final state contains several soft jets. Additionally, the paper focuses on multivariate analysis to enhance signal sensitivity, with carefully optimized input variables.

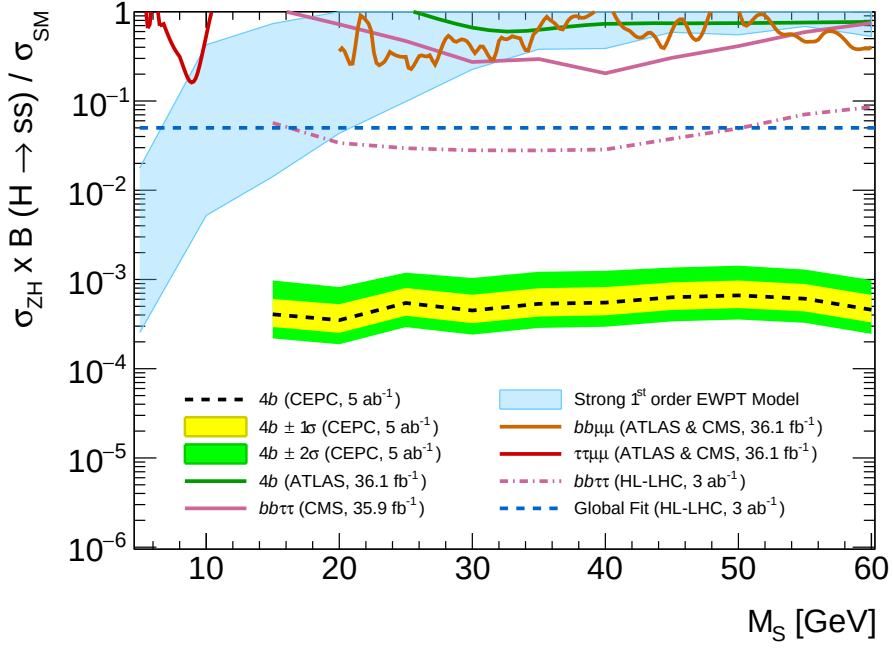


Figure 6–10 The ratio of expected upper limits at 95% CL on the $\sigma_{ZH} \times B(H \rightarrow ss)$ and SM cross-section (σ_{SM}) as a function of singlet mass (M_s). The expected limits obtained from the BDT analysis are represented by the black dotted line with 1σ (yellow) and 2σ (green) uncertainty bands. The blue-shaded region in the plot indicates points that predict a strong first-order electroweak phase transition with successful tunneling, as determined by numerical scans^[147]. The plot also displays the current (solid) and projected (dashed) sensitivities of the LHC in the $\tau\tau\mu\mu$ (red)^[172-173], $bb\mu\mu$ (orange)^[174-175], $bb\tau\tau$ (pink)^[176-177], and $4b$ (green)^[178] channels. For the $bb\mu\mu$ and $\tau\tau\mu\mu$ channels, the best limit between ATLAS and CMS is shown at each mass point. Additionally, the HL-LHC projection for the indirect limit on the total exotic branching fraction is displayed as the blue dashed line^[179].

Table 6–4 The expected 95% CL upper limit for the product of the signal's cross-section times branching ratio relative to the Standard Model cross-section. The results are presented for the combined electron e^+e^-H and muon $\mu^+\mu^-H$ channels using the multivariate BDT approach.

Expected 95% CL upper limits	
M_s [GeV]	$\sigma_{ZH} \times \text{B}(H \rightarrow ss)/\sigma_{\text{SM}}$
15	4.07×10^{-4}
20	3.50×10^{-4}
25	5.45×10^{-4}
30	4.49×10^{-4}
35	5.34×10^{-4}
40	5.50×10^{-4}
45	6.32×10^{-4}
50	6.63×10^{-4}
55	6.09×10^{-4}
60	4.58×10^{-4}

Chapter 7 Conclusion

7.1 Conclusion

In this research, an observation of the electroweak production of the $W\gamma jj$ process, including detailed measurements of both fiducial and differential cross-sections, is conducted. This study utilized data collected by the ATLAS detector at the Large Hadron Collider (LHC) at a center-of-mass energy of $\sqrt{s} = 13$ TeV, with a total integrated luminosity of 140 fb^{-1} . The $W\gamma jj$ process offers a unique opportunity to explore the quartic gauge couplings through the vector boson scattering mechanism. Specifically, this process is sensitive to the $WW\gamma Z$ and $WW\gamma\gamma$ couplings, making it an excellent probe for examining the electroweak gauge symmetry breaking within the Standard Model.

Advanced neural network techniques were employed to observe the electroweak $W\gamma jj$ production, achieving a significance well above six standard deviations. The measured fiducial cross-section for this process was found to be $13.2 \pm 2.5 \text{ fb}$, aligning with the Standard Model leading-order predictions from MADGRAPH 5 +PYTHIA 8 and SHERPA. Differential cross-sections were also measured across six kinematic observables within a more stringent fiducial phase space. These observables are particularly sensitive to the quartic gauge couplings and the CP-violating (CPV) structures of the $WW\gamma Z$ and $WW\gamma\gamma$ couplings.

To account for detector inefficiencies and resolution effects, an iterative Bayesian unfolding method was used to correct the data. The resulting unfolded distributions were then compared with theoretical predictions from MADGRAPH 5 +PYTHIA 8 and SHERPA 2.2.12. While the leading-order predictions generally fell within the uncertainty range, MADGRAPH 5 +PYTHIA 8 tended to overshoot the measurements at high invariant mass (m_{jj}) and transverse momentum ($p_{T,jj}$), whereas SHERPA 2.2.12 showed reasonable agreement but slightly underestimated the data across all six observables. This comprehensive analysis provides significant insights into the electroweak interactions and the underlying mechanisms of gauge symmetry breaking.

Additionally, we introduced a search for the production of Higgs boson pairs via VBF production in the $bbbb$ final state. This second analysis also utilizes data from the ATLAS detector with an integrated luminosity of 140 fb^{-1} from pp collisions at the LHC. The focus

of this analysis is on the Lorentz-boosted regime, where each Higgs boson is reconstructed as a large-R jet. This strategy demonstrates high sensitivity to anomalous κ_{2V} values that produce energetic Higgs bosons. Machine learning techniques are applied in both b-tagging for large-R jets and signal-background discrimination using boosted decision trees (BDT). As a result, the data are found to be consistent with the background-only hypothesis. The observed (expected) constraints obtained are $0.55 < \kappa_{2V} < 1.49$ ($0.37 < \kappa_{2V} < 1.67$) at 95% CL. A value of $\kappa_{2V} = 0$ is excluded with an observed (expected) significance of 3.8 (3.3) standard deviations. Furthermore, a search was performed for the first time for a new heavy spin-0 resonance through VBF HH production in a mass range between 1 TeV and 5 TeV. No significant excess is observed, and exclusion limits are set on the production cross-section.

A search for exotic decays of the Higgs boson is also covered in this dissertation, with a particular focus on the Higgs produced in association with a Z boson that decays leptonically. The analysis utilized simulated data from 5000 fb^{-1} of e^+e^- collisions at $\sqrt{s} = 240 \text{ GeV}$ at the CEPC. A *LightGBM*-based boosted decision tree was employed to discriminate signal from background events, using the BDT score as the final discriminant for statistical analysis. This method improved sensitivity by a factor ranging from 2 to 4 compared to the standard cut-and-count analysis. Upper limits on the ZH production cross-section times branching ratio were set. The study of the $4b$ final state at the CEPC could conclusively test the possibility of a strongly first-order electroweak phase transition in the extended Standard Model with a light singlet of mass as low as 15 GeV, showing significantly higher sensitivity than what can be achieved at the LHC for this low mass range.

Studies on hadronic calorimeter for the DarkSHINE experiment are also presented in this dissertation. The design of hadronic calorimeter is optimized to meet the requirements of hadron rejection. Both transverse size and absorber thickness layout are optimized to achieve the best rejection power. The final design saves the material budget compared to the initial design. The simulation also shows good performance in terms of hadron rejection.

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Appendix A Supplementary Material for Chapter 4

A.1 Monte Carlo Samples

Sample	DSID	Filtereff	$\sigma[nb]$
EWK $W\gamma$ jj			
Sh_2212_lvgammajj	700709	1.00E+0	1.78E+0
MGaMcAtNloPy8EG_EWKVgamma	363270	1.00E+0	8.40E-1
MGaMcAtNloPy8EG_EWKVgamma	363271	1.00E+0	8.40E-1
MGaMcAtNloPy8EG_EWKVgamma	363272	1.00E+0	8.40E-1
QCD $W\gamma$ jj			
Sh_2211_munugamma	700402	1.00E+0	3.65E+2
Sh_2211_enugamma	700403	1.00E+0	3.65E+2
Sh_2211_taubugamma	700404	1.00E+0	3.65E+2
MGPY8EG_enugamma_01jNLO	504678	1.00E+0	1.94E+2
MGPY8EG_munugamma_01jNLO	504679	1.00E+0	1.94E+2
MGPY8EG_taubugamma_01jNLO	504680	1.00E+0	1.52E+2
Top Backgrounds			
PowhegPythia8EvtGen_A14_Wt_DR_inclusive_top	410646	1.00E+0	3.79E+1
PowhegPythia8EvtGen_A14_Wt_DR_inclusive_antitop	410647	1.00E+0	3.79E+1
PhPy8EG_A14_tchan_BW50_lept_top	410658	1.00E+0	3.70E+1
PhPy8EG_A14_tchan_BW50_lept_antitop	410659	1.00E+0	2.22E+1
PowhegPythia8EvtGen_A14_singletop_schan_lept_top	410644	1.00E+0	2.03E+0
PowhegPythia8EvtGen_A14_singletop_schan_lept_antitop	410645	1.00E+0	1.27E+0
MGPY8EG_A14NNPDF23_tWgamma	500334	1.00E+0	1.23E-1
MadGraphPythia8EvtGen_A14NNPDF23_tWgamma_GamFromDec	412006	1.00E+0	2.88E-1
MadGraphPythia8EvtGen_A14NNPDF23_tgamma_nonallhadronic	410389	1.00E+0	4.62E+0
aMcAtNloPy8EG_A14NNPDF23_tgammaSM_tchan_4fl_NLO	412147	1.00E+0	1.14E+0
Single Photon			
Sherpa_222_NNPDF30NNLO_SinglePhoton_pty_17_35	364541	1.00E+0	4.15E+5
Sherpa_222_NNPDF30NNLO_SinglePhoton_pty_35_70	364542	1.00E+0	4.40E+4
Sherpa_222_NNPDF30NNLO_SinglePhoton_pty_70_140	364543	1.00E+0	4.53E+3
Sherpa_222_NNPDF30NNLO_SinglePhoton_pty_140_280	364544	1.00E+0	3.76E+2
Sherpa_222_NNPDF30NNLO_SinglePhoton_pty_280_500	364545	1.00E+0	2.19E+1
Sherpa_222_NNPDF30NNLO_SinglePhoton_pty_500_1000	364546	1.00E+0	1.46E+0
Sherpa_222_NNPDF30NNLO_SinglePhoton_pty_1000_E_CMS	364547	1.00E+0	2.99E-2
EWK $Z\gamma$			
MGaMcAtNloPy8EG_EWKVgamma	363266	1.00E+0	1.62E-1
MGaMcAtNloPy8EG_EWKVgamma	363267	1.00E+0	5.21E-2

Sample	DSID	Filtereff	$\sigma[nb]$
MGaMcAtNloPy8EG_EWKVgamma	363268	1.00E+0	5.20E-2
Sh_2212_llgammajj_Min_N_TChannel	700708	1.00E+0	1.66E-1
Diboson			
Sh_2212_III	700600	1.00E+0	1.30E+0
Sh_2212_IIIv	700601	1.00E+0	4.66E+0
Sh_2212_IIvv_os	700602	1.00E+0	1.21E+1
Sh_2212_IIvv_ss	700603	1.00E+0	2.22E-2
Sh_2212_Ivvv	700604	1.00E+0	3.11E+0
Sh_2212_vvvv	700605	1.00E+0	5.78E-1
Sherpa_222_NNPDF30NNLO_III	364250	1.00E+0	1.25E+0
Sherpa_222_NNPDF30NNLO_IIIv	364253	1.00E+0	4.57E+0
Dijet			
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ1WithSW	364701	2.42E-2	7.84E+10
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ2WithSW	364702	9.82E-3	2.43E+9
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ3WithSW	364703	1.17E-2	2.65E+7
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ4WithSW	364704	1.34E-2	2.55E+5
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ5WithSW	364705	1.45E-2	4.55E+3
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ6WithSW	364706	9.45E-3	2.58E+2
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ7WithSW	364707	1.11E-2	1.62E+1
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ8WithSW	364708	1.02E-2	6.25E-1
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ9WithSW	364709	1.23E-2	1.96E-2
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ10WithSW	364710	5.89E-3	1.20E-3
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ11WithSW	364711	2.65E-3	4.22E-5
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ12WithSW	364712	4.30E-4	1.04E-6
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ0W	361020	9.75E-1	7.84E+10
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ1W	361021	6.72E-4	7.84E+10
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ2W	361022	3.34E-4	2.43E+9
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ3W	361023	3.20E-4	2.65E+7
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ4W	361024	5.31E-4	2.55E+5
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ5W	361025	9.24E-4	4.55E+3
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ6W	361026	9.43E-4	2.58E+2
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ7W	361027	3.94E-4	1.62E+1
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ8W	361028	1.02E-2	6.25E-1
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ9W	361029	1.21E-2	1.96E-2
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ10W	361030	5.91E-3	1.20E-3
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ11W	361031	2.67E-3	4.23E-5
Pythia8EvtGen_A14NNPDF23LO_jetjet_JZ12W	361032	4.26E-4	1.04E-6
W+jets			
Sh_2211_Wenu_maxHTpTV2_BFilter	700338	9.38E-3	2.17E+4

Sample	DSID	Filtereff	$\sigma[nb]$
Sh_2211_Wenu_maxHTpTV2_CFilterBVeto	700339	1.49E-1	2.17E+4
Sh_2211_Wenu_maxHTpTV2_CVetoBVeto	700340	8.44E-1	2.17E+4
Sh_2211_Wmunu_maxHTpTV2_BFilter	700341	9.80E-3	2.18E+4
Sh_2211_Wmunu_maxHTpTV2_CFilterBVeto	700342	1.46E-1	2.18E+4
Sh_2211_Wmunu_maxHTpTV2_CVetoBVeto	700343	8.44E-1	2.18E+4
Sh_2211_Wtaunu_L_maxHTpTV2_BFilter	700344	9.01E-3	7.68E+3
Sh_2211_Wtaunu_L_maxHTpTV2_CFilterBVeto	700345	1.46E-1	7.68E+3
Sh_2211_Wtaunu_L_maxHTpTV2_CVetoBVeto	700346	8.47E-1	7.68E+3
Sh_2211_Wtaunu_H_maxHTpTV2_BFilter	700347	8.68E-3	1.41E+4
Sh_2211_Wtaunu_H_maxHTpTV2_CFilterBVeto	700348	1.43E-1	1.41E+4
Sh_2211_Wtaunu_H_maxHTpTV2_CVetoBVeto	700349	8.47E-1	1.41E+4
Sh_2211_mumugamma	700398	1.00E+0	1.03E+2
Sh_2211_eegamma	700399	1.00E+0	1.03E+2
Sh_2211_tautaugamma	700400	1.00E+0	1.03E+2
Sh_2211_nunugamma	700401	1.00E+0	5.64E+1
Z+jets			
Sh_2211_Zee_maxHTpTV2_BFilter	700320	2.49E-2	2.22E+3
Sh_2211_Zee_maxHTpTV2_CFilterBVeto	700321	1.30E-1	2.22E+3
Sh_2211_Zee_maxHTpTV2_CVetoBVeto	700322	8.46E-1	2.22E+3
Sh_2211_Zmumu_maxHTpTV2_BFilter	700323	2.44E-2	2.22E+3
Sh_2211_Zmumu_maxHTpTV2_CFilterBVeto	700324	1.30E-1	2.22E+3
Sh_2211_Zmumu_maxHTpTV2_CVetoBVeto	700325	8.46E-1	2.22E+3
Sh_2211_Ztautau_LL_maxHTpTV2_BFilter	700326	2.49E-2	2.75E+2
Sh_2211_Ztautau_LL_maxHTpTV2_CFilterBVeto	700327	1.25E-1	2.75E+2
Sh_2211_Ztautau_LL_maxHTpTV2_CVetoBVeto	700328	8.50E-1	2.75E+2
Sh_2211_Ztautau_LH_maxHTpTV2_BFilter	700329	2.44E-2	1.01E+3
Sh_2211_Ztautau_LH_maxHTpTV2_CFilterBVeto	700330	1.25E-1	1.01E+3
Sh_2211_Ztautau_LH_maxHTpTV2_CVetoBVeto	700331	8.50E-1	1.01E+3
Sh_2211_Ztautau_HH_maxHTpTV2_BFilter	700332	2.46E-2	9.33E+2
Sh_2211_Ztautau_HH_maxHTpTV2_CFilterBVeto	700333	1.25E-1	9.33E+2
Sh_2211_Ztautau_HH_maxHTpTV2_CVetoBVeto	700334	8.50E-1	9.33E+2
EWK Wjj			
Sherpa_221_NNPDF30NNLO_Wenu2jets_Min_N_TChannel	308096	1.00E+0	6.81E+0
Sherpa_221_NNPDF30NNLO_Wmunu2jets_Min_N_TChannel	308097	1.00E+0	6.80E+0
Sherpa_221_NNPDF30NNLO_Wtaunu2jets_Min_N_TChannel	308098	1.00E+0	6.80E+0
EWK Zjj			
Sherpa_221_NNPDF30NNLO_Zee2jets_Min_N_TChannel	308092	1.00E+0	6.32E-1
Sherpa_221_NNPDF30NNLO_Zmm2jets_Min_N_TChannel	308093	1.00E+0	6.34E-1
Sherpa_221_NNPDF30NNLO_Ztautau2jets_Min_N_TChannel	308094	1.00E+0	6.33E-1

