

Searches for New Physics in Top-Antitop Associated Production Processes and Mechanical Design and Thermal Performance of the CMS Inner Tracker Endcap Pixel Upgrade

Dissertation

zur

Erlangung der naturwissenschaftlichen Doktorwürde
(Dr. sc. nat.)

vorgelegt der

Mathematisch-naturwissenschaftlichen Fakultät

der

Universität Zürich

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Zürich, 2024



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Abstract

Three analyses in top-antitop associated production processes are presented. The measurements are based on data collected in proton-proton collisions at $\sqrt{s} = 13$ TeV by the CMS experiment at the CERN LHC, corresponding to an integrated luminosity of 138 fb^{-1} .

The first measurement is a search for new physics in the production of one or more top quarks with additional leptons, jets, and b jets in the context of Effective Field Theory (EFT). EFT effects are incorporated into the event weights of the simulated samples, allowing detector-level predictions that account for correlations and interference effects among EFT operators and between EFT operators and Standard Model (SM) processes. The Wilson Coefficients (WCs) corresponding to 26 EFT operators were simultaneously fit to the data. In all cases, the data is found to be consistent with the SM expectations.

Also, a measurement of the Charge-Parity (CP) structure of the Yukawa coupling between the Higgs (H) boson and top quarks at tree level, when the H boson is produced in association with one (tH) or two ($t\bar{t}H$) top quarks, is presented. The analysis targets events where the H boson decays to leptons and the top quark(s) decay either leptonically or hadronically. Separation of CP-even from CP-odd scenarios is achieved by applying machine learning techniques to final states characterized by the presence of at least two leptons. No significant CP-odd contribution is observed and the results are compatible with predictions for the SM H boson.

In addition, the first differential measurement of the production of H bosons in association with either one (tH) or two ($t\bar{t}H$) top quarks in final states with electrons, muons and taus is performed. The sensitivity of the analysis is improved by using machine learning methods to separate the signal from backgrounds. The H boson transverse momentum and the mass of the $t\bar{t}H$ system are reconstructed, and differential cross sections for $t\bar{t}H$ production are calculated at particle level, assuming a lack of new physics effects. The measurement is performed in terms of the H boson p_T as well as in terms of the mass of the $t\bar{t}H$ system. Also, a measurement of the H trilinear coupling is performed. At the moment of publishing, this analysis is undergoing the internal review process of the CMS experiment; as such, the plots are marked as 'Work in Progress', and the data, numbers, and discussions presented here may differ from the paper's final version.

Lastly, the TEPX section of the inner tracker of the CMS experiment for the high-luminosity LHC is presented and studies on the current development of said part are discussed. Several design choices surrounding the mechanical and thermal design were tested and their optimal configuration was selected.

Acknowledgements

As I culminate this incredible journey of my PhD at the CMS Experiment at CERN, I am filled with deep gratitude towards many who have made this journey not only possible but also immensely rewarding.

I want to thank the entire UZH group, as their collaborative spirit, encouragement and invaluable inputs have created an inspiring and supportive working environment.

Special thanks also goes to Stefanos Leontsinis and Sergio Sanchez for their guidance and support. As my supervisors, their encouragement, support and mentorship has been crucial in navigating the challenges of scientific research. Their exceptional character and ability to create opportunities for growth have greatly enriched my PhD experience and aided my professional growth.

Special thanks also goes to Prof. Dr. Florencia Canelli for the opportunity to join her group to pursue my PhD for providing the opportunity to work on such many diverse projects and her continuous support.

I also want to thank the people in my committee Prof. Dr. Nicola Serra and Prof. Dr. Gino Isidori.

Lastly, I would also like to thank my parents and family, for supporting me along my studies.

Special thanks goes to my wife Janina, who supported me more than one could wish for and listened to countless hours of me rambling about physics.

To all of you, thank you for being a part of my journey. Your contributions have not only aided in my academic pursuits but have also been a source of personal growth and inspiration.