Sample	DSID	Filtreff	$\sigma[nb]$
EWK-QCD $W\gamma$ jj Interference			
MGPY8EG_Wenu_INTWg	501840	1.00E+0	1.83E-2
MGPY8EG_Wmnu_INTWg	501841	1.00E+0	1.82E-2
MGPY8EG_Wtnu_INTWg	501842	1.00E+0	1.82E-2
EFT Samples			
MGPY8EG_wgjj_T0_QUAD	509492	1.00E+0	2.78E-2
MGPY8EG_wgjj_M0_INT_2	510220	1.00E+0	9.25E-6
MGPY8EG_wgjj_M0_QUAD_2	510221	1.00E+0	1.27E-4
MGPY8EG_wgjj_M1_INT_2	510222	1.00E+0	-1.17E-5
MGPY8EG_wgjj_M1_QUAD_2	510223	1.00E+0	5.32E-5
MGPY8EG_wgjj_M2_INT_2	510224	1.00E+0	9.36E-6
MGPY8EG_wgjj_M2_QUAD_2	510225	1.00E+0	1.07E-3
MGPY8EG_wgjj_M3_INT_2	510226	1.00E+0	-4.53E-5
MGPY8EG_wgjj_M3_QUAD_2	510227	1.00E+0	4.69E-4
MGPY8EG_wgjj_M4_INT_2	510228	1.00E+0	-3.05E-5
MGPY8EG_wgjj_M4_QUAD_2	510229	1.00E+0	3.02E-4
MGPY8EG_wgjj_M5_INT_2	510230	1.00E+0	-7.07E-6
MGPY8EG_wgjj_M5_QUAD_2	510231	1.00E+0	4.43E-4
MGPY8EG_wgjj_M7_INT_2	510234	1.00E+0	3.04E-6
MGPY8EG_wgjj_M7_QUAD_2	510235	1.00E+0	1.70E-5
MGPY8EG_wgjj_T0_INT_2	510236	1.00E+0	-1.89E-4
MGPY8EG_wgjj_T0_QUAD_2	510237	1.00E+0	1.87E-2
MGPY8EG_wgjj_T1_INT_2	510238	1.00E+0	-8.89E-4
MGPY8EG_wgjj_T1_QUAD_2	510239	1.00E+0	3.74E-2
MGPY8EG_wgjj_T2_INT_2	510240	1.00E+0	-4.75E-4
MGPY8EG_wgjj_T2_QUAD_2	510241	1.00E+0	4.63E-3
MGPY8EG_wgjj_T5_INT_2	510242	1.00E+0	-2.50E-4
MGPY8EG_wgjj_T5_QUAD_2	510243	1.00E+0	4.18E-2
MGPY8EG_wgjj_T6_INT_2	510244	1.00E+0	-7.24E-4
MGPY8EG_wgjj_T6_QUAD_2	510245	1.00E+0	5.47E-2
MGPY8EG_wgjj_T7_INT_2	510246	1.00E+0	-4.16E-4
MGPY8EG_wgjj_T7_QUAD_2	510247	1.00E+0	8.30E-3
MGPY8EG_wgjj_T0_ALL_2	510248	1.00E+0	1.67E+0
MGPY8EG_wgjj_T1_ALL_2	510249	1.00E+0	1.69E+0

A.2 Sample Overlap Removal

Samples with photons in the matrix element are subject to cuts on photon transverse momentum and ΔR with the lepton. To avoid double counting, dedicated photon samples are combined with samples without photons, and an overlap removal procedure is applied. The VGammaORTool algorithm defines the overlap region with $p_T(\gamma) > 17$ GeV and $\Delta R(l, \gamma) > 0.3$. True photons must have $p_T > 3$ GeV and not originate from baryons, mesons, τ leptons, or π^0 , and must come from the generator. Leptons must be true, stable particles from the generator and not originate from a hadron or radiated photon. Events with photons and leptons satisfying these criteria fall in the overlap region. Some remaining events in the Zjets and ttbar samples with two truth leptons but only one reconstructed lepton are only considered for overlap removal if $\Delta R(\gamma, l) > 0.2$.

A.3 Event selection

The event yields along with the Monte Carlo predicted yields for both the electron and muon channels are detailed in Tables A–2 and A–3.

Sample	Baseline	2nd lepton veto	$ M_Z - M_{\gamma\gamma} > 10\text{GeV}$	MET>30GeV	$M_{W}^* > 30\text{GeV}$	$\Delta\phi(j1(2), MET) > 0.4$	$pT_{j1(2)} > 50$	B jet veto	$M_{jj} > 500$	$\Delta Y(jj) > 2$
Data 2015+2016	155545	143776	72292	43361	36907	29975	12886	6289	X	X
Sh2212 EWK evjj	828.704	822.549	725.381	533.326	451.266	367.966	235.442	192.099	98.653	88.5649
Madgraph EWK evjj	2044.59	2007.31	1745.95	1286.57	1111.43	904.747	467.015	251.092	141.593	131.752
Sh2211 QCD evjj	30594.2	30326.3	26365.8	17908.4	15539	12830.6	4207.28	3384.52	613.501	480.033
Madgraph QCD evjj	32846.7	32604.4	28478.8	19446.4	16102.6	13409.8	4640.32	3878.24	694.229	532.496
EWK-QCD inter. evjj	72.3131	71.3852	62.0985	49.037	46.0801	32.8126	30.1646	25.4493	10.3679	3.37017
EWK eejj	208.853	49.6225	40.3308	13.6339	11.3427	7.1665	4.61129	3.87018	2.01862	1.81944
QCD eejj	16905.1	9028.14	6738.24	2399.04	1754.63	1270.77	350.941	291.169	51.5981	43.4871
VV	362.374	268.19	179.475	144.088	127.708	107.877	42.6258	34.9718	6.88264	5.35712
tty	8848.92	7237.85	6269.13	5074.28	4266.11	3602.43	2624.84	245.131	26.2696	22.9641
tq γ	1010.71	981.012	828.807	630.211	547.903	444.118	229.132	34.7218	12.8762	12.6493
tW γ	506.865	428.785	375.142	292.975	241.844	204.501	124.978	22.7006	1.85438	1.46081
Single Top										
Total MC (Sh2211)	59338.04	49213.83	41584.4	27044.99	22985.88	18868.24	7850.01	4234.63	824.02	659.71
Total MC (Madgraph)	62806.43	52676.69	44717.97	29336.23	24209.65	19984.22	8514.63	4787.35	947.69	755.36
Data 2017	235463	219196	100751	61858	52696	43056	16048	7763	X	X
Sh2212 EWK evjj	933.697	925.924	817.854	608.763	515.552	422.639	266.791	219.684	110.221	99.2818
Madgraph EWK evjj	2401.2	2357.28	2040.98	1513.36	1303.62	1076.23	569.902	307.039	168.771	159.851
Sh2211 QCD evjj	39321.7	39007	33897.7	23611.6	20483.1	16944.7	5052.05	4066.19	704.605	553.745
Madgraph QCD evjj	42302.6	42018.2	36597.3	25625.9	21467.2	17905	5654.11	4743.27	815.186	628.755
EWK-QCD inter. evjj	89.6508	88.2193	78.6523	62.0274	54.6771	37.8374	36.1964	29.7713	12.3883	3.99715
EWK eejj										
QCD eejj	22595.6	12442.6	9090.74	3692.91	2727.8	2086.88	440.523	357.535	64.4045	55.0325
VV	471.899	349.588	234.812	192.064	169.135	143.792	49.5134	41.3448	9.07612	7.15367
tty	10159.9	8305.37	7179.06	5864.23	4920.49	4142.84	3047.5	284.608	33.1797	30.0685
tq γ	1189.45	1149.39	992.24	758.951	676.001	571.026	277.425	44.1198	19.4343	18.8335
tW γ	589.54	497.279	438.436	346.955	288.467	245.024	150.388	28.0169	2.40897	1.91055
Single Top										
Total MC (Sh2211)	75351.44	62765.37	52729.49	35137.5	29835.22	24594.74	9320.39	5071.27	955.72	770.02
Total MC (Madgraph)	79799.84	67207.93	56652.22	38056.4	31607.39	26208.63	10225.56	5835.7	1124.85	905.6
Data 2018	295665	274594	128929	78420	66889	54490	20632	10096	X	X
Sh2212 EWK evjj	1277.31	1267.76	1120.46	829.676	704.042	575.397	365.864	300.441	148.371	133.179
Madgraph EWK evjj	3236.07	3181.47	2762.89	2059.87	1773.66	1454.55	758.576	405.386	222.558	207.609
Sh2211 QCD evjj	52298.1	51883.2	45010.1	31046.3	26954.2	22283.3	6897.87	5524.16	958.605	755.536
Madgraph QCD evjj	57108.2	56637.5	49315.1	34237.7	28514.1	23889.1	7811.91	6580.1	1096.34	906.226
EWK-QCD inter. evjj	125.195	123.157	109.843	83.9899	78.6038	56.3873	50.2886	41.7215	16.6227	4.71086
EWK eejj	321.803	80.3128	65.504	24.6265	20.4352	13.6942	8.78538	7.34203	3.76285	3.43717
QCD eejj	30313.7	16717	12262.3	4834.38	3495.23	2647.24	618.71	497.628	91.5566	79.6652
VV	646.653	481.317	321.459	259.401	229.143	194.259	66.6078	55.911	11.4167	8.91099
tty	13750	11278.7	9769.34	7956.82	6674.45	5615.13	4100.37	385.566	45.6187	40.3853
tq γ	1588.35	1541.91	1308.62	1002.82	890.529	734.796	393.574	55.8697	23.3435	21.5989
tW γ	797.394	670.964	588.026	464.74	389.318	328.778	204.507	38.0729	3.96254	3.30367
Single Top										
Total MC (Sh2211)	101118.5	84044.32	70555.65	46502.75	39435.95	32448.98	12706.58	6906.71	1303.26	1050.73
Total MC (Madgraph)	107887.36	90712.33	76503.08	50924.35	42065.47	34933.93	14013.33	8067.6	1515.18	1275.85

Table A–2 The event yields for the electron channel, along with predicted yields from Monte Carlo (MC) simulations at various stages of the event selection, are presented. The baseline stage includes criteria for data quality, primary vertex, as well as the presence of good leptons and photons, supplemented by ΔR constraints.

Sample	Baseline	2nd lepton veto	$ M_{\ell\ell} - M_{\ell\ell} > 10 GeV$	MET>30GeV	$M_{W}^* > 30 GeV$	$\Delta\phi(j1(2), MET) > 0.4$	$pT_{j1(2)} > 50$	B jet veto	$M_{jj} > 500$	$\Delta Y(jj) > 2$
Data 2015+2016	79138	66228	55618	38777	33151	27468	11877	5647	X	X
Sh2212 EWK $\mu\nu jj$	803.525	797.078	706.059	521.98	449.121	365.13	224.044	188.19	96.2678	86.3828
Madgraph EWK $\mu\nu jj$	2076.65	2040.66	1774.55	1320.61	1147.42	943.062	479.395	259.264	141.054	132.848
Sh2211 QCD $\mu\nu jj$	30938.6	30671.2	26664.1	18308.7	15944.8	13221.3	4223.14	3391.67	604.032	487.155
Madgraph QCD $\mu\nu jj$	32994.1	32738.1	28617.6	19659.7	16518.5	13693.1	4557.85	3837.52	596.678	490.554
EWK-QCD inter. $\mu\nu jj$	73.3463	72.5963	63.0417	50.251	47.2233	33.7197	30.695	25.7369	9.52187	2.77324
EWK $\mu\mu$	180.41	12.2585	10.8468	4.48805	3.58719	2.39238	1.51886	1.30703	0.683674	0.624231
QCD $\mu\mu jj$	14804	5301.88	3378.51	1486.24	1099.78	834.907	213.227	170.388	29.2089	23.8933
VV	241.798	179.727	152.414	124.594	110.679	93.4833	35.5507	29.4968	5.88892	4.60793
t γ	8625.86	7046.31	6088.53	4941.37	4150.92	3503.28	2529.94	241.41	24.8214	22.3173
tq γ	990.915	961.633	822.017	628.526	549.683	460.297	253.743	31.8861	10.2519	9.64606
tW γ	482.516	408.537	359.322	281.999	235.365	199.862	121.675	22.6018	2.19027	1.75889
Single Top										
Total MC (Sh2211)	57140.97	45451.22	38244.84	26348.15	22591.16	18714.37	7633.53	4102.69	782.87	639.16
Total MC (Madgraph)	60469.6	48761.7	41266.83	28497.78	23863.16	19764.1	8223.59	4619.61	820.3	689.02
Data 2017	106645	88782	73945	52207	44932	37226	14192	6723	X	X
Sh2212 EWK $\mu\nu jj$	890.064	882.044	779.224	585.017	498.538	408.22	246.189	201.308	104.107	93.8038
Madgraph EWK $\mu\nu jj$	2329.07	2286.78	1991.32	1493.5	1296.77	1070.2	544.532	292.215	164.806	153.739
Sh2211 QCD $\mu\nu jj$	39470.2	39156.7	33930.9	23614.9	20632.5	17030.3	4885.67	3915.73	690.85	558.736
Madgraph QCD $\mu\nu jj$	42059.8	41740.5	36321	25528	21359.3	17869.9	5388.54	4553.78	802.003	645.277
EWK-QCD inter. $\mu\nu jj$	86.7142	85.8709	76.1505	59.8375	55.633	40.0816	33.9373	27.802	10.1019	3.23685
EWK $\mu\mu$										
QCD $\mu\mu jj$	20309.2	7294.81	4433.26	2221.91	1660.18	1317.71	263.582	212.281	37.8648	31.0084
VV	334.147	249.603	211.034	176.135	156.41	133.951	43.521	35.7587	7.29217	5.65177
t γ	9642.25	7877.55	6810.08	5556.77	4673.06	3945.16	2877.5	272.197	29.5104	26.6607
tq γ	1104.48	1071.66	919.396	725.139	631.745	517.233	277.619	37.798	14.5811	14.3721
tW γ	550.3	459.349	401.477	317.064	263.506	221.425	134.104	22.9038	2.05687	1.71558
Single Top										
Total MC (Sh2211)	72387.36	57077.59	47561.52	33256.77	28571.57	23614.08	8762.12	4725.78	896.36	735.19
Total MC (Madgraph)	76415.96	61066.12	51163.72	36078.36	30096.6	25115.66	9563.34	5454.74	1068.22	881.66
Data 2018	137830	114729	95872	67835	58436	48356	18593	8535	X	X
Sh2212 EWK $\mu\nu jj$	1200.17	1190.9	1052	784.826	672.414	547.121	335.033	281.13	143.709	129.58
Madgraph EWK $\mu\nu jj$	3096.64	3042.55	2640.62	1977.63	1714.09	1416.49	726.895	383.482	211.832	199
Sh2211 QCD $\mu\nu jj$	51882	51481.1	44630.2	31002.4	27057.7	22452.2	6657.03	5338.36	924.914	747.394
Madgraph QCD $\mu\nu jj$	55792.4	55389.4	48179.5	33644.2	28428	23743.8	7216.68	6152.25	1063.41	848.85
EWK-QCD inter. $\mu\nu jj$	115.239	113.718	100.551	78.6945	72.718	51.6619	47.0108	39.5667	15.1677	4.95408
EWK $\mu\mu$	274.93	18.6118	16.509	7.37883	6.01585	4.31179	2.65234	2.18575	1.23227	1.09252
QCD $\mu\mu jj$	26274.5	9452.19	5773.65	2775.55	2095.95	1656.13	376.805	294.271	52.7771	43.3118
VV	430.252	321.308	274.629	226.501	201.721	172.353	54.9581	46.2571	9.79293	7.72059
t γ	12879	10514.6	9091.38	7421.14	6238.16	5251.55	3840.98	373.285	42.093	37.5406
tq γ	1499.72	1460.83	1234.76	957.96	841.136	687.473	378.52	49.2343	21.0518	19.4849
tW γ	726.714	609.893	535.312	420.288	350.086	299.355	184.77	34.1442	3.29693	2.65114
Single Top										
Total MC (Sh2211)	95282.53	75163.15	62708.99	43674.74	37535.9	31122.16	11877.76	6458.43	1214.03	993.73
Total MC (Madgraph)	101089.4	80923.1	67846.91	47509.34	39947.88	33283.12	12829.27	7374.68	1420.65	1164.61

Table A–3 Event yields and predicted yields from Monte Carlo (MC) simulations for the muon channel are detailed at various stages of the event selection process. The ‘Baseline’ stage encompasses checks for data quality and primary vertex adequacy, alongside established criteria for good leptons and photons, and includes ΔR measurements.

A.4 Jet fake photon

A.4.1 Template fit method

Various functions were evaluated to best describe each template's shape. The most effective fits were achieved using a double-sided crystal ball for prompt photons and a Novosibirsk function for jet-fake photons. The crystal ball function, which combines a Gaussian core with a power-law tail, is formulated as follows:

$$f_{CB} = \begin{cases} \exp\left(-\frac{(E-E_0)^2}{2\sigma^2}\right) & \text{if } \frac{E-E_0}{\sigma} > -\alpha \\ \left(\frac{n}{|\alpha|}\right)^n \exp\left(-\frac{|\alpha|^2}{2}\right) \left(\frac{n}{|\alpha|} - |\alpha| - \frac{E-E_0}{\sigma}\right)^{-n} & \text{if } \frac{E-E_0}{\sigma} \leq -\alpha \end{cases} \quad (\text{A-1})$$

where E_0 denotes the Gaussian mean, σ the width, α the cutoff parameter, and n the power of the tail. A double-sided crystal ball is simply two crystal ball functions that share the same mean and width.