1 Introduction

Since the beginning of time, mankind has sought to understand the world around us and how it works. Over the millennia, we have adapted and improved our model of nature to include more and more phenomena and make more accurate predictions, with the ultimate goal of eventually deriving a theory of everything. As early as 430 BC, Greek philosophers came up with the idea of "atomos", which means indivisible. Their idea was that everything is made up of fundamental, indivisible building blocks that create the world we experience and live in.

Just over 2000 years later, in the 19th century, the chemist John Dalton discovered that matter actually appeared to combine into discrete units of weight. This was the first glimpse of the fundamental building blocks of matter. These efforts ultimately led to the development of the Standard Model of Particle Physics (SM), which provides a unified model of all fundamental particles and the interactions between them. At the time the SM was formulated, many of the postulated particles had not yet been discovered. Only through the continuous and dedicated work of many scientists, and major improvements in detector technology, has it been possible to search for and discover the predicted particles. This search led to the discovery of the Higgs (H) boson by the ATLAS and CMS experiments [1–3] at CERN’s Large Hadron Collider (LHC) [4] in 2012. This marked the discovery of the last particle of the SM, more than 47 years after its prediction [5, 6].

Despite its many remarkable successes, there are both theoretical and experimental reasons to suggest that the SM is not the final and most fundamental theory of nature.

Several observations, both within and outside particle physics, fall outside what would be expected from the SM, suggesting the existence of further physics beyond the SM. The search for new physics is one of the driving forces of modern particle physics, with two main approaches to the search for new physics. The first is the direct search for new physics in the form of new particles or interactions, while the second is the search for deviations from the predictions of the SM.

In this thesis, analyses using both approaches are presented. The first approach, by precisely measuring processes in top quark production in association with additional leptons. Here top quark interactions are measured in the context of 26 dimension-six Effective Field Theory (EFT) operators that can affect processes involving top quarks produced with additional charged leptons. The second approach involves two measurements of top-antitop production associated with a Higgs boson in multilepton final states. The first measurement will test the Charge-Parity (CP) structure of top Higgs Yukawa coupling. The second measurement is a precision measurement of the $t\bar{t}H$ cross section. This analysis explores the idea of measuring the cross section differentially, which allows us to gain sensitivity to processes that change the kinematical shapes instead of just the total cross section.

All three studies used data collected by the CMS experiment [7, 8] collected in the years between 2016 and 2018 at the LHC.

In addition, this thesis also presents the continuous efforts of upgrading and designing the Inner Tracker (IT) of the CMS detector to prepare for the higher data rates and challenging

radiation levels of the High Luminosity LHC [9]. More specifically it focuses on the end-cap part of the inner silicon pixel detector (TEPX).

On the analysis measuring top quark production in association with additional leptons in the context of EFT operators, my work focused mainly on improving the sensitivity to the four four-heavy quark operators by introducing and optimizing a new Signal Region (SR). Also, I motivated the introduction of a $t\bar{t}$ control region in future iterations of the analysis to better constrain EFT operators affecting $t\bar{t}$ processes. On the analysis measuring $t\bar{t}H$ processes in the context of CP invariance, I worked on the optimization on how to differentiate between CP-even and CP-odd behaviour, as well as on the event selection, binning studies and overall validation our data and objects via dedicated control and validation regions. For the analysis measuring $t\bar{t}H$ processes differentially, my work consisted of the development of the framework in which the analysis is performed in, binning studies, validation of data and objects via control and validation regions, to training Deep Neural Networks (DNN) to differentiate between signal and background processes and regress the transverse momentum (p_T) of the H boson. My work on the TEPX consisted of validating and optimizing the thermal design of the TEPX detector. The work itself consisted of simulating the behaviour of the TEPX disks under load and then setting up and maintaining a test bench to test prototypes of these disks and compare the results with the simulations.

The structure of this thesis is as follows:

Chap. 2 discusses the SM as well as possible physics beyond the SM, focusing on the parts relevant to top and top Higgs physics.

Chap. 3 describes the LHC accelerator, the CMS detector and the collection of proton-proton collision data.

After that, Chap. 4 focuses on top quark production in association with additional leptons in the context of EFT operators measurement.

Chap. 5 presents a CP measurement of the top-Higgs Yukawa coupling in $t\bar{t}H$ multilepton final states.

Chap. 6 presents a differential measurement of the $t\bar{t}H$ cross section in multilepton final states.

Chap. 7 presents the studies carried out on the TEPX inner tracker upgrade for the High Luminosity LHC at CMS.

Additionally, in Chap. A of the appendix, a study on a global event description in high energy physics using concepts of optimal transport with a graph neural network to reduce Pile-Up is shown.

2 The Standard Model of particle physics and beyond

2.1 Overview

Everything we know of is composed out of elementary particles that interact according to a set of natural rules. According to our current understanding, elementary particles correspond to excited states of quantum fields. Quantum Field Theory (QFT) provides the mathematical framework to describe these fields. The Standard Model of particle physics (SM) [10] is a renormalizable and gauge invariant QFT that includes all particles and their interactions observed to date. The full set of SM particles can be seen in Fig. 2.1.

According to the SM, particles interact via the strong, weak and electromagnetic forces and the interactions are mediated by bosons, particles with integer spin. The strong force is mediated by gluons while the electromagnetic force is mediated by photons. The massive Z and $W^\pm$ are the mediators of the electroweak force.

Fermions have a spin of $1/2$ and are divided into quarks and leptons. The quarks and leptons are each divided into three generations which are assumed to be copies of each other except for their mass differences.

The discovery of the Higgs (H) boson in 2012 marked a milestone in particle physics, as it was the last piece missing in the SM. Simultaneously, the discovery of the H boson opened many new ways to probe the SM via its special connection to other SM particles and its role in the mass determination of other particles. Especially the top quark, due to its high mass, features a very high coupling to the H boson which offers interesting ways to probe the H boson.

However, even though the SM has proven to provide great predictions for many processes, it does not provide a complete explanation of our universe. Questions, like the strong CP problem [12, 13] or the hierarchy problem [14–16] remain unanswered for example. Problems like these motivate new studies of SM processes and the development of new theories Beyond the SM (BSM) like Effective Field Theory (EFT) extensions of the SM.

2.2 Electroweak Interaction

Between 1960 and 1970, Glashow, Weinberg and Salam [14, 17, 18] developed the theory of Electroweak (EWK) interactions to the SM. It combines Quantum Electrodynamics (QED) ($U(1)_Y$) with the weak interaction ($SU(2)_L$).

In the EWK theory, interactions are mediated by three massive spin 1 W bosons (W^1 , W^2 and W^3), where each has its respective component of isospin (I_3) $+1$, -1 and 0 . As such, they are responsible for transformations in the $SU(2)_L$ isospin phase space. A unique characteristic of the EWK interaction is, that W^1 and W^2 only interact with left-handed particles and right-