The Novosibirsk function, which models the tail-heavy distribution, is described by:

$$f_N = e^{-0.5\left(\frac{(\ln(q_y))^2}{\Lambda^2} + \Lambda^2\right)} \quad (\text{A-2})$$

where

$$q_y = 1 + \frac{\Lambda(x - x_0)}{\sigma} \cdot \frac{\sinh(\Lambda\sqrt{\ln 4})}{\Lambda\sqrt{\ln 4}} \quad (\text{A-3})$$

Here, x_0 represents the peak position, σ the width, and Λ characterizes the distribution's tail. The pdfs $f_T(x|\theta_T)$ and $f_{NT}(x|\theta_{NT})$ denote the double-sided crystal ball for tight photons and the Novosibirsk function for non-tight photons, respectively, where x signifies the photon isolation and θ the adjustable parameters of the fit.

The real photon template is derived by conducting an unbinned fit on the isolation distribution of tight, truth-matched photons from Monte Carlo simulations using a double-sided crystal ball function. The fit minimizes the negative log-likelihood, expressed as:

$$-\ln \mathcal{L} = -\ln \prod_i f_T(x|\theta_T) \quad (\text{A-4})$$

where i indexes each event.

For constructing a jet-faking photon template, data from a fake-enriched control region—defined by one of the non-tight photon identification points—is fitted with a Novosibirsk

function. The corresponding minimized negative log-likelihood is:

$$-\ln \mathcal{L} = -\ln \prod_i f_{NT}(x|\theta_{NT}) \quad (\text{A-5})$$

with i again indicating the number of events.

The resultant templates are then combined, and their normalizations are adjusted to match data containing a tight photon. In this phase, the template parameters are floated but constrained by multivariate Gaussians, determined by the mean and sigma from the best fits of the templates. The negative log-likelihood for this step is:

$$-\ln \mathcal{L} = -\ln \prod_i [f_T(x|\theta_T)f_{NT}(x|\theta_{NT})G(\theta_T|\sigma_{\theta_T})G(\theta_{NT}|\sigma_{\theta_{NT}})] \quad (\text{A-6})$$

where G represents the multivariate Gaussian constraints, and i spans all events.

A.4.2 Uncertainties

Statistical Error on yield: Statistical uncertainty in the yield reflects the limited data available in the regions where the real and fake photon templates are fitted. This uncertainty is carried over to the final analysis by allowing the template fitting parameters to fluctuate during the fit to real photon data. These fluctuations are controlled by Gaussian constraints, which are based on the optimal mean and width obtained from the template fits, as detailed in the previous likelihood expressions. The uncertainties in the yields are calculated by integrating the final shape of the jet-faking photon template while adjusting the final parameters within their uncertainties.

Real Photon Leakage The standard methodology does not consider the contamination of real photons into the non-tight control region. To address this, a systematic adjustment includes an additional template in the non-tight fit to represent real photons that are present but fail tight identification. This template, referred to as the leakage template, is modeled using a double-sided crystal ball function and is derived from Monte Carlo simulations of real photons that do not meet tight criteria. Due to the limited statistics of the Monte Carlo data, a single leakage template is used across all regions instead of individual templates for each bin..

The minimization of the negative log likelihood for the fit to non-tight photon data is then defined as:

$$-\ln \mathcal{L} = -\ln \prod_i f_{NT}(x|\theta_{NT})f_L(x|\theta_L)G(\theta_L|\sigma_{\theta_L}) \quad (\text{A-7})$$

where G represents the Gaussian constraint based on the optimal fit parameters and their uncertainties from the fit to Monte Carlo real photons that fail tight identification.

Real photon leakage is treated as a systematic uncertainty rather than a nominal component in the jet faking photon fit. This is due to the fact that varying the photon loose identification to assess systematic errors associated with the choice of control region leads to a reduction in the amount of data available in the non-tight region. Moreover, the large number of fit parameters required when including the leakage template makes the fit unstable and yields unrealistic shapes for the jet faking photon when the leakage template is included.

Photon loose identification definition systematic: As mentioned in Section 3.4, four distinct definitions of Loose' ID can be utilized to establish a control region enriched with jet-faking photons. Loose' 2, which permits two criteria failures, closely resembles the actual data and is therefore considered the most biased. Conversely, Loose' 5 allows up to five criteria failures, making it the least biased. To address potential biases introduced by the selection of the Loose' definition, the template fitting method is applied using each Loose' ID definition in addition to the nominal Loose' 4. The range of outcomes from these variations is used to define the uncertainty associated with the choice of the jet faking photon enriched control region.

Real Photon Isolation Modelling Uncertainty The predominant source of real photons in Monte Carlo simulations comes from QCD $W\gamma jj$ events, which are utilized in this estimation. Given the potential imperfections in the isolation modeling of real photons, a theoretical uncertainty is applied. Although an alternative generator in the madgraph sample is available, its limited statistics may cause variations in the template shapes due simply to inadequate sample size. Instead, systematic variations are introduced by modifying the factorization and renormalization scales in the QCD $W\gamma jj$ sample. The variations $(\mu_F, \mu_R) = (0.5, 0.5)$ and $(\mu_F, \mu_R) = (2.0, 2.0)$ are implemented to establish upper and lower bounds on this uncertainty. It should be noted that the fitting process allows for adjustments in the real

photon shape parameters to better match the data, thereby compensating for any potential mis-modeling of photon isolation. Consequently, this systematic uncertainty is considered minimal.

A.5 Jet fake muon

A.5.1 Fake Factor Calculation in the Dijet Region

Defining tight and anti-tight muon criteria is pivotal for estimating fake muons using the fake factor method, as these definitions impact both the statistical reliability and the purity of the dataset utilized for calculating the muon fake factor. To accurately estimate the fake factor F , it is crucial to utilize a dataset enriched with jet-originated fake muons. Detailed analysis has been conducted to confirm the purity of these jet-dominated regions before proceeding with the calculation of F . The criteria for tight muons align with the general muon definition in this study, whereas the anti-tight criteria involve reversing either the isolation cut or the σ_{d_0} for muons. The specific requirement $d_0/\sigma_{d_0} < 20$ is employed to exclude significant outliers while retaining the bulk of the data.

Dijet data is selected to estimate the fake factor due to its substantial statistical volume. This selection is based on the premise that the final state includes at least one muon and one jet, with the jet and muon scattering back-to-back, and the jet's momentum exceeding 30 GeV. The fake factor F for muons is calculated by determining the ratio of the number of events with tight muons to those with anti-tight muons. Main backgrounds such as events involving W or Z bosons decaying into leptons are minimized through stringent cuts on the missing transverse momentum and the reconstructed transverse momentum of the W boson. Additional backgrounds from top quarks and dibosons are also considered and subtracted. The detailed selection criteria are delineated in Table A-4, with specific cuts on $\Delta R(\mu, j_0)$ and $\Delta\phi(\mu, j_0)$ designed to maximize the dijet signal-to-background ratio. Discrepancies between data and MC can be attributed to imprecise MC simulations of dijet events featuring a faked muon, prompting the use of data minus W/Z jets MC samples for accurate fake factor calculation.

Dijet Event Selection
Passes single muon triggers
$N_\mu = 1$ and $p_T^\mu > 20$ GeV
$N_{jet} \geq 1$ and $p_T^{j_0} > 30$ GeV
b-jet veto
$E_T^{miss} < 20$ GeV
$m_T^W < 20$ GeV
$ \Delta R(\mu, j_0) > 2.8$
$ \Delta\phi(\mu, j_0) > 2.8$

Table A–4 Dijet event selection criteria for the fake factor calculation of jets faking muons

A.5.2 Systematic uncertainties

There are multiple sources of systematic uncertainty in estimating the background from jets mimicking muons. First, the compositional differences between dijet and γ jets MC samples, lead to variability in calculated fake factors, contributing to systematic uncertainties. Second, in determining the distributions of fake and anti-tight muons, Sherpa QCD $W\gamma$ MC samples are compared with Madgraph QCD MC samples to assess uncertainties, with additional checks on W/Z +jets MC samples by altering scale factors and PDFs. Third, the selection criteria for dijet events, such as variations in missing transverse energy and the transverse momentum of the W boson and leading jet, introduce variability in the fake factor calculation. Lastly, the binning choices for the muon's p_T and η are evaluated using an alternative binning method, and discrepancies from the nominal fake factor are considered for systematic uncertainties.

A.6 Lepton fake photon

Fitting results are depicted in Figures A–1 and A–2, conducted around a ± 20 GeV range of the Z mass peak at 91.118 GeV. The signal is integrated within a 10 GeV window around this peak. The final fake rate, inclusive of statistical uncertainties derived from the fit results, is presented in Figures A–3 and A–4.

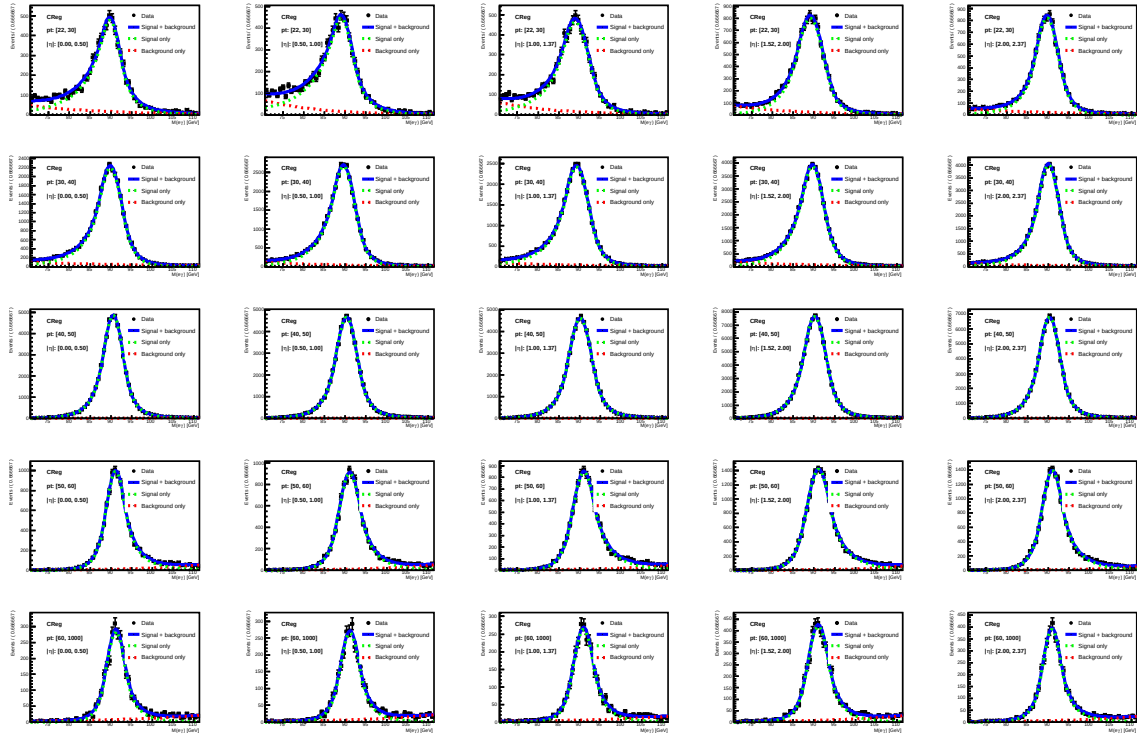
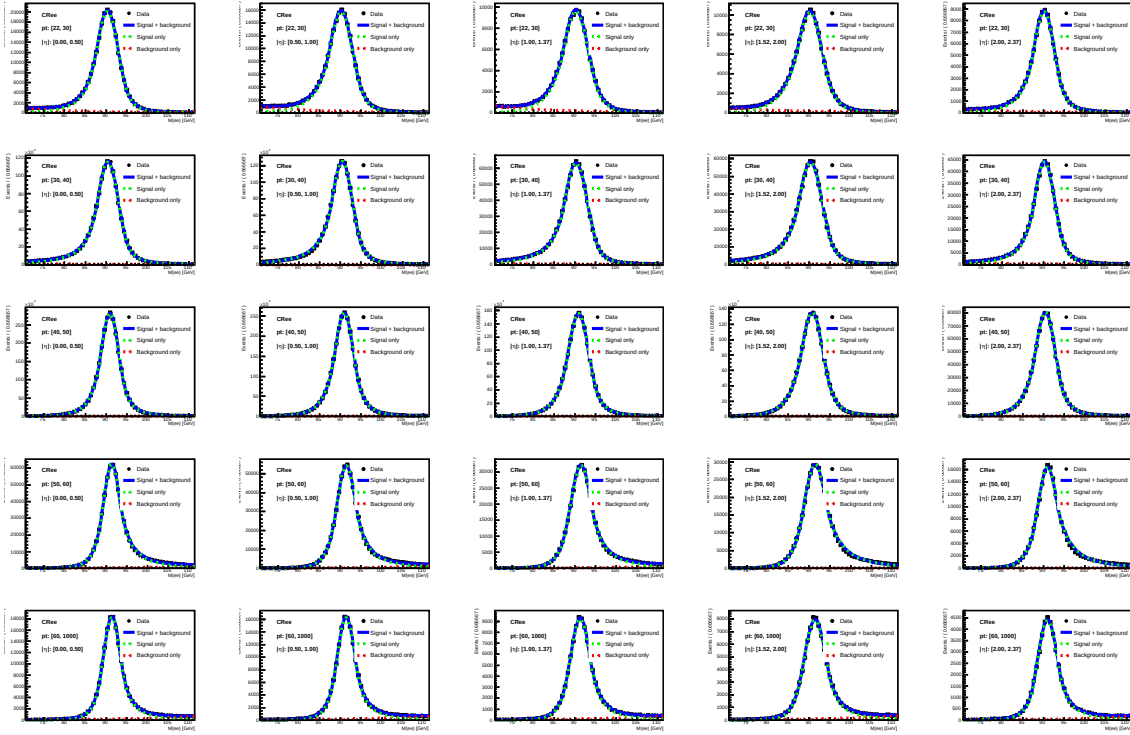
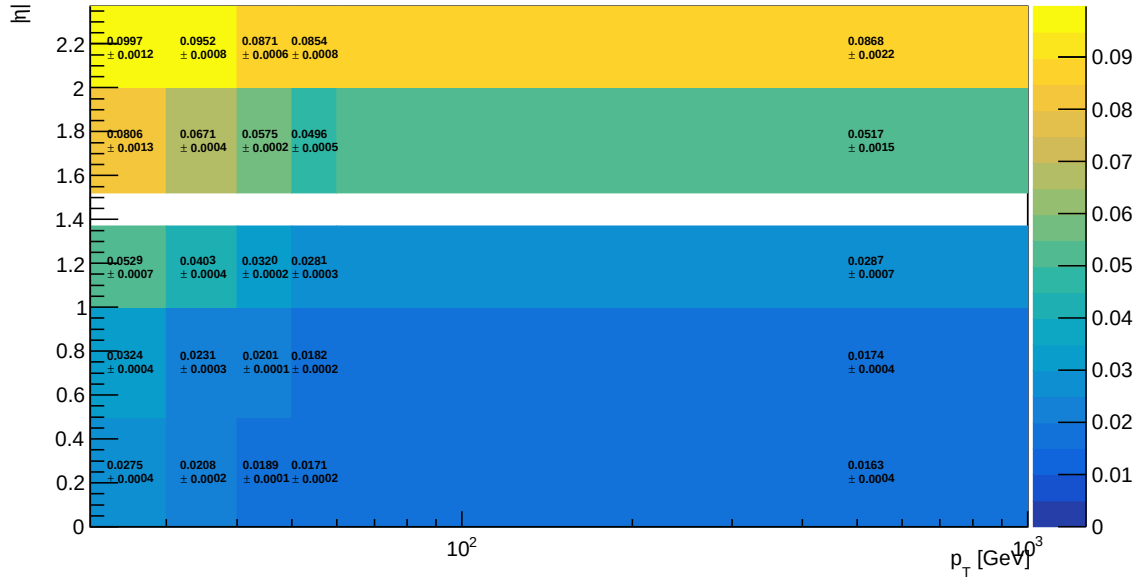


Figure A-1 Signal and background fits for each probe electron $|\eta|$ and p_T bin in CReg.^[94]

Figure A-2 Signal and background fits for each probe electron $|\eta|$ and p_T bin in CRee.^[94]Figure A-3 Nominal electron to photon fake rate in 2D, including statistical uncertainty.^[94]

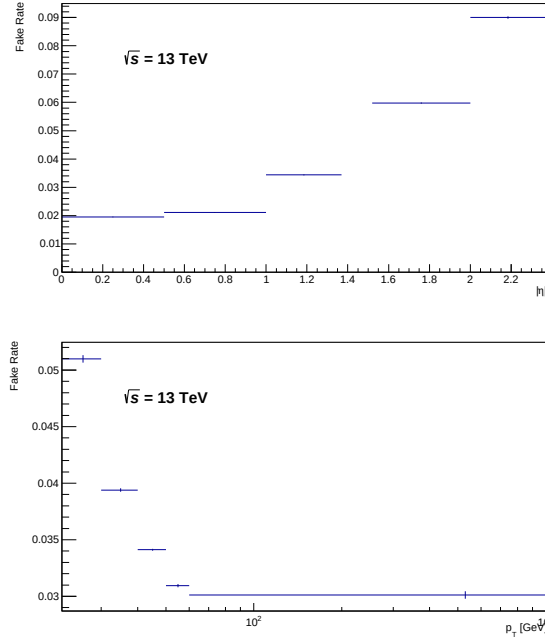


Figure A-4 Nominal electron to photon fake rate in p_T and η , including statistical uncertainty.^[94]

A.7 Signal Extraction

Uncertainties in signal extraction procedure are described in the following sequence:

A.7.1 Bias and Fit Stability Checks

To ensure the fitting framework's stability and unbiased nature, various checks were performed. These checks are crucial for confirming that the framework behaves consistently under diverse conditions and is free from systematic biases.

A.7.2 Fit Instabilities and the Choice of $f(x)$

During the analysis, it was observed that defining $f(x)$ as a linear function sometimes caused significant fluctuations in the extracted EW yield, particularly noticeable in the last bin of m_{jj} . This was attributed to small statistical variations in the pre-fit QCD- $W\gamma jj$ templates or the Asimov dataset.