Standard Model of Elementary Particles

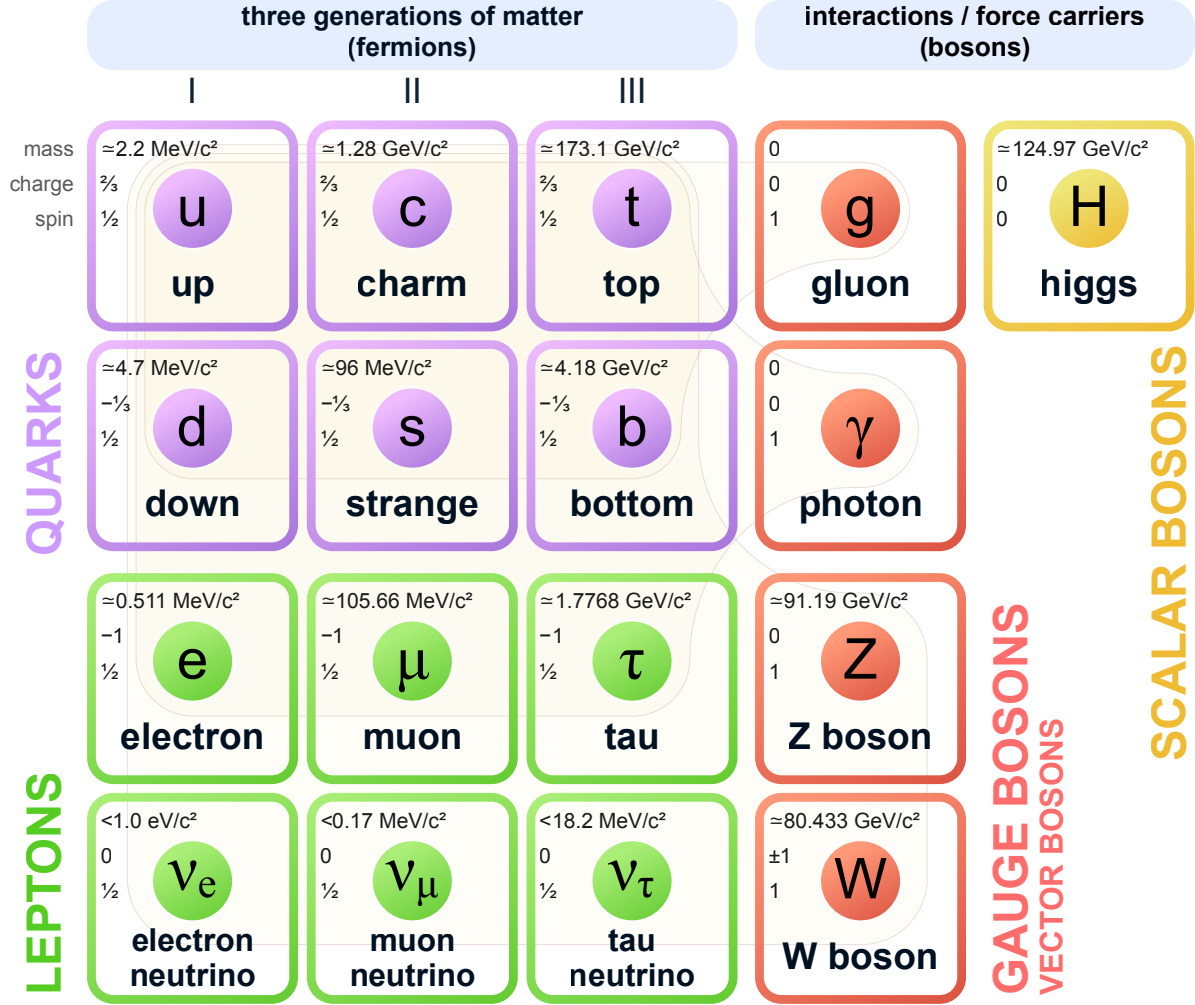


Figure 2.1: Complete set of SM particles. Taken from [11]

handed antiparticles¹. Left-handed fermions have an isospin of either $+1/2$ (up, charm, top and neutrinos) or $-1/2$ (down, strange, bottom and charged lepton partner of corresponding neutrino) while right-handed fermions have an isospin of 0. Antiparticles on the other hand, have the sign of their isospin reversed. As a result, the EWK interactions violate Charge Parity (CP) symmetry, which so far is the only sector where CP violation has been observed. An in depth discussion of CP violation can be found in Sec. 2.7.2. As W^1 and W^2 are responsible for the conversion of isospin states within each generation, it directly follows that only left-handed particles and right-handed antiparticles are able to change flavors. An example of such a conversion in isospin would be the decay of a top quark ($I_3 = +1/2$) into a b quark ($I_3 = -1/2$) via the emission of a W^1 boson ($I_3 = +1$).

The differentiation between left- and right-handedness is represented by considering the left- and right-handed projections of the matter fields:

¹Left- and right-handedness is based on chirality, an intrinsic property of particles.

$$\psi_L = \frac{1}{2} (1 - \gamma^5) \psi, \quad \psi_R = \frac{1}{2} (1 + \gamma^5) \psi \quad (2.1)$$

Subsequently, from there, left-handed particles are represented as doublets and right-handed particles as singlets:

$$L = \begin{pmatrix} u_L \\ d_L \end{pmatrix}, \quad u_R, \quad d_R \quad (2.2)$$

The full Lagrangian for the $SU(2)_L$ weak interaction can then be written as:

$$\mathcal{L} = -\frac{1}{4} W_{\mu\nu}^i W_i^{\mu\nu} + i\bar{u}_R \gamma^\mu \partial_\mu u_R + \bar{d}_R \gamma^\mu \partial_\mu d_R + i\bar{L} \gamma^\mu D_\mu L \quad (2.3)$$

with $W_{\mu\nu}^i = \partial_\mu W_\nu^i - \partial_\nu W_\mu^i - g_W \epsilon^{ijk} W_\mu^j W_\nu^k$ and $D_\mu = \partial_\mu + ig_W \frac{\sigma_i}{2} W_\mu^i$. However, simply requiring invariance under $SU(2)_L$ symmetry does not allow for mass terms in the Lagrangian. Sec. 2.3 describes, how mass terms are added to the Lagrangian in detail.

The $U(1)_Y$ symmetry then corresponds to the electromagnetic interaction, mediated by photons. It can be described by the Lagrangian:

$$\mathcal{L} = \sum_{\psi=L,u_R,d_R} \bar{\psi}(x) (i\gamma_\mu \partial^\mu - Y g_Y B_\mu) \psi(x) - \frac{1}{4} B^{\mu\nu} B_{\mu\nu} \quad (2.4)$$

For this symmetry the hypercharge Y is conserved.

Finally, the $SU(2)_L \times U(1)_Y$ symmetry introduces four degrees of freedom. These can then be related to mass eigenstates corresponding to the $W^\pm$ and Z bosons and the photon.

$$W^\pm = \frac{1}{\sqrt{2}} (W^1 \mp iW^2) \quad (2.5)$$

$$\begin{pmatrix} \gamma \\ Z^0 \end{pmatrix} = \begin{pmatrix} \cos(\theta_W) & \sin(\theta_W) \\ -\sin(\theta_W) & \cos(\theta_W) \end{pmatrix} \begin{pmatrix} B \\ W_3 \end{pmatrix} \quad (2.6)$$

Where θ_W can be described as via the ratio between the Z and $W^\pm$ boson masses:

$$\cos(\theta_W) = \frac{m_W}{m_Z} \quad (2.7)$$

2.3 Spontaneous Symmetry Breaking of the Electroweak Symmetry

Eq. (2.3) shows the Lagrangian that emerges by requiring invariance under $SU(2)_L$ [19]. However, as mentioned above, simply adding mass terms would destroy the $SU(2)_L$ symmetry. On the other hand, experiments show that the corresponding particles do have mass. Conventionally, this is interpreted as the $SU(2)_L$ symmetry being broken, meaning that while the symmetry exists at high energies, it spontaneously breaks at lower energies. To add mass terms to the Lagrangian, a complex spin 0 field h is introduced:

$$\mathcal{L}_H = \partial_\mu \phi^\dagger \partial^\mu \phi + \rho^2 \phi^\dagger \phi - \lambda(\phi^\dagger \phi)^2 \quad (2.8)$$

140 In addition, a Yukawa interaction term is added between fermions and the scalar doublet:

$$\mathcal{L}_{\text{Yukawa}} = -y_u(\bar{L}H u_R + \bar{u}_R H L) - y_d(\bar{L}H d_R + \bar{d}_R H L) \quad (2.9)$$

141 Note that since there are no right-handed neutrinos in the SM (since they don't interact with
142 anything), the right term is not present for leptons. Adding the above terms to the Lagrangian
143 keeps it invariant under local $SU(2)_L \times U(1)_Y$ symmetry.