To investigate these instabilities, the shift in the extracted EW yield for each toy simulation

was analyzed:

$$\Delta N_{EW}^i = \frac{N_{EW}^{Nominal} - N_{EW}^i}{N_{EW}^{Nominal}}, \quad (A-8)$$

where N_{EW}^i corresponds to the yield when the QCD- $W\gamma jj$ template or Asimov dataset is perturbed. These variations are visualized in Figure A-5, depicting a 2D histogram of 1000 toys. The x-axis represents the shift in the QCD- $W\gamma jj$ template from nominal, and the y-axis shows the corresponding shift in the extracted EW yield.

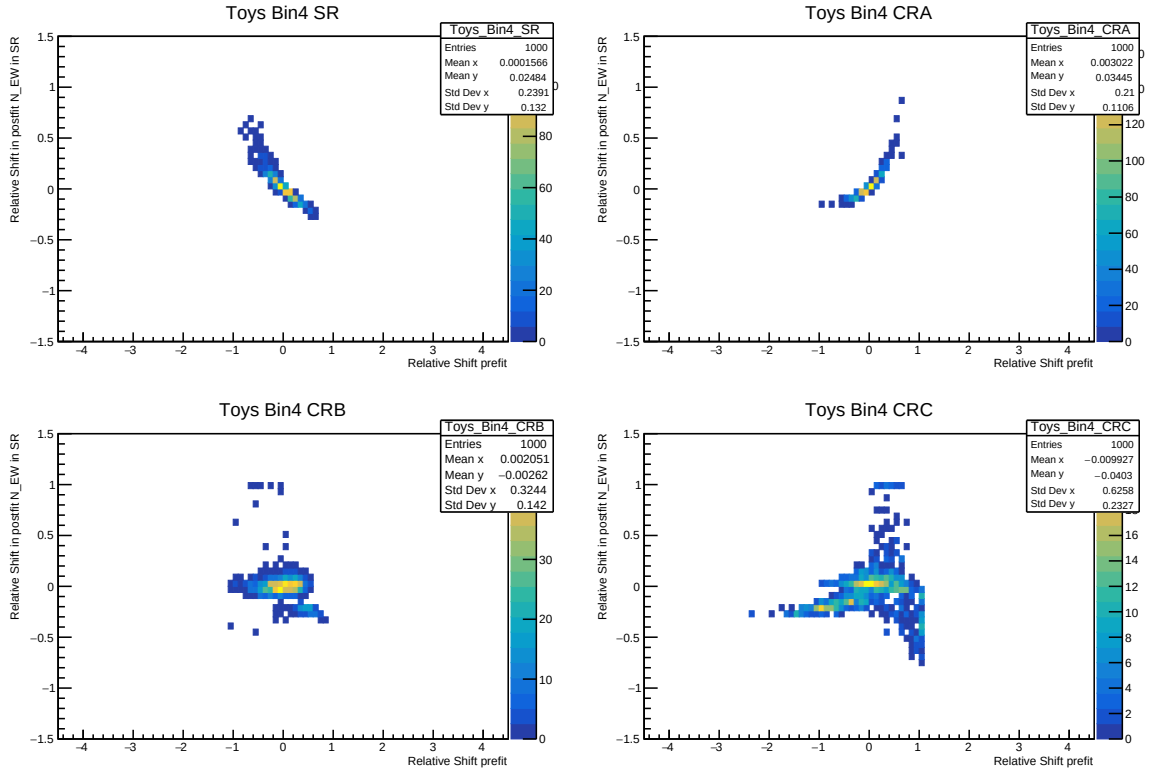


Figure A-5 The relative shift in the extracted electroweak yield in the last bin of m_{jj} , showing the impact of small fluctuations in the QCD template on the fit outcome. The largest variances are observed in this bin when using a linear definition for $f(x)$. The Asimov dataset is constructed using the Madgraph5 QCD- $W\gamma jj$ template to highlight these instabilities. [94]

The observed instability is partly due to poor MC statistics in the critical bins of the QCD- $W\gamma jj$ distribution, where even a minimal shift can lead to substantial variations in the EW yield. Notably, in the CRC, a likely shift in the QCD prediction by just a few events can result in an average deviation of approximately 25% in the extracted yield. This effect underscores the inadequacy of using a linear $f(x)$ in situations with sparse data, leading to

exaggerated fluctuations in the model output.

A more stable behavior is observed when $f(x)$ is defined as a constant. Figure A–6 demonstrates this stability by comparing the effects of statistical fluctuations on the extracted yield when $f(x)$ is constant.

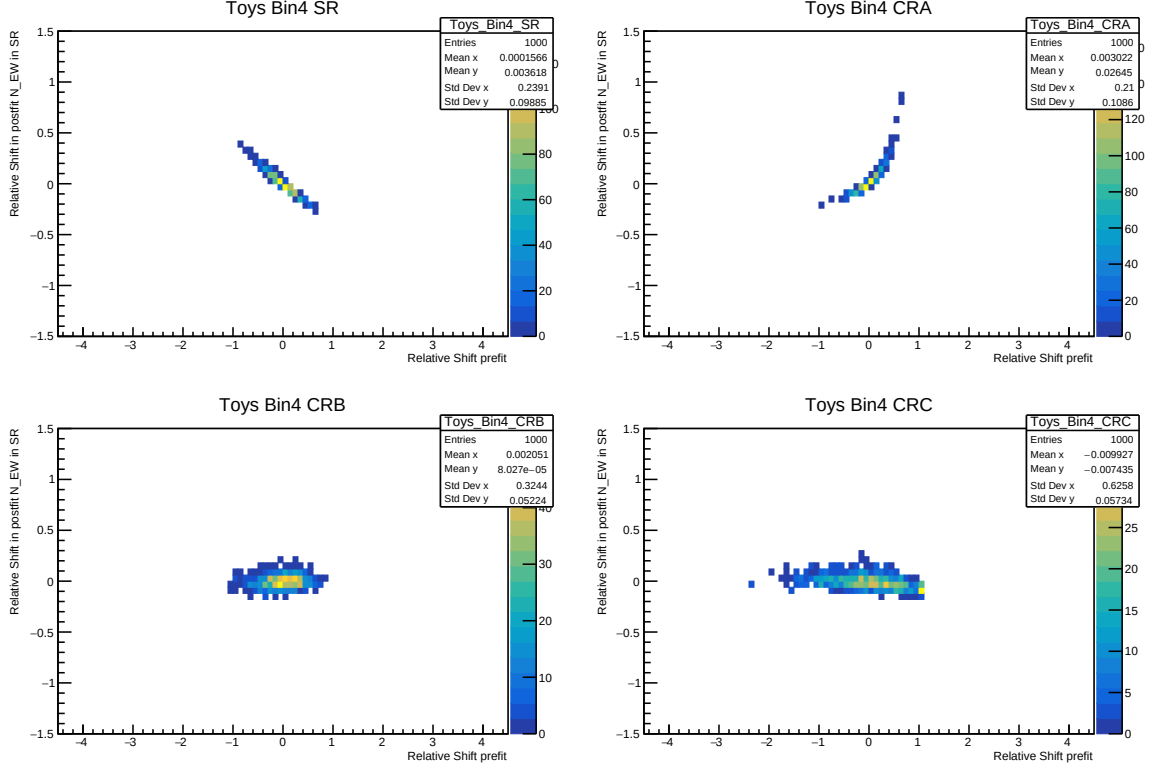


Figure A–6 Analysis of relative yield variations in the fourth bin of m_{jj} using a constant $f(x)$. The adjustment to a constant function significantly reduces the impact of poor QCD statistics on the stability of the fit. ^[94]

This analysis suggests that using a constant value for $f(x)$ not only stabilizes the fitting process but also improves the statistical precision of the extracted yield by reducing the influence of fluctuations in data-sparse regions. This adjustment is essential for maintaining the robustness of the fit across all bins, especially when dealing with limited data points in the background-dominated bins.

A.7.3 Statistical uncertainties in the data

To determine the statistical uncertainty in the data, 10000 toy distributions are created from the Asimov sample, where for each toy, the bin contents are sampled from a Poisson

distribution of mean equal to the original bin contents. The RMS of the resulting yields divided by the mean of the data toys is taken as the relative uncertainty in the data, R^{stat} . The relative uncertainty is multiplied by the central value for the extracted EW yield (see equation 4–29 for the definition of the central value) to get the final absolute uncertainty due to data.

The integrated extracted EW yields, and data statistical uncertainties for m_{jj} , $p_{T,jj}$ and $\Delta\phi_{jj}^{\text{signed}}$ are 231.9 ± 39.6 , 232.1 ± 34.3 , 236.9 ± 27.8 respectively, whereas the input signal template has an integrated yield in the SR of 236.90. Note that it is difficult for the total absolute statistical uncertainties to be directly compared between observables because the statistical resolution of the extracted yield in a given bin is dependent on every other bin due to the correlations induced between bins by $f(x)$. Additionally, the statistical precision of the $\Delta\phi_{jj}^{\text{signed}}$ extracted yield is expected to be better than the other observables due to the fact that the bin-dependent factors b_L are shared between symmetric bins.

$$R^{\text{stat}} = \frac{\text{RMS}_{\text{Data}}(N_{\text{EW, Sherpa}, i})}{\langle N_{\text{EW, Sherpa}, i} \rangle_{\text{Data}}} \quad (\text{A-9})$$

A.7.4 MC statistical uncertainties

The MC stat uncertainty is evaluated by creating 10000 *bootstraps* of all the MC templates in the SR and in all CRs. A bootstrap is a replica fluctuated according to a unit Poisson distribution in such a way as to keep track of correlations.

The signal extraction is performed separately for each bootstrap. After extracting the signal, the relative MC stat uncertainty is given by

$$R_{\text{MC Stats}}^{\text{syst}} = \frac{\text{RMS}_{\text{MC}}(N_{\text{EW, Sherpa}, i})}{N_{\text{EW, Nominal}}} \quad (\text{A-10})$$

where RMS_{QCD} represents the RMS over all the bootstraps where the QCD- $W\gamma jj$ templates were varied.

A.7.5 Experimental systematic uncertainties

A complete list of experimental uncertainties is given here:

- JES uncertainties coming from:
 - The `EffectiveNP` nuisance parameters which capture the uncertainties from the absolute in-situ calibrations (γ/Z +jet and multi-jet balance).

- Other JES uncertainties coming from the eta-intercalibration, pileup, flavour-related, and punch-through uncertainty sources.
- JER uncertainties coming from:
 - The `EffectiveNP` nuisance parameters which capture uncertainties from the noise term and di-jet in-situ sources.
 - Differences between the MC and data JER.
- Muon and Electron/ γ energy scale and resolution sources.
- PRW and MET systematic uncertainties

The *bootstrapping* method is crucial for assessing the final systematic uncertainties on the extracted electroweak (EW) yields. This technique distinctly separates the contributions of statistical and systematic factors. For instance, consider a scenario where one set of Monte Carlo (MC) events uses the Jet Energy Scale (JES) at its nominal value, while another set operates with a slightly adjusted JES. Despite this alteration, the events remain completely correlated, differing only in the scaling applied to jet energies and p_T .

This correlation highlights a critical point: the standard error propagation methods, which presume uncorrelated uncertainties, are not applicable here. Instead, the *bootstrapping* method is employed, generating $N_{\text{bootstraps}}$ pseudo-experiments for both the nominal scenario and each systematic variation. In this process, each MC event weight is multiplied by a random number drawn from a unit Poisson distribution, ensuring the preservation of correlations between the nominal and systematic experiments. This is achieved by using the same random number seed for sampling the Poisson distribution across corresponding events in both setups. Without maintaining these correlations, the variance between nominal and systematic results would be inflated by statistical noise, significantly skewing the perceived statistical uncertainty. A total of $N_{\text{bootstraps}} = 10000$ is deemed sufficient for robust analysis in this context.

The significance of statistical uncertainties on systematic errors cannot be understated, as they provide insight into the statistical significance of observed systematic variations—essentially determining whether differences between nominal and varied templates are statistically driven. To manage this, a significance threshold, σ_{thresh} , is established. Systematic uncertainties exceeding this threshold relative to their statistical uncertainty are considered statistically significant. The analysis tests three threshold levels—1.6, 1.0, and 0—to decide the inclusion level of systematic uncertainties, opting to retain all identified uncertainties

regardless of their individual statistical significance due to their minimal overall impact.

Primary sources of experimental uncertainties include Jet Energy Resolution (JER) and JES. Systematic variations are evaluated using 1000 bootstraps¹ for the nominal and each experimental systematic condition. Each experimental nuisance parameter, such as “JER_EffectiveNP__1up,” affects the QCD- $W\gamma jj$, EW- $W\gamma jj$, and prompt background yields consistently across samples, illustrating the correlated nature of these experimental uncertainties. The systematic uncertainty for any variation is quantified by averaging the deviations from the nominal across all bootstraps and normalizing this by the mean of the nominal bootstraps. The relative experimental uncertainty on the central EW yield value is denoted as $R_{\text{exp}}^{\text{sys}}$, with $N_{\text{EW},i}^{\text{exp}}$ representing the extracted EW yield for a given systematic variation during bootstrap i , and $N_{\text{EW},i}^{\text{Nom}}$ for the nominal scenario.

$$R_{\text{exp}}^{\text{sys}} = \frac{\langle N_{\text{EW},i}^{\text{Nom}} - N_{\text{EW},i}^{\text{exp}} \rangle}{\langle N_{\text{EW},i}^{\text{Nom}} \rangle}, \quad \Delta R_{\text{exp}}^{\text{sys}} = \frac{\text{RMS}(N_{\text{EW},i}^{\text{Nom}} - N_{\text{EW},i}^{\text{exp}})}{\langle N_{\text{EW},i}^{\text{Nom}} \rangle}. \quad (\text{A-11})$$

The statistical uncertainties on $R_{\text{exp}}^{\text{sys}}$, denoted as $\Delta R_{\text{exp}}^{\text{sys}}$, are calculated by subtracting each systematic bootstrap from the nominal bootstrap and computing the RMS of the resulting distributions. The systematic uncertainties are then refined through a Linear Gaussian Kernel smoothing algorithm. This algorithm begins by dividing the x-axis range into 100 discrete points. A linear interpolation is performed through all permutations of pairs of coordinates from the histogram bin values. Each line is evaluated at x , producing y_i , with the error on y_i , ϵ_i , determined by propagating the errors of the histogram bins. A weight, calculated as the product of $1/\epsilon_i^2$ and two Gaussian kernels with adjustable widths centered on each x-axis value of the coordinate pair, is then assigned to each y_i . The weighted average of all y_i values yields the final smoothed value at x . The Gaussian kernel width begins at 0.5 and is incrementally adjusted until the smoothed values achieve statistical significance at a maximum level of 1σ , as verified by a chi-squared test. The resultant smoothed graph, which includes 100 coordinate values, is reassessed at the original histogram bin centers to produce the finalized smoothed histogram.

For uncertainties not subjected to bootstrapping, such as those related to fakes estimates (excluding the photon-ID uncertainties from jets faking photons) and non- $W\gamma$ samples, the

¹ Computational constraints limit the number of bootstraps to 1000 for most uncertainties, except for generator choice variations.

Root TH1::Smooth(3) function is utilized. This function performs three iterations of the “353QH, twice” algorithm, as detailed in the 1974 Cern School of Computing proceedings^[180]. This running median smoothing algorithm combines a series of operations as indicated by its nomenclature, where the integers represent window sizes, “Q” stands for quadratic interpolation, “H” indicates the use of the Hann function, and “twice” implies that the sequence is processed twice.

A.7.6 Data-driven Background Uncertainties

Uncertainties in the data-driven background estimates, as detailed in Section 4.4, are incorporated into the extracted EW yield by adjusting the data-driven background template within the fit according to these uncertainties. Statistical uncertainties for these templates are treated similarly to MC statistical uncertainties in the likelihood, i.e., they are included in the formulation of the Poisson constraints. Furthermore, statistical variations are explicitly considered as up and down shifts when adjusting the templates. Notably, no bootstrapping is conducted for uncertainties on data-driven backgrounds, nor is smoothing applied to the final uncertainties on the extracted EW yield, to prevent potential oversmoothing given the absence of bootstrapping to assess their statistical significance.

A.7.7 Generator Choice

The uncertainty due to the choice of QCD- $W\gamma jj$ generator, denoted as $R_{\text{Gen Choice}}^{\text{sys}}$, is quantified before any smoothing by extracting the EW yield in the SR using different QCD- $W\gamma jj$ templates across 10000 bootstraps. The difference in the yield is computed for each pair of bootstraps, and the average difference is calculated. This average is then normalized by the central value to determine the relative uncertainty:

$$R_{\text{Gen Choice}}^{\text{sys}} = \frac{\langle N_{\text{EW},i}^{\text{Nom, Sherpa}} - N_{\text{EW},i}^{\text{Nom, MG5}} \rangle}{\langle N_{\text{EW},i}^{\text{Nom, Sherpa}} \rangle}, \quad \Delta R_{\text{Gen Choice}}^{\text{sys}} = \frac{\text{RMS}(N_{\text{EW},i}^{\text{Nom, Sherpa}} - N_{\text{EW},i}^{\text{Nom, MG5}})}{\langle N_{\text{EW},i}^{\text{Nom, Sherpa}} \rangle} \quad (\text{A-12})$$

Here, the index i spans all bootstraps, with Sherpa and Madgraph bootstraps being uncorrelated. The statistical uncertainty on $R_{\text{Gen Choice}}^{\text{sys}}$, indicated by $\Delta R_{\text{Gen Choice}}^{\text{sys}}$, is calculated by taking the RMS of the differences for each bootstrap pair. This approach underscores the significant error bars and the limited statistical precision of the Madgraph5 QCD- $W\gamma jj$

sample, as depicted in Figure A–7.