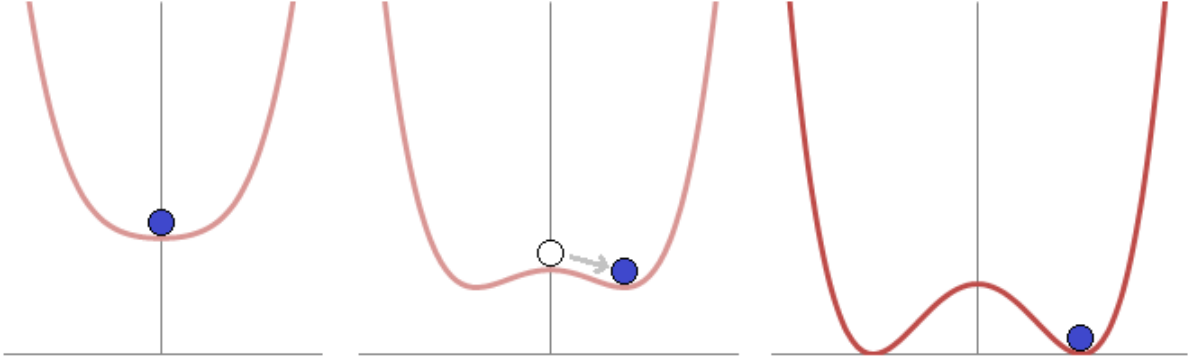


Figure 2.2: The diagram on the left shows a two-dimensional representation of the potential at high energy ($\rho > 0$) before the symmetry breaking occurs. The middle and right diagrams show a two-dimensional representation of the potential once the symmetry breaking occurs at lower energy ($\rho < 0$). Taken from [20].

144 Expanding the two-dimensional diagram from Fig. 2.2, the potential takes on a sombrero like
145 shape. As a result, there are infinite choices for the minimum of the potential. A convenient
146 choice, which is usually taken, is:

$$\Phi_{\min} = \begin{pmatrix} 0 \\ \sqrt{\frac{\rho^2}{2\lambda}} \end{pmatrix} \equiv \begin{pmatrix} 0 \\ \sqrt{\frac{v}{\sqrt{2}}} \end{pmatrix} \quad (2.10)$$

147 Where v corresponds to the new vacuum value. From there the unitary gauge follows as:

$$\Phi_{\text{un}} = \begin{pmatrix} 0 \\ \sqrt{\frac{v+h}{\sqrt{2}}} \end{pmatrix} \quad (2.11)$$

148 One way to interpret this is that of the original four degrees of freedom that appear in our
149 complex scalar doublet, three of them are already represented in our $SU(2)_L$ symmetry. As
150 such, these three are not physical and cannot be measured. The remaining one, however, is a
151 physical field h , called the H field.

152 Finally, this brings new terms to the Lagrangian, which can be interpreted as mass terms.

$$\mathcal{L} = \underbrace{\frac{1}{4}v^2 g'^2 (W^+)_{\mu}(W^-)^{\mu}}_{=M_W^2} + \underbrace{\frac{1}{8}v^2 (g^2 + g'^2) Z_{\mu}^2}_{=\frac{1}{2}M_Z^2} + \underbrace{\frac{1}{8}v^2 0}_{M_{\text{photon}}=0} \cdot A_{\mu}^2 \quad (2.12)$$

This also allows us to derive an equation for the mass of the H boson:

$$m_H = \sqrt{2\lambda}v \quad (2.13)$$

Finally, the Yukawa coupling also introduces mass term for fermions:

$$m_{\psi} = \frac{y_{\psi}v}{\sqrt{2}} \quad (2.14)$$

2.4 CKM Matrix

So far, the way we have formulated the Lagrangian, it only takes one generation of particles into account. However, looking at Fig. 2.1, we can see that there are actually three separate generations of particles. To consider all three generations at once, the Yukawa interaction term of Eq. (2.9) is extended by considering a group of quarks Q_{Li} , u_{Ri} and d_{Ri} . The Yukawa interaction for quarks then becomes:

$$\mathcal{L}_{\text{Yukawa}} = -Y_{ij}^d \bar{Q}_{Li} H d_{Rj} - Y_{ij}^u \bar{Q}_{Li} \epsilon H^* u_{Rj} \quad (2.15)$$

Where the Yukawa coupling $Y^{u,d}$ now becomes a 3×3 complex matrix. Also, the indices i and j both span all three flavors and ϵ corresponds to the 2×2 antisymmetric tensor. This has a few implications. Similarly as before, the Higgs field still assumes its vacuum expectation value, allowing fermions to become massive. Since the Yukawa coupling $Y^{u,d}$ is not a diagonal matrix, the mass eigenstates do not correspond to the gauge eigenstates. Thus, the coupling to the $W^{\pm}$ bosons does not only occur between the same generation. Instead, couplings between generations emerge, that allow the fermions to change between generations. These couplings are described by the Cabibbo Kobayashi Maskawa (CKM) matrix:

$$V_{\text{CKM}} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \quad (2.16)$$

Where the entries of the CKM matrix can be found by diagonalizing the $Y^{u,d}$ matrix. While the elements of the CKM matrix are free parameters, they are still not independent of each other as the matrix must be unitary. The need for unitarity results in six constraints, which do not fully constrain the system. Therefore, experimentally measuring the elements of the CKM matrix exactly, is a viable strategy to test the consistency of the SM.