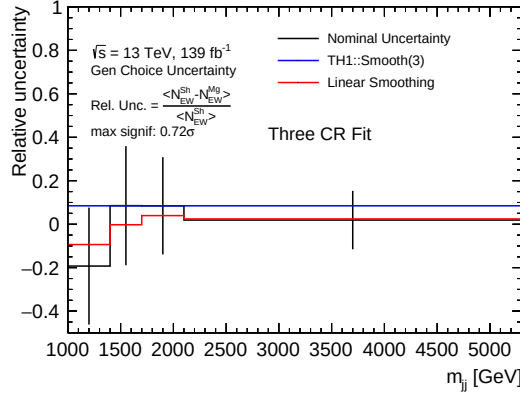


Figure A–7 Illustration of QCD generator choice uncertainties for m_{jj} before and after smoothing. The substantial error bars highlight the limited statistical resolution of the generator choice uncertainty.^[94]

A.7.8 Other theoretical uncertainties

The theoretical uncertainties evaluated include scale, PDF, and α_s uncertainties. These are considered for QCD $Z\gamma$, EWK $W\gamma jj$, and QCD $W\gamma jj$ backgrounds. Uncertainties on fakes estimates, interference effects between QCD- $W\gamma jj$ and EW- $W\gamma jj$, and MC statistical uncertainties are also assessed.

To assess scale uncertainties, the signal is extracted using nominal templates across 1000 bootstraps, as well as templates that reflect systematic variations in scale for the EW and QCD $W\gamma jj$ backgrounds. The nominal systematic uncertainty for each combination of factorization scale (μ_F) and renormalization scale (μ_R) is computed as follows:

$$R_{(\mu_F, \mu_R)}^{\text{sys}} = \frac{\langle N_{\text{EW},i}^{\text{Nom}} - N_{\text{EW},i}^{(\mu_F, \mu_R)} \rangle}{\langle N_{\text{EW},i}^{\text{Nom}} \rangle}. \quad (\text{A-13})$$

Following this, systematic uncertainties are smoothed post-fitting each bootstrap.

PDF uncertainties are addressed by extracting the signal across 100 different PDF variations for each sample and calculating the RMS of the extracted yields per bin to derive the final uncertainty due to PDF choice. PDF uncertainties for non- $W\gamma$ backgrounds are negligible and thus not presented. The α_s uncertainties are quantified by averaging the differences between yields from upper and lower variations, and all other systematic uncertainties with bidirectional variations are symmetrized similarly.

The interference between QCD- $W\gamma jj$ and EW- $W\gamma jj$ is quantified by comparing the extracted N_{EW} using an Asimov dataset, which includes the interference, to the nominal $N_{EW, \text{Nominal}}$, which excludes the interference effect.

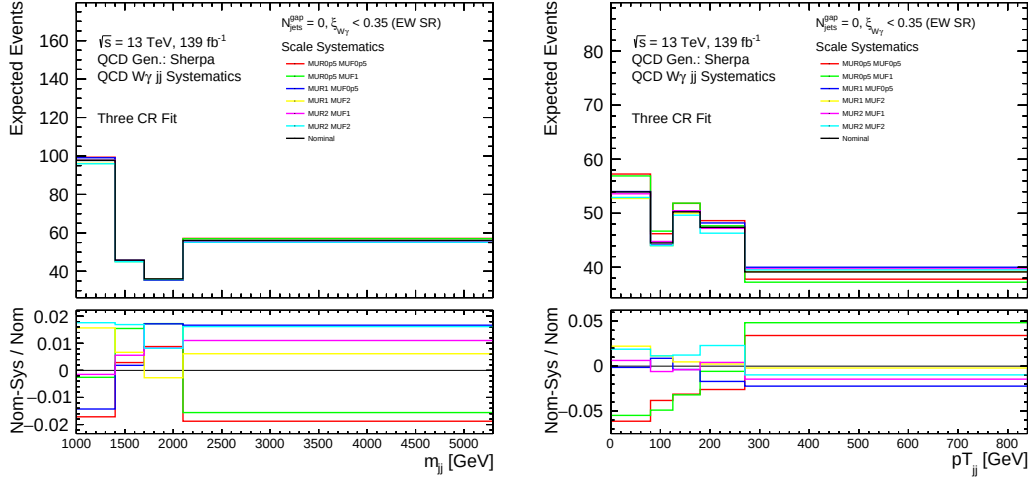


Figure A-8 Final smoothed scale uncertainties for the 3CR observables as derived from QCD scale variations for m_{jj} and $p_{T,jj}$.^[94]

When unfolding detector effects from these systematic uncertainties, individual scale and PDF variations are unfolded separately, rather than using an envelope or RMS approach prior to unfolding.

Table A-5 presents all final extracted yields and uncertainties using the nominal method, alongside a CRC method cross-check.

A.8 Unfolding

A.8.1 Technical closure test

The technical closure test is critical for verifying that the unfolding framework performs as expected. This test uses a distribution from electroweak (EW) signal MC samples as inputs to the unfolding process, rather than actual data collected from detectors. The effectiveness of this approach is assessed by comparing the unfolded distribution to the truth-level MC distribution. If the reconstructed distribution is sourced directly from the same signal prediction, the unfolding procedure should ideally reproduce the exact truth-level distribution.

Results of the technical closure test could be found in Figure A-9. For this test, the

Var	CRA or CRC	Bin	Yield	Data Stat	Exp Syst	Theory Syst	Total Syst
m_{jj}	CRA	1	96.03	34.48%	8.74%	20.66%	22.44%
m_{jj}	CRA	2	45.6	32.48%	9.3%	15.97%	18.48%
m_{jj}	CRA	3	35.77	29.39%	9.2%	13.68%	16.49%
m_{jj}	CRA	4	56.19	20.03%	3.81%	10.99%	11.63%
pT_{jj}	CRA	1	53.7	28.28%	12.62%	16.99%	21.17%
pT_{jj}	CRA	2	44.52	31.94%	7.56%	17.16%	18.75%
pT_{jj}	CRA	3	50.1	32.93%	8.36%	13.72%	16.06%
pT_{jj}	CRA	4	47.01	32.44%	5.47%	11.45%	12.69%
pT_{jj}	CRA	5	38.79	37.29%	7.35%	27.97%	28.92%
$\Delta\phi_{jj}^{signed}$	CRA	1	35.78	30.07%	8.13%	17.46%	19.26%
$\Delta\phi_{jj}^{signed}$	CRA	2	22.71	34.84%	7.65%	15.21%	17.03%
$\Delta\phi_{jj}^{signed}$	CRA	3	59.21	29.99%	6.64%	14.34%	15.81%
$\Delta\phi_{jj}^{signed}$	CRA	4	59.1	30.12%	6.64%	14.34%	15.81%
$\Delta\phi_{jj}^{signed}$	CRA	5	22.63	35.22%	7.65%	15.21%	17.03%
$\Delta\phi_{jj}^{signed}$	CRA	6	36.15	29.23%	8.13%	17.34%	19.15%
pT_l	CRA	1	49.12	33.95%	8.12%	19.26%	20.9%
pT_l	CRA	2	51.67	29.88%	7.61%	16.65%	18.31%
pT_l	CRA	3	47.04	32.46%	8.63%	13.57%	16.08%
pT_l	CRA	4	44.29	31.45%	9.63%	12.34%	15.65%
pT_l	CRA	5	41.75	34.51%	5.38%	22.62%	23.26%
$\Delta\phi_{l\gamma}^{signed}$	CRA	1	23.18	39.35%	7.87%	15.19%	17.11%
$\Delta\phi_{l\gamma}^{signed}$	CRA	2	20.73	36.83%	6.99%	11.49%	13.45%
$\Delta\phi_{l\gamma}^{signed}$	CRA	3	29.83	36.06%	7.08%	15.04%	16.62%
$\Delta\phi_{l\gamma}^{signed}$	CRA	4	43.78	32.04%	6.63%	13.82%	15.33%
$\Delta\phi_{l\gamma}^{signed}$	CRA	5	43.9	31.84%	6.63%	13.82%	15.33%
$\Delta\phi_{l\gamma}^{signed}$	CRA	6	29.97	35.92%	7.08%	15.04%	16.62%
$\Delta\phi_{l\gamma}^{signed}$	CRA	7	20.71	36.69%	6.99%	11.49%	13.45%
$\Delta\phi_{l\gamma}^{signed}$	CRA	8	23.4	38.82%	7.87%	14.98%	16.92%
ly_m	CRA	1	96.6	29.84%	8.6%	18.6%	20.49%
ly_m	CRA	2	51.73	29.55%	6.81%	13.85%	15.43%
ly_m	CRA	3	34.54	33.05%	5.52%	15.08%	16.06%
ly_m	CRA	4	27.05	32.81%	5.14%	14.48%	15.37%
ly_m	CRA	5	24.25	37.97%	7.08%	12.72%	14.56%

Table A–5 Extracted EW $W\gamma jj$ event counts using the CRA fitting approach, detailing both statistical and systematic uncertainties. MC statistical uncertainties are encompassed within the theoretical uncertainty calculations.

Var	CRA or CRC	Bin	Yield	Data Stat	Exp Syst	Theory Syst	Total Syst
m_{jj}	CRA	1	124.95	34.55%	7.77%	15.47%	17.31%
m_{jj}	CRA	2	77.92	21.21%	7.41%	11.98%	14.09%
m_{jj}	CRA	3	37.99	31.9%	7.86%	16.86%	18.6%
m_{jj}	CRA	4	80.75	16.33%	2.89%	9.95%	10.36%
pT_{jj}	CRA	1	73.84	25.79%	11.55%	16.27%	19.95%
pT_{jj}	CRA	2	73.28	24.69%	7.39%	15.43%	17.11%
pT_{jj}	CRA	3	74.21	27.42%	8.04%	12.48%	14.85%
pT_{jj}	CRA	4	52.58	35.15%	6.46%	13.38%	14.86%
pT_{jj}	CRA	5	37.99	40.64%	8.35%	22.15%	23.68%
$\Delta\phi_{jj}^{signed}$	CRA	1	49.32	27.97%	7.68%	15.48%	17.29%
$\Delta\phi_{jj}^{signed}$	CRA	2	20.24	42.46%	7.31%	15.79%	17.4%
$\Delta\phi_{jj}^{signed}$	CRA	3	96.01	24.18%	6.15%	11.03%	12.63%
$\Delta\phi_{jj}^{signed}$	CRA	4	72.69	31.92%	6.9%	13.45%	15.12%
$\Delta\phi_{jj}^{signed}$	CRA	5	23.78	35.79%	8.19%	14.56%	16.7%
$\Delta\phi_{jj}^{signed}$	CRA	6	43.91	30.78%	8.61%	17.82%	19.79%
pT_l	CRA	1	70.04	32.14%	8.72%	18.05%	20.05%
pT_l	CRA	2	59.72	31.41%	9.14%	17.97%	20.16%
pT_l	CRA	3	58.55	35.75%	10.12%	15.47%	18.48%
pT_l	CRA	4	57.13	30.15%	10.25%	13.59%	17.02%
pT_l	CRA	5	53.52	30.95%	5.67%	17.54%	18.43%
$\Delta\phi_{l\gamma}^{signed}$	CRA	1	35.21	32.76%	6.08%	15.4%	16.56%
$\Delta\phi_{l\gamma}^{signed}$	CRA	2	37.06	26.29%	5.9%	11.93%	13.31%
$\Delta\phi_{l\gamma}^{signed}$	CRA	3	36.54	37.95%	7.19%	21.45%	22.62%
$\Delta\phi_{l\gamma}^{signed}$	CRA	4	68.79	26.55%	8.35%	18.3%	20.11%
$\Delta\phi_{l\gamma}^{signed}$	CRA	5	35.27	47.66%	8.87%	26.23%	27.69%
$\Delta\phi_{l\gamma}^{signed}$	CRA	6	30.31	44.85%	8.56%	25.99%	27.37%
$\Delta\phi_{l\gamma}^{signed}$	CRA	7	29.25	31.41%	7.3%	15.03%	16.71%
$\Delta\phi_{l\gamma}^{signed}$	CRA	8	29.73	37.76%	7.57%	18.21%	19.72%
ly_m	CRA	1	119.11	32.08%	9.0%	23.42%	25.09%
ly_m	CRA	2	57.71	36.72%	7.33%	21.97%	23.16%
ly_m	CRA	3	39.88	34.94%	6.03%	18.62%	19.57%
ly_m	CRA	4	40.74	28.73%	5.75%	17.88%	18.78%
ly_m	CRA	5	29.47	40.83%	9.68%	20.12%	22.33%

Table A–6 Total number of extracted EW $W\gamma jj$ events using the CRA fit method, along with their statistical and systematic uncertainties. MC statistical uncertainties are incorporated within the theoretical uncertainties.

reconstructed distribution from SHERPA + PYTHIA8 EW MC samples is unfolded using MC-based inputs, allowing for a direct evaluation of the unfolding framework's accuracy and reliability.

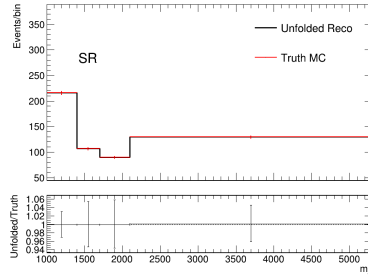


Figure A–9 Technical closure test for m_{jj} in the electron and muon combined channel after SR selections. The reconstructed distribution from SHERPA + PYTHIA8 electroweak MC samples is unfolded with MC-based response matrices. The unfolded distribution (in black) perfectly matches the signal distribution at truth-level (in red). The lower pad is showing ratios of unfolded distribution to the truth-level distribution.^[94]

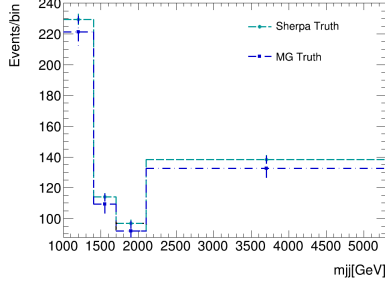
A.8.2 Hidden variable test

This closure test, referred to as the hidden variables test, focuses on the effects in MC shapes that are not accounted for in the detector simulation uncertainties. It involves assessing the unfolding results using an alternative MadGraph sample. This test also acts as a verification of generator choice uncertainties, where the Asimov extracted yields from MadGraph are unfolded using a MadGraph-specific unfolding matrix.

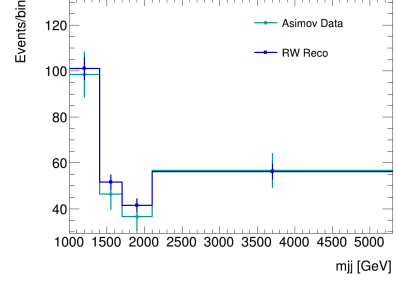
Prior to unfolding, the MadGraph sample is re-weighted to ensure that the shapes of the observables at the truth level are consistent between the two MC samples. The unfolding matrix, constructed from the MadGraph signal sample, is adjusted row by row using factors calculated by dividing the truth-level Sherpa signal distribution by the truth-level MadGraph signal distribution. This adjustment ensures that the truth distributions from the MadGraph and Sherpa unfolding matrices matches each other at the same level.

The reweighted truth-level distributions are depicted in Figure A–10. The reweighted reconstruction-level distributions are also presented in Figure A–10. Subsequently, the Asimov extracted signal yield is unfolded using both the reweighted MadGraph matrix and the nominal Sherpa matrix. The results of these unfoldings are illustrated in Figure A–10. The

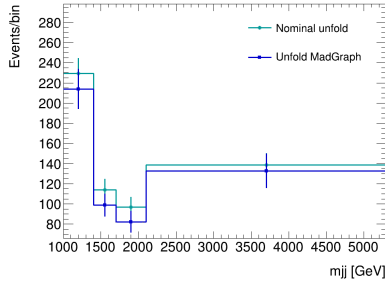
relative differences between these two unfolded distributions are quantified and included as an uncertainty in the final unfolded results, which are shown in the same figure.



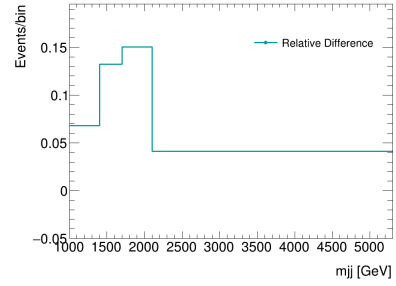
(a) Truth level distribution of both Madgraph and Sherpa.



(b) Reweighted MadGraph distribution at reco level.



(c) Unfolded distribution with reweighted MadGraph response.



(d) Relative difference between reweighted distribution and nominal unfolded distribution.

Figure A–10 Distributions of m_{jj} : (a) Truth level distribution of both Madgraph and Sherpa, (b) Reweighted MadGraph distribution at reco level, (c) Unfolded distribution with reweighted MadGraph response, and (d) Relative difference between reweighted distribution and nominal unfolded distribution.^[94]

A.8.3 Data-driven closure test

An essential aspect of verifying the integrity of the unfolding procedure is the implementation of a data-driven closure test. This test is only applicable post-unblinding and serves to cross-check against biases, ensuring that uncertainties are not double-counted.

The process involves reweighting the electroweak (EW) $W\gamma$ MC distribution to enhance agreement between the reconstructed distribution and the observed data. The reweighted distribution is then unfolded using the original MC inputs. Systematic uncertainty is quantified by comparing the reweighted truth-level distribution with the distribution obtained post-unfolding. The discrepancy between these distributions indicates any potential bias inherent in the unfolding procedure itself.

Reweightings is achieved by adjusting each column of the response matrix with a specific weight. This weight is derived by dividing the data by the original reconstructed distribution from the EW $W\gamma$ MC sample. As a result, the reweighted reconstruction-level distribution aligns precisely with the reconstructed data distribution. This reweighted distribution is subsequently unfolded using the nominal response matrix. The difference observed is interpreted as the bias from the unfolding process and is included as one of the systematic uncertainties.

The weights for this process are calculated by dividing the distribution of the extracted EW $W\gamma$ process from the data by the original MC-based reconstructed distribution. This ratio is then used as the weighting factor for the reweighting process. The weighting factors are illustrated in Figure A–11.

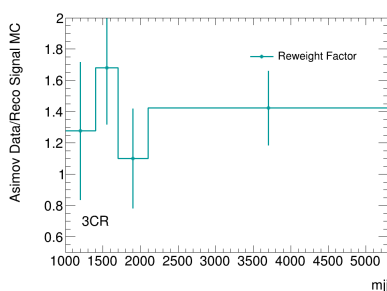


Figure A–11 Weights for the data-driven closure test which is calculated from data divided by the reconstruct MC-based EW $W\gamma$ distribution for m_{jj} after the SR selection.^[94]

The data-driven closure test involves comparing the reweighted truth-level distribution against the unfolded reweighted distribution. These distributions are presented in Figure A–

12. The unfolded distribution, which results from the unfolding of the reweighted reconstructed distribution, is evaluated against the reweighted truth-level distribution to assess the accuracy of the unfolding process.

Further, the relative uncertainties derived from this comparison are depicted in Figure A–13. These uncertainties demonstrate that the unfolding process introduces minimal bias into this term. This result confirms the reliability of the unfolding method and is subsequently incorporated as one of the systematic uncertainties in the final unfolded distribution.

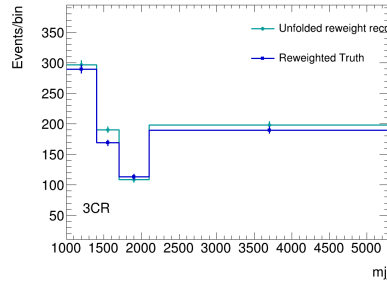


Figure A–12 Distribution of unfolded reweighted reco-level distribution and reweighted truth-level distribution for m_{jj} after the SR selection.^[94]

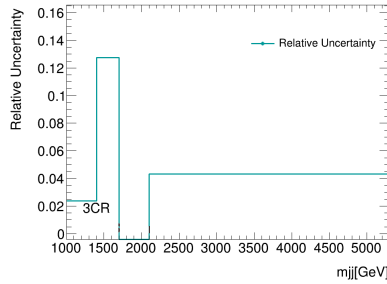


Figure A–13 Relative uncertainty of unfolded reweighted reco-level distribution and reweighted truth-level distribution for m_{jj} after the SR selection. The uncertainty is included in results as systematic uncertainty.^[94]

A.9 Systematic uncertainties

A.10 Smoothing

Large uncertainties could result in unreliable physics outcomes. And the statistics is not always sufficient to fully cover the uncertainty. To address this issue, a smoothing technique

is applied in this analysis to avoid this large effect issue. The algorithm follows:

1. A threshold δM is defined from the statistical uncertainty on the systematic variation and the statistical uncertainty on the nominal sample.
2. For each bin i and its neighbor $i - 1$, calculate

$$x_{i-1,i} = \left| \frac{S_i - N_i}{N_i} - \frac{S_{i-1} - N_{i-1}}{N_{i-1}} \right| \quad (\text{A-14})$$

and the relative statistical uncertainty

$$\delta x_{i-1,i} = \sqrt{\frac{\delta M_i^2}{N_i^2} + \frac{\delta M_{i-1}^2}{N_{i-1}^2}} \quad (\text{A-15})$$

where S_i and N_i are the number of events in bin i in the variation and the nominal sample, respectively.

3. If $x_{i-1,i} < \delta x_{i-1,i}$ for at least one bin then neighboring bins $b - 1$ and b with the highest ratio $\frac{\delta x_{b-1,b}}{x_{b-1,b}}$ are merged.
4. This is done until no bin satisfies $x_{i-1,i} < \delta x_{i-1,i}$.
5. The TH1 Smooth algorithm described in^[181] is applied.

For correlated sources of events $\delta M = \max(\delta S, \delta N)$ while for uncorrelated sources of events $\delta M = \sqrt{\delta S^2 + \delta N^2}$ where δS and δN are the statistical uncertainty on the systematic variation and the nominal sample, respectively. TRExFitter offers this technique if one uses it with the option of *Smoothing* : 40 for correlated systematics and *Smoothing* : 400 for uncorrelated systematics.

A.11 Theoretical uncertainties

All of the MC samples used in this analysis for background and signal processes should be corrected for the theoretical uncertainties. Uncertainties from missing higher order terms of the interaction cross section calculation is one of the sources. And the other one is coming from the underlying PDFs used in the MC samples. An uncertainty on the value of strong coupling constant α_s is included as for samples at NLO (i.e. QCD $W\gamma jj$ and QCD $Z\gamma jj$). In order to cross check the process, another QCD sample generated with MadGraph is also used for the analysis.

A.12 Scale Uncertainties

The estimation of the missing higher orders in the perturbative expansion of the partonic cross section is carried out through scale variations. These variations involve adjusting the renormalization and factorization scales by a factor of two, which serves as an approximation for the higher order terms in the cross section calculation. For each Monte Carlo simulation, six scale combinations are evaluated: $(\mu_F, \mu_R) = (0.5, 0.5), (0.5, 1.0), (1.0, 0.5), (1.0, 2.0), (2.0, 1.0), (2.0, 2.0)$. Following the PMG guidelines, variations where $(\mu_F, \mu_R) = (0.5, 2.0)$ or $(2.0, 0.5)$ are excluded. The range of these scale variations provides the upper and lower bounds used as systematic uncertainties, following PMG protocols. The PMGSystematicsTool is employed to integrate these variations. In the context of Sherpa 2.2.11 samples, specifically QCD $W\gamma jj$ and QCD $Z\gamma jj$, scale variations also extend to the parton shower calculations, aligning the scale changes in the parton shower with those in the matrix element, in accordance with the recommendations in^[182].

A.13 PDF and α_S uncertainties

Uncertainties associated with the parton distribution functions (PDFs) used in Monte Carlo simulations arise from experimental uncertainties in the datasets employed for PDF fitting and from the uncertainty in the functional forms of these fits. To estimate the impact of these uncertainties, the PDFs are varied, with NNPDF3.0 serving as the standard set for all samples analyzed. These variations are aggregated following the protocols outlined in^[183] and^[184], utilizing the PMGSystematicsTool. Furthermore, alternative PDF sets (NNPDF3.1, CT14, MSHT, PDF4LHC) are evaluated against the nominal set, and any discrepancies not accounted for by the nominal PDF's uncertainties are addressed by assigning additional uncertainties.

For the QCD $W\gamma jj$ and QCD $Z\gamma jj$ samples, uncertainties related to the value of the strong coupling constant, α_S , are also considered. These affect the cross-section calculations integral to PDF fits, and are incorporated by employing the same PDF set calculated with two different α_S values. The resultant uncertainties are then merged with the PDF uncertainties using the PMG Systematics tool.

Additionally, theoretical systematic variations for the Sherpa signal samples, particularly

in the signal regions utilized in the neural network fit, are depicted in Figure A–14.

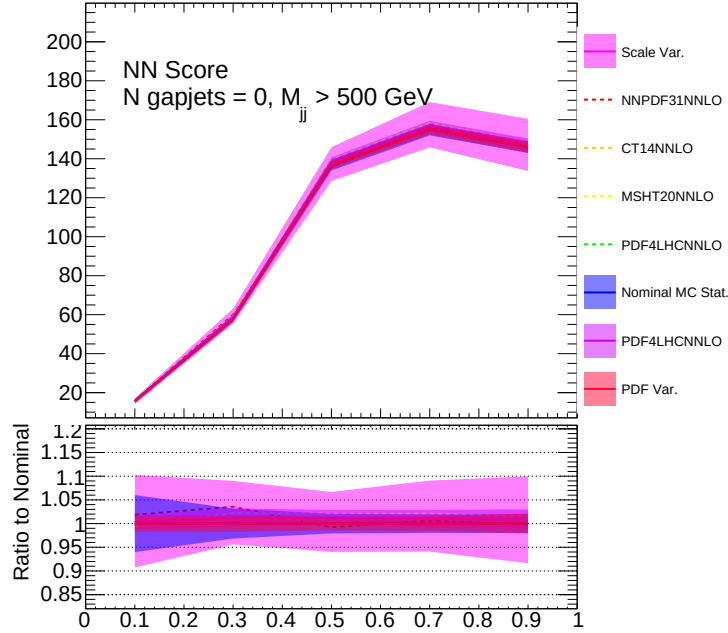


Figure A–14 Theory systematic variations, as combined by the PMGSystematicsTool.^[94]

Theory systematics are comprehensively applied across all Monte Carlo estimated backgrounds.

A.14 QCD generator choice uncertainty

The predicted distribution from Sherpa and MadGraph QCD samples are different and the difference is large. In order to account for QCD mismodelling, the difference between these two generators is taken into account as a systematic uncertainty. Shape difference and normalization difference are both taken care of with different nuisance parameters.

To eliminate the effect of double counting of jet experimental uncertainties, MC to MC calibrations are applied.

A.15 Electroweak generator choice uncertainty

Similarly, we use EW samples from MadGraph generator to account for the different signal predictions. Only shapes are treated as a source of systematic uncertainties.

A.16 Experimental uncertainties

Experimental uncertainties are calculated in accordance with the most recent recommendations from the CP group. For each experimental systematic uncertainty, the template used for Monte Carlo predictions is modified by $\pm 1\sigma$. The considerations include:

- Photons: ID and isolation efficiency scale factor uncertainties.
- Electrons: ID, isolation, reconstruction and trigger efficiency scale factor uncertainties.
- Egamma: Resolution and scale uncertainties.
- Muons: ID, Isolation, reconstruction, TTVA, trigger efficiency scale factor uncertainties.
- Jets: Energy scale and resolution, Eta calibration, flavor tagging efficiencies, precision flavor uncertainties, vertex tagging, btagging uncertainties.
- MET: MET soft track resolution and scale.
- PRW: Uncertainties scale factors used for pileup reweighting.
- Luminosity

A.17 Results

A.17.1 Expected Results

Figure A–7 is recoding event yields after the fit for each of the processes.

	Signal Region	Control Region
EWK $W\gamma jj$	514.84 ± 83.46	121.44 ± 28.11
EWK $Z\gamma jj$	11.64 ± 1.00	6.61 ± 0.76
QCD $W\gamma jj$	1628.76 ± 111.42	1974.24 ± 137.97
Top Bkg.	110.32 ± 18.52	188.22 ± 38.02
QCD $Z\gamma jj$	115.39 ± 33.77	144.43 ± 68.88
$j \rightarrow \gamma$	402.40 ± 47.02	408.42 ± 56.11
$e \rightarrow \gamma$	147.78 ± 5.59	172.19 ± 6.12
$j \rightarrow l$	115.57 ± 16.06	113.27 ± 9.85
pileup γ	0 ± 0	11.18 ± 0.16
Total	3046.71 ± 63.86	3140 ± 95.27
Data	X	3143

Table A–7 Yields after fit to asimov dataset in the signal region and data in the control region

The fitted norm factors are shown in table A–8. As expected, the signal strength is fitted to 1 while the QCD norm factor fitted in the background only fit to the control region is recovered.

Parameter	Value
μ_{EW}	$1.00^{+0.17}_{-0.17}$
μ_{QCD}	$1.03^{+0.36}_{-0.36}$

Table A–8 Electroweak signal strength and QCD normalization after fit to asimov data

All systematic uncertainties outlined in section 4.8 are included in the fit. The normalization component of the theoretical uncertainties on the signal sample is excluded since the signal acceptance is determined by the data. The constraining of some nuisance parameters demonstrates the data’s ability to refine these uncertainties. Overconstrained nuisance parameters likely arise from asymmetric errors on these parameters. It is important to note that nuisance parameters exclusively affecting the signal are not adjusted during the fit.

The influence of each nuisance parameter is assessed by conducting the fit with individual nuisance parameters held constant and comparing these results to the nominal fit which could be found in appendix A.17.

Figure A–15 presents the profile of the negative log-likelihood as it varies with the electroweak signal strength parameter. The test statistic value at $\mu = 0$ is utilized to calculate the

expected significance.

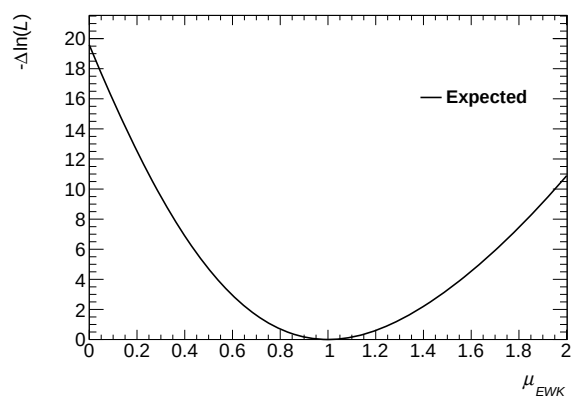


Figure A-15 Likelihood scan for the parameter of interest. The scan is shown for fits with and without systematic uncertainties included.^[94]

The expected significance is 6.26σ . Figure A-16 displays the relative effects of systematic and theoretical uncertainties on the parameter of interest.

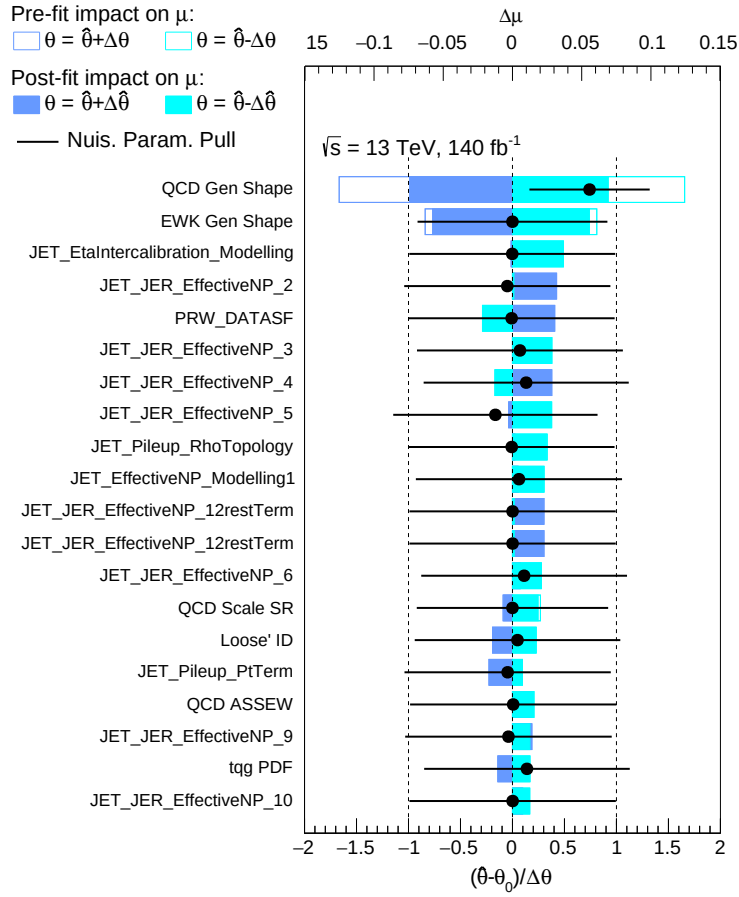


Figure A-16 The effect of individual nuisance parameters on the parameter of interest.^[94]

The pre-fit and post-fit plots for the five highest-ranked training variables are displayed in the Signal region in Figure A-17. Generally, an improved agreement is observed post-fit across all five variables.

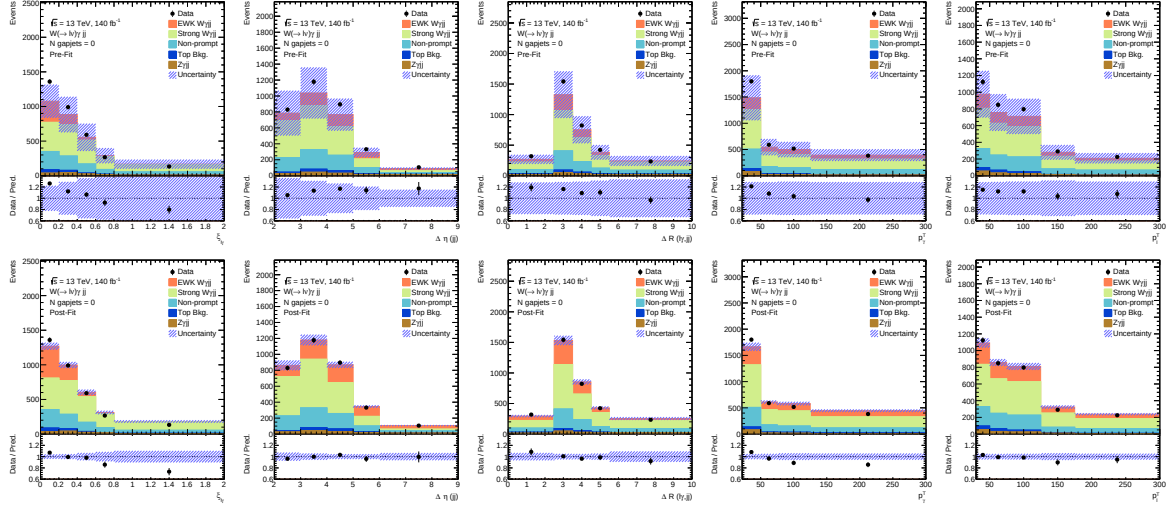


Figure A–17 Pre-fit and post-fit plots for five training variables of the neural network in the Signal region are presented. These plots include all theoretical and systematic uncertainties related to Monte Carlo backgrounds and data-driven estimates as discussed in sections 4.8 and 4.4.^[94]

A.17.2 Fiducial volume definition

- The event must include at least one prompt photon (as determined by `MCTruthClassifier::isPrompt`) with $p_T > 22$ GeV and $|\eta| < 2.5$, excluding the transition region $1.37 < |\eta| < 1.52$. Photon isolation energy must be $E_{iso} < 0.2p_{T_\gamma}$, calculated at the truth level as the sum of transverse momenta of stable particles within a radius $R = 0.4$ around the photon, excluding neutrinos.
- There must be one prompt electron or muon (defined by `MCTruthClassifier::isPrompt`) with $p_T > 30$ GeV and $|\eta| < 2.5$, excluding leptons from tau decays and considering dressed p_T . The region $1.37 < |\eta| < 1.52$ is also excluded for electrons. Additionally, the mass of the lepton-photon system must be within 10 GeV of the Z mass, mirroring the reconstructed level selection.
- At least two jets with $p_T > 50$ GeV and $|\eta| < 4.4$ must be present, using the `AntiKt4TruthDressedWZJets` container. A jet is defined as a cluster of stable particles excluding prompt leptons, neutrinos, and photons associated with prompt leptons.
- The event must have $E_T^{\text{miss}} > 30$ GeV, calculated at the truth level from the transverse momentum of all non-interacting objects.
- $M_W^T > 30$ GeV, determined from the truth lepton's transverse momentum and the truth E_T^{miss} .

- The event must satisfy angular separations: $\Delta\Phi(j_1(2), MET) > 0.4$, $\Delta R(j_0, j_1) > 0.4$, $\Delta R(j_{0,1}, \gamma) > 0.4$, $\Delta R(j_{0,1}, l) > 0.4$, and $\Delta R(\gamma, l) > 0.4$.
- There should be no b-jets in the event, identified by the GhostBHadronsFinalCount decoration.
- The dijet mass M_{jj} must exceed 500 GeV, and the rapidity difference $\Delta Y(j, j)$ must be greater than 2.

A.18 EFT

S, O, and M denote scalar-like, tensor-like, and mixed scalar-like and tensor-like operators. Only tensor-like and mixed operators effect the couplings which could be detected by this measurement. The operators could be shown as

$$O_{M0} = Tr[W_{\mu\nu}W^{\mu\nu}] \times [(D_\beta\phi)^\dagger D^\beta\phi] \quad (A-16)$$

$$O_{M1} = Tr[W_{\mu\nu}W^{\mu\beta}] \times [(D_\beta\phi)^\dagger D^\mu\phi] \quad (A-17)$$

$$O_{M2} = Tr[B_{\mu\nu}B^{\mu\nu}] \times [(D_\beta\phi)^\dagger D^\beta\phi] \quad (A-18)$$

$$O_{M3} = Tr[B_{\mu\nu}B^{\mu\beta}] \times [(D_\beta\phi)^\dagger D^\mu\phi] \quad (A-19)$$

$$O_{M4} = [(D_\mu\phi)^\dagger W_{\beta\nu}D^\mu\phi] \times B^{\beta\nu} \quad (A-20)$$

$$O_{M5} = [(D_\mu\phi)^\dagger W_{\beta\nu}D^\nu\phi] \times B^{\beta\mu} \quad (A-21)$$

$$O_{M7} = [(D_\mu\phi)^\dagger W_{\beta\nu}W^{\beta\nu}D^\mu\phi] \quad (A-22)$$

$$O_{T0} = Tr[W_{\mu\nu}W^{\mu\nu}] \times Tr[W_{\alpha\beta}W^{\alpha\beta}] \quad (A-23)$$

$$O_{T1} = Tr[W_{\alpha\nu}W^{\mu\beta}] \times Tr[W_{\mu\beta}W^{\alpha\nu}] \quad (A-24)$$

$$O_{T2} = Tr[W_{\alpha\mu}W^{\mu\beta}] \times Tr[W_{\beta\nu}W^{\nu\alpha}] \quad (A-25)$$

$$O_{T3} = Tr[W_{\mu\nu}W_{\alpha\beta}] \times Tr[W^{\alpha\nu}W^{\mu\beta}] \quad (A-26)$$

$$O_{T4} = Tr[W_{\mu\nu}W_{\alpha\beta}] \times B^{\alpha\nu}B^{\nu\beta} \quad (A-27)$$

$$O_{T5} = Tr[W_{\mu\nu}W^{\mu\nu}] \times B_{\alpha\beta}B^{\alpha\beta} \quad (A-28)$$

$$O_{T6} = Tr[W_{\alpha\nu}W^{\mu\beta}] \times B_{\mu\beta}B^{\alpha\nu} \quad (A-29)$$

$$O_{T7} = Tr[W_{\alpha\mu}W^{\mu\beta}] \times B_{\beta\nu}B^{\nu\alpha} \quad (A-30)$$

where D^β and D_β denote the covariant derivatives, W represents the $SU(2)_L$ field strength tensor, B signifies the $U(1)_Y$ field strength tensor, and ϕ refers to the Higgs field.

Dimension-5, dimension-7, and dimension-9 operators, which violate lepton and baryon number conservation, are excluded from this study. Dimension-6 operators, which can introduce charged anomalous triple gauge couplings (aTGC), are heavily constrained by vector boson fusion measurements and thus are considered with caution. CP conservation-violating operators also emerge at dimension-6, influencing both the QCD and electroweak vertices relevant to this analysis. Furthermore, while CP-violating operators appear at dimension-8, currently, no MadGraph model incorporates these operators, limiting the scope of simulations possible for these interactions.

Note that when an additional operator is included in the Standard Model Lagrangian, the matrix element is modified accordingly:

$$A = A_{SM} + f_j A_j \quad (A-31)$$

where A_{SM} is the Standard Model amplitude and A_j represents the amplitude associated with the new operator, introduced with a coupling constant f_j . The squared amplitude is then given by:

$$|A|^2 = |A_{SM} + f_j A_j|^2 = |A_{SM}|^2 + f_j \text{Re}(A_{SM} A_j^*) + f_j^2 |A_j|^2 \quad (A-32)$$

This expression encompasses contributions from the interference between the Standard Model and the new operator, which scales linearly with f_j , and a term derived solely from the new operator, scaling quadratically with f_j . These are respectively referred to as the linear or interference term and the quadratic or EFT-only term.

An important consideration is that linear terms from operators of higher dimensions than 8 are suppressed by the same factor, Λ^4 , as the quadratic terms of dimension-8 operators. Consequently, these linear terms can contribute similarly to the cross section as the dimension-8 quadratic terms. It should be noted that operators higher than dimension-8 are currently not incorporated in existing Monte Carlo generators and are thus not included in this analysis.

Appendix B Hadronic calorimeters for DarkSHINE and CEPC experiments

B.1 Hadronic Calorimeter of DarkSHINE

B.1.1 Introduction

Astronomical observations have shown the universe contains dark matter (DM)^[185-186], which interacts gravitationally but not electromagnetically. DM particles interact with Standard Model (SM) particles through new mechanisms, explained by the "freeze-out" process^[187]. This process stabilizes DM density as the universe expands and cools, allowing DM across a mass spectrum from MeV to TeV, including Light Dark Matter (LDM) and Weakly Interactive Massive Particles (WIMP)^[188-194].

WIMP searches are extensive, using experiments like AMS^[195], DAMPE^[196], LHC, BESIII^[197], XENON^[198-199], and PandaX^[200], nearing the neutrino floor^[201]. LDM research is crucial, focusing on the dark photon (A') as a mediator^[202-206]. Experiments like NA64^[207], BESIII^[208], and LDMX^[209-211] search for dark photons.

The DarkSHINE experiment^[212] aims to detect dark photons using an 8 GeV electron beam from SHINE^[213-215]. DarkSHINE targets dark photons with masses from MeV to GeV. The detector includes a Silicon Tracker, Electromagnetic Calorimeter (ECAL), and Hadronic Calorimeter (HCAL), with a tungsten target between tagging and recoil trackers (Figure B-1).

The silicon tracker in a 1.5 T magnetic field reconstructs electron trajectories and momenta. It includes a tagging tracker with seven silicon strip layers and a recoil tracker with six, separated by a tungsten target. ECAL, with 11 layers of LYSO (Ce) crystal scintillators, absorbs electron and photon energy for precise measurements. HCAL, a Fe-Sc type sampling calorimeter, uses iron absorbers and plastic scintillator strips to detect particles.

Electrons interacting with the target produce dark photons, carrying part of the electron's energy and decaying into undetected DM particles. The remaining energy is carried by the recoil electron, absorbed by ECAL. Dark photons may also decay visibly, reducing the cross section^[212]. HCAL vetoes background events, like neutrons and muons, detected in HCAL but not ECAL.

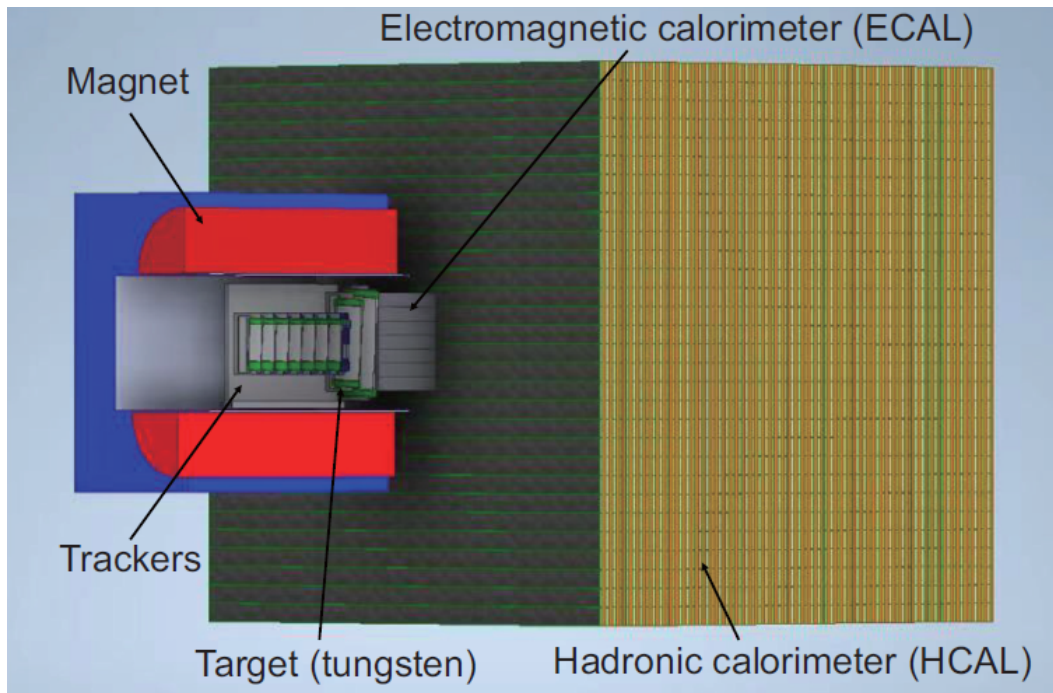


Figure B-1 DarkSHINE detector sketch. Electron direction is left to right. Red material with blue brace is the dipole magnet. The tagging tracker is at the center, the recoil tracker at the edge. The target is in the middle. ECAL follows the tracker, then HCAL^[212].

B.1.2 Optimization of the design

Hadronic calorimeter is an important part of the detector system, it handles the detection of background events who behaves like signal events with missing energy. The HCAL should be capable of vetoing the background events with high efficiency. A good design of HCAL ensures the success of the experiment. The optimization study uses the DarkSHINE software, a comprehensive simulation and analysis framework integrating functions like detector simulation, signal digitization, event display, reconstruction, and data analysis. An upcoming update will incorporate machine learning^[216]. Built on GEANT4 v10.6.3^[160], this package efficiently handles data flow across different stages.

GEANT4, a toolkit for simulating particle interactions with matter, is crucial for HCAL development and optimization. It supports various physics processes and complex geometries, widely used in high-energy physics.

Two simulation strategies are used. First, target particles are directly simulated to hit HCAL, providing large statistics and calculating veto efficiency. Second, complete sim-

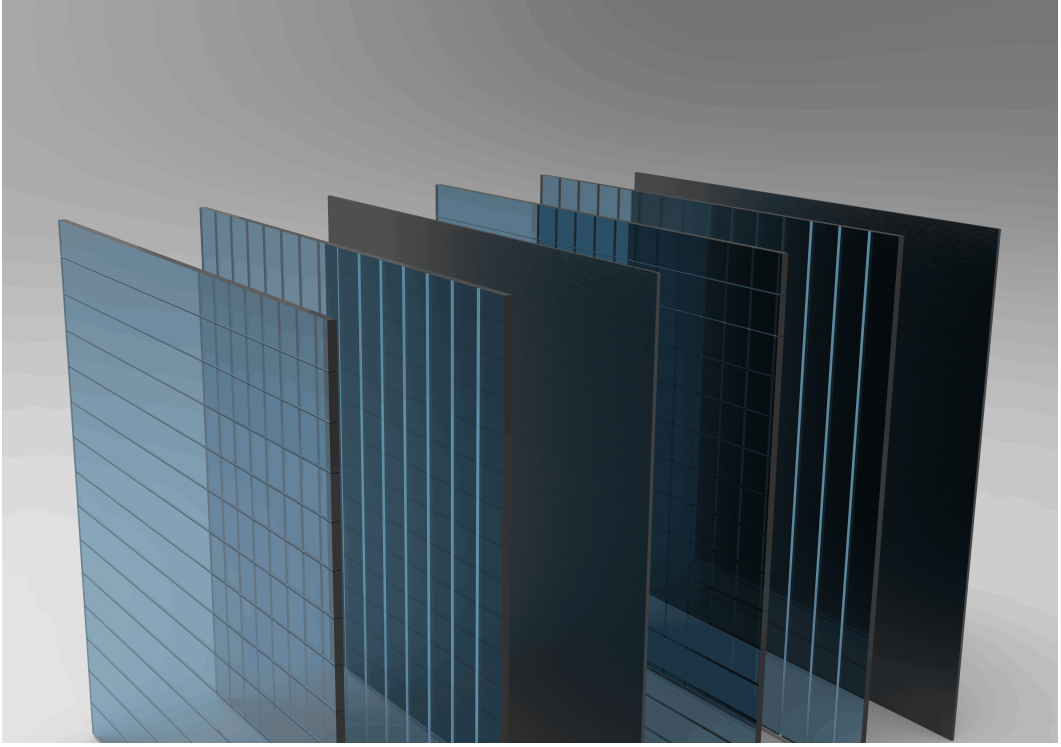


Figure B-2 XY-crossing scintillator structures. Transparent parts are scintillator layers, opaque parts are iron layers. Each scintillator layer has x- and y-direction sub-layers.

ulations evaluate veto efficiency of rare processes involving neutrons or muons with bias functions.

The DarkSHINE experiment uses HCAL variables $E_{\text{HCAL}}^{\text{total}}$ and $E_{\text{HCAL}}^{\text{MaxCell}}$ to veto muons and hadronic particles. $E_{\text{HCAL}}^{\text{total}}$ is the total energy in HCAL, and $E_{\text{HCAL}}^{\text{MaxCell}}$ is the highest energy deposition in a cell. A 5 cm scintillator unit width is used. The optimized cut values are:

- $E_{\text{HCAL}}^{\text{total}} < 30 \text{ MeV}$;
- $E_{\text{HCAL}}^{\text{MaxCell}} < 0.1 \text{ MeV}$.

To meet the $< 10^{-5}$ veto inefficiency requirement, 10^6 events are used for each test point, with results treated as 1×10^{-6} veto inefficiency if 0 out of 10^6 events survive, ensuring logarithmic axis validity.

B.1.2.1 Transverse Size

The transverse dimensions of the HCAL, determining its coverage angle, are crucial for vetoing neutral particles and analyzing rare processes. Coverage angle considers trajectories of secondary particles and shower dimensions. Larger HCAL size offers benefits but must

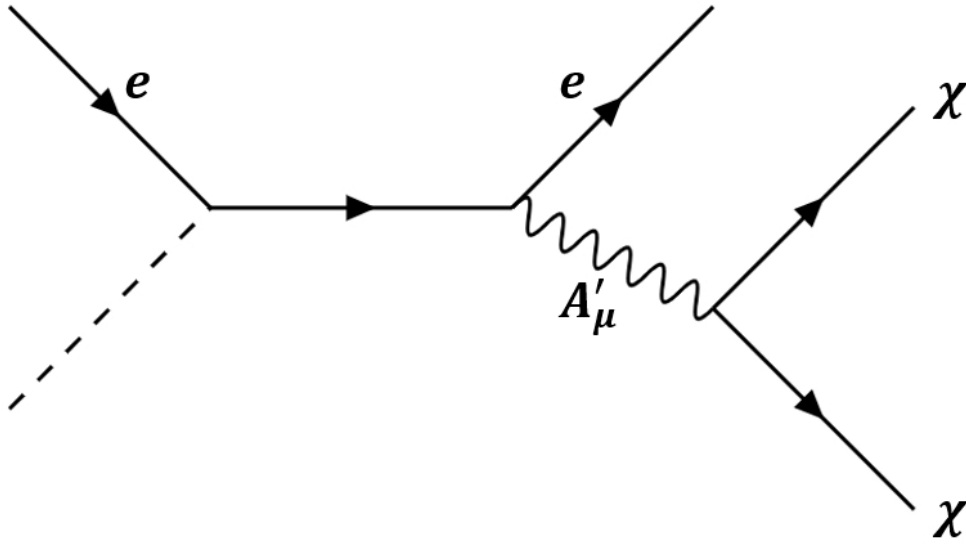


Figure B-3 Feynman diagram of DarkSHINE signal process, including bremsstrahlung production and invisible decay of dark photons^[212].

balance physical requirements, budget, and weight constraints. As a sampling calorimeter, HCAL needs sufficient components in the shower cluster to be vetoed by selection criteria. An optimal smaller size reduces budget and weight while meeting exclusion efficiency criteria.

HCAL performance is evaluated by direct particle injection tests, monitoring secondary particles in alignment with the beam. This approach helps understand how lateral size impacts efficiency across various scenarios.

This study explores HCAL transverse sizes from 4 m×4 m to 1 m×1 m. Simulations cover particle energies from 100 MeV to 3000 MeV, maintaining a constant total absorber thickness of 10λ to avoid bias. The HCAL design includes four modules in a two-by-two configuration, with scintillator strips half the transverse side length and 5 cm width, ensuring sensitivity and manageable size. This modular design aids future construction and installation.

Simulation results in Figure B-4 show the relationship between HCAL's transverse size and veto efficiency. The Y-axis represents veto inefficiency, and the X-axis denotes incident particle energy. Larger HCAL sizes improve veto power, with the 1.5 m design chosen for SHINE facility weight limits.

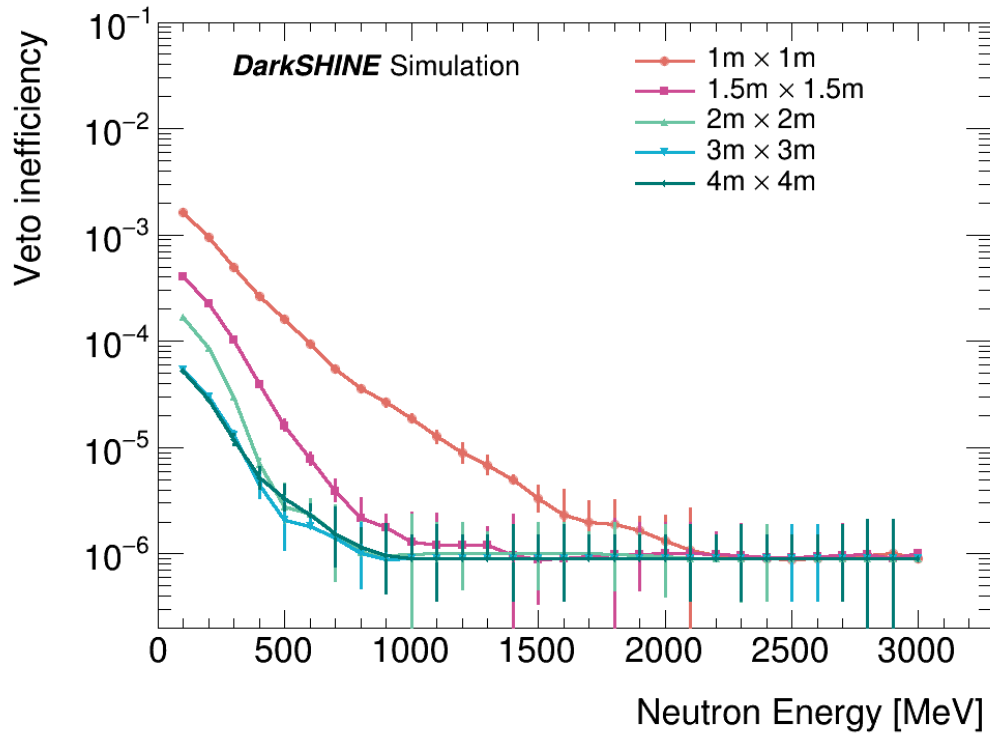


Figure B-4 Veto inefficiency vs. incident neutron energy. Larger HCAL sizes show better veto power. The 1.5 m design is chosen for SHINE facility weight limits.

In conclusion, larger HCAL sizes offer better performance for high-energy neutrons (2 GeV to 3 GeV) and low-energy neutrons. The 1.5 m×1.5 m design meets the requirement with veto inefficiency below 10^{-3} , balancing interaction length and weight for the SHINE facility.

B.1.2.2 Absorber thickness

The detector design can vary significantly based on experimental requirements. Homogeneous detectors use a single material for detection and absorption, offering high energy resolution, while sampling detectors use alternating layers of active and passive materials, providing efficiency and versatility for high-energy particles. The DarkSHINE HCAL is a sampling detector designed to capture high-energy neutrons while allowing low-energy neutrons to reach the scintillators.

Various absorber thicknesses were simulated, ranging from 10 mm to 100 mm per layer. Veto inefficiency as a function of detector depth is shown in Figure B-5 for neutron energies of 100, 500, and 2000 MeV. Each curve represents total absorber thickness from 100 mm to

1600 mm.

A 10 mm absorber is optimal for 100 MeV neutrons, with 70 layers achieving an inefficiency of $<10^{-5}$ for high-energy neutrons when enough layers are used. Thicker absorbers require fewer layers for the same interaction length, thinner absorbers are good for low energy neutrons but are not sufficient for high energy neutrons. Figure B–6 shows veto inefficiency for 10 mm and 50 mm absorbers at different beam energies, demonstrating that increased thickness reduces the number of layers needed.

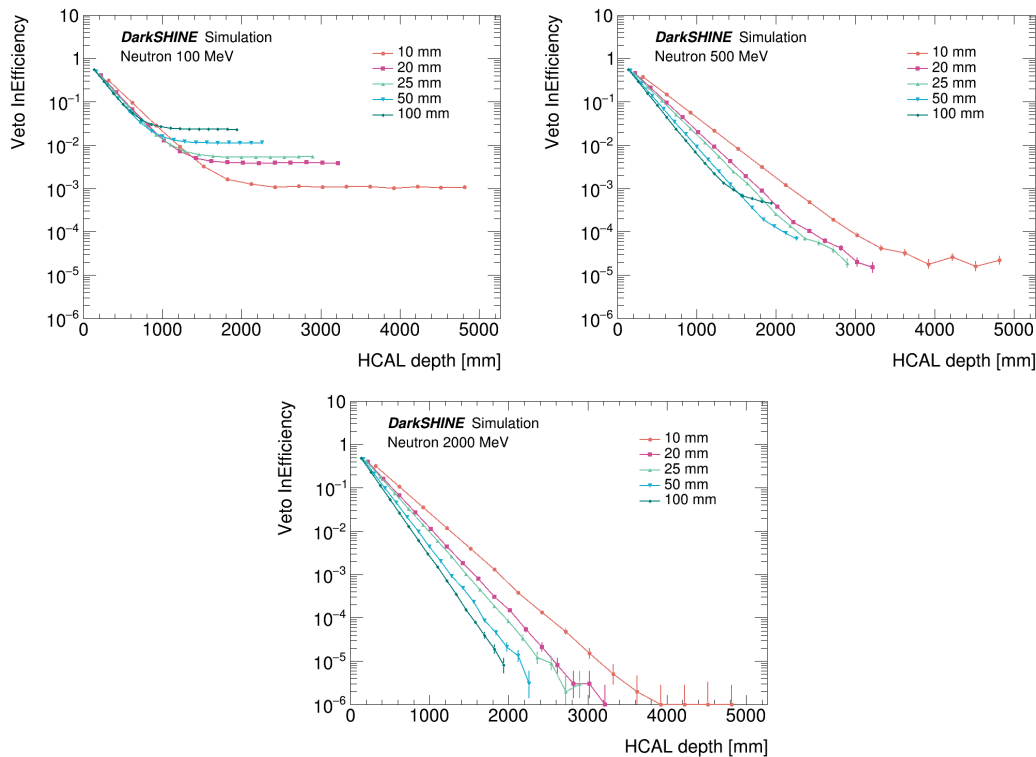


Figure B–5 Veto inefficiency vs. detector depth for different absorber thicknesses. Thinner absorbers enhance low-energy neutron veto efficiency, while thicker absorbers are better for high-energy neutrons within a smaller depth range.

The optimized DarkSHINE HCAL design uses a thinner absorber in the front to capture low-energy neutrons and a thicker absorber in the back to minimize material usage. This design employs 70 layers of 10 mm absorber and 18 layers of 50 mm absorber, achieving a total thickness of 10λ and meeting physical requirements.

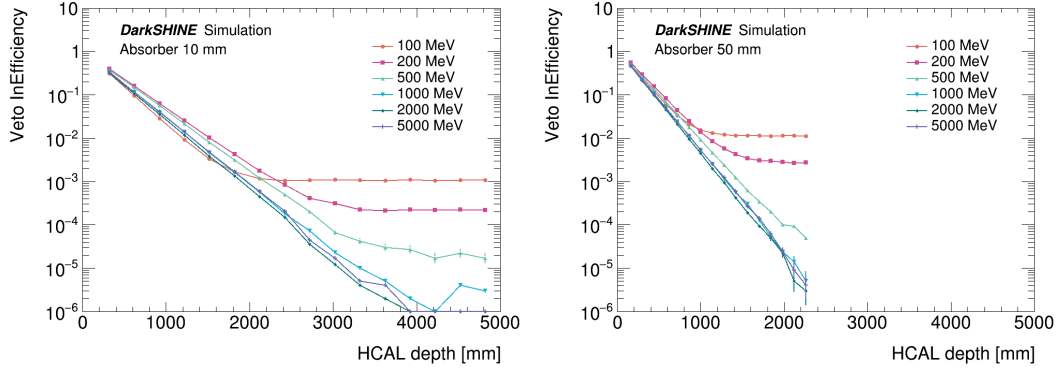


Figure B-6 Veto inefficiency vs. detector depth for different beam energies. 10 mm and 50 mm absorber thickness results are shown. Each point represents the same total absorber thickness but different HCAL depths.

B.1.3 Performance

As stated before, the previous study used neutron veto inefficiency as the primary indicator. However, it is crucial to evaluate the performance for all relevant particles entering HCAL. The veto inefficiency of various hadronic particles through the optimized DarkSHINE HCAL was assessed by simulating different incident particles with distinct energies, increasing the number of events to 10^7 . The particles tested included neutrons, k^0 (short- and long-lived), π^0 , and protons. The results are shown in Table B-1.

The HCAL shows a performance gradient in veto capabilities, particularly for neutrons of different energies. Lower energy neutrons (100 MeV) are absorbed in the first few absorber layers, precluding secondary particle detection. Higher energy neutrons (500 MeV) show decreased veto inefficiency, aligning with design objectives. For energies >1000 MeV, the HCAL maintains low veto inefficiency for various hadronic particles, indicating superior discrimination capabilities. However, kaons at 2 GeV exhibit slightly higher inefficiency due to long-lived K^0 particles and deeper showers.

The differential behavior among particle types within the HCAL highlights the complex interactions between particles and detector materials. These findings validate the optimized HCAL design for the DarkSHINE experiment and provide insights into particle detection and background event mitigation in high-energy physics research.

Table B–1 Veto inefficiency of HCAL for different hadronic particles and energies. Events with multiple hadronic particles can be more easily vetoed by HCAL, assuming independent veto power for each particle in an event.

Veto InEff $\times E-06$	n	k^0
100[MeV]	$1170^{+10.9}_{-10.8}$	$31600^{+55.5}_{-55.4}$
500[MeV]	$18.4^{+1.46}_{-1.36}$	$5.40^{+0.839}_{-0.733}$
1000[MeV]	$3.70^{+0.714}_{-0.606}$	$3.70^{+0.714}_{-0.606}$
2000[MeV]	$2.70^{+0.626}_{-0.516}$	$11.5^{+1.19}_{-1.08}$

π^0	p	μ
$7.30^{+0.958}_{-0.852}$	$30700^{+61.5}_{-61.3}$	$409^{+6.49}_{-6.39}$
$0.1^{+0.184}_{-0}$	$8.04^{+1.34}_{-1.16}$	$15.0^{+1.33}_{-1.22}$
$0.1^{+0.184}_{-0}$	$0.1^{+0.958}_{-0}$	$2.00^{+0.555}_{-0.443}$
$0.1^{+0.188}_{-0}$	$0.1^{+2.78}_{-0}$	$0.1^{+0.184}_{-0}$

B.1.4 Conclusion

The design and optimization of the hadronic calorimeter (HCAL) for the DarkSHINE experiment have been meticulously conducted, focusing on factors like absorber thickness, scintillator placement, and side HCAL requirements. These parameters were optimized considering weight and budget constraints while meeting physical requirements.

The optimized HCAL design features iron absorber layers and scintillator layers. The transverse dimensions are $1.5 \text{ m} \times 1.5 \text{ m}$, with 10λ thick iron layers along the beam direction. The first 70 layers are 1 cm thick, and the last 18 layers are 5 cm thick. Each absorber is followed by a 1 cm thick plastic scintillator layer with 5 cm wide strips. The scintillator strips in adjacent layers are perpendicular to each other. An additional scintillator layer is placed between the ECAL and the first iron layer. A side HCAL surrounding the ECAL is also incorporated.

This novel HCAL design offers enhanced veto power for various rare processes, including electron-nuclear and photon-nuclear reactions, especially those with neutral hadrons and muons in the decay final states. The optimized HCAL is crucial for the DarkSHINE experiment and demonstrates the importance of advanced hadronic calorimetry techniques in particle physics experiments.

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List of Research Achievements

First-Author Publications

[1] **WANG Z, et al.** Design of hadronic calorimeter for DarkSHINE experiment. arXiv:2311.01780 [physics.ins-det] (**Nucl. Sci. Tech.** 35, 148 (2024), DOI: 10.1007/s41365-024-01502-5)

[2] **WANG Z, et al.** Probing Electroweak Phase Transition at CEPC via Exotic Higgs Decays with 4b Final States. **LHEP** 2023 (2023) 436, DOI: 10.31526/lhep.2023.436

[3] **WANG Z, et al.** Study of Electroweak Phase Transition in Exotic Higgs Decays at the CEPC. **SnowMass2021 White Paper**. arXiv:2203.10184 [hep-ex]

ATLAS Collaboration Papers with my major contributions

[1] **ATLAS Collaboration.** Fiducial and differential cross-section measurements of electroweak $W\gamma jj$ production in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector. arXiv:2403.02809 [hep-ex] (accepted by **Eur. Phys. J. C, ATLAS Standard Model Closure Talk**)

[2] **ATLAS Collaboration.** Search for pair production of boosted Higgs bosons via vector-boson fusion in the $b\bar{b}b\bar{b}$ final state using pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector. arXiv:2404.17193 [hep-ex] (accepted by **Phys. Lett. B, ATLAS Internal Note Editor**)

ATLAS Collaboration Conference Note

[1] **ATLAS Collaboration.** Search for pair production of boosted Higgs bosons in the $b\bar{b}b\bar{b}$ final state in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector, **ATLAS-CONF-2024-003**

Proceedings

[1] **WANG Z**, Search for $H \rightarrow aa \rightarrow 4b$ exotic decays and VBF $HH \rightarrow 4b$ with CEPC and ATLAS, NPPP 330 (2023) 51, DOI: 10.1016/j.nuclphysbps.2023.04.026(Proceeding of **Higgs Potential 2023** Conference)

[2] **WANG Z**, Observation and differential cross-section measurements of electroweak $W\gamma jj$ production in pp collisions at $\sqrt{s} = 13\text{TeV}$ with the ATLAS detector (**NPPP** 346 (2024) 11, DOI:10.1016/j.nuclphysbps.2024.06.009 (Proceeding of CLHCP2024 Conference))

Other co-authored Publications

[1] **CHEN J, et al.** Prospective study of light dark matter search with a newly proposed DarkSHINE experiment[J]. **Sci. China-Phys. Mech. Astron.**, 66(1): 211062 (2023), DOI: 10.1007/s11433-022-1983-8

[2] **DUAN Y, et al.** Scintillator tile batch test of CEPC AHCAL. **Journal of Instrumentation**, 2022, 17(05): P05006. DOI: 10.1088/1748-0221/17/05/P05006

[3] **SONG S, et al.** Study of residual artificial neural network for particle identification in the CEPC high-granularity calorimeter prototype. **Journal of Instrumentation**, 2024, 19(04): P04033. DOI: 10.1088/1748-0221/19/04/P04033

[4] **ZHANG H, et al.** Design and test for the CEPC muon subdetector based on extruded scintillator and SiPM. **Journal of Instrumentation**, 2024, 19(06): P06020. DOI: 10.1088/1748-0221/19/06/P06020

[5] **SHI Y, et al.** Development of the CEPC analog hadron calorimeter prototype. (**NST-**

2024-0526, submitted to Nuclear Science and Techniques)

[6] **ZHAO Z, et al.** Design of a LYSO Crystal Electromagnetic Calorimeter for DarkSHINE Experiment. arXiv:<http://export.arxiv.org/abs/2407.17800> (**NST-2024-0554**, submitted to Nuclear Science and Techniques)

Selected International Conference Talks

[1] **2022 July:** *Search for $H \rightarrow aa \rightarrow 4b$ exotic decays and VBF $HH \rightarrow 4b$ with CEPC and ATLAS*, **Plenary Talk @ Higgs Potential 2022**, Beijing, China

[2] **2022 August:** *Search for $HH \rightarrow 4b$ production and $H \rightarrow aa \rightarrow 4b$ exotic decays with ATLAS and CEPC*, **Plenary Talk @ TDLI-PKU BSM workshop 2022:Electroweak lights the way**, Shanghai, China

[3] **2023 July:** *Dark SHINE—a new initiative to search for light dark matter at SHINE facility*, **Parallel Talk @ The 2nd International Conference on Axion Physics and Experiment (Axion 2023)**, Xi'an, China

[4] **2024 July:** *VBF/VBS measurements in ATLAS*, **Parallel Talk @ 29th International Symposium on Particles, Strings and Cosmology(PASCOS2024)**, Quy Nhon, Vietnam()

Selected Domestic Conference Talks

[1] **2022 August:** *Search for $HH \rightarrow 4b$ production and $H \rightarrow aa \rightarrow 4b$ exotic decays with ATLAS and CEPC*, **Parallel Talk @ 11th CPS HEP biennial Conference 2022**, Dalian, China

[2] **2023 August:** *Design and Unit Test for DarkSHINE HCAL Calorimeter*, **Parallel Talk @ 21st Nuclear Electronics and Nuclear Detection Technology Conference**, Enshi, China

[3] **2023 November:** *Observation and differential cross-section measurements of electroweak $W\gamma jj$ production in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, **Parallel Talk** @ The 9th Chinese LHC Physics Workshop (**CLHCP2023**), Shanghai, China

[4] **2024 August:** *Search for pair production of boosted Higgs bosons via vector-boson fusion in the $bbbb$ final state using pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*, **Parallel Talk** @ **14th CPS HEP biennial Conference 2024**, Qingdao, China

Important Talks in ATLAS Collaboration

[1] **2023 May:** *Boosted VBF $HH4b$ Status Report* ATLAS HDBS/DiHiggs Analysis Status Report, CERN

[2] **2023 May:** *W VBS SM Closure* ATLAS Standard Model Plenary Analysis Closure Talk, CERN

Academic Prize and Honors

[1] **2023:** 粒子天体物理与宇宙学教育部重点实验室优秀研究生奖