2.5 Quantum Chromodynamics

Quantum Chromodynamics (QCD) describes the strong interactions of the SM. It is a gauge theory based on the symmetry of the 3-dimensional special unitary group $SU(3)_C$. It is a non-abelian group with 8 generators T^a , which are usually represented by the Gell-Mann matrices, where each of the 8 matrices corresponds to one of the 8 gluons.

The conserved hyperparameter under this symmetry is called color charge. There are three color charges, usually associated with red, green and blue. The only particles that have color charge are quarks and gluons. As such, all other particles are unaffected by the strong force. Quarks carry exactly one color, while antiquarks carry anti-color. Gluons, on the other hand carry one color and one anti-color simultaneously, and are therefore able to change the color charge of quarks.

The QCD Lagrangian is defined as follows:

$$\mathcal{L} = \bar{\psi}(x) [i\gamma^\mu \partial_\mu - g_s \gamma^\mu T_a G_\mu^a - m] \psi(x) - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} \quad (2.17)$$

Where the field strength tensor $G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a - g_s f^{abc} G_\mu^b G_\nu^c$ and f^{abc} correspond to the structure constants of the group (the generators of the adjoint representation). The indices a, b and c each run over the 8 types of gluons. The third term of the field introduces the ability of gluons to interact with each other (self-interaction). Finally, g_s corresponds to the coupling constant of the strong interaction. Often, however, instead of g_s , $\alpha_s = \frac{g_s^2}{4\pi}$ is used.

The $SU(3)_C$ group exhibits special behaviour related to the scaling of α_s . At the level of one loop, α_s scales as follows:

$$\frac{d\alpha_s}{dQ^2} = -\frac{\alpha_s^2}{12\pi Q^2} (33 - 2n_f) \quad (2.18)$$

where n_f corresponds to the number of accessible flavors and Q corresponds to the energy scale of the interaction. Note, that for $n_f \leq 3$, α_s decreases with increasing Q . As a result, the strong force is stronger at large distances and weaker at short distances. Only at high energies does the opposite occur, where the strength of the strong force becomes progressively weaker due to the scaling of α_s and can be described by perturbative QCD. At lower energies, however, non-perturbative QCD is needed to describe the behaviour of the strong force.

An interesting property of color-charged particles is, that they can achieve a color-neutral state by combining with other particles. This combination of particles no longer interacts via the strong force. There are two ways of achieving color neutrality. The first requires all three colors to be equally represented. This is usually achieved by combining three quarks with different color charges, which then form a boson. However, more exotic states of matter such as pentaquarks are also possible [21]. The second way to achieve color neutrality is to combine a quark and an antiquark so that their color charges cancel each other out to form a meson.

As such, they cannot exist as independent particles and will always form into colorless bound states like baryons and mesons (quantum confinement) as it is always energetically favourable to stay in these bound states. Even if one were to try to split these bound particles into individual particles, the energy used to split them would simply result in a new quark-antiquark pair forming to return to colorless states (hadronization). The only exception are top quarks, which decay before hadronization.

Hadronization also has a direct impact on high-energy experiments as it is the cause of jet formation. Jets are cones of particles produced by the separation of color-charged particles. Due to the separation of a color-charged particle from other color-charged particle, it is no longer able to form a color-neutral state. The separated particles begin to radiate large amounts of partons (gluons and quarks) in a process called a parton shower. The radiated particles then form color-neutral bound states in the form of hadrons. This so-called hadronization leads to a clustering of particles all moving in roughly the same direction as the original parton, as shown in Fig. 2.3. This clustered spray of particles is then called a jet.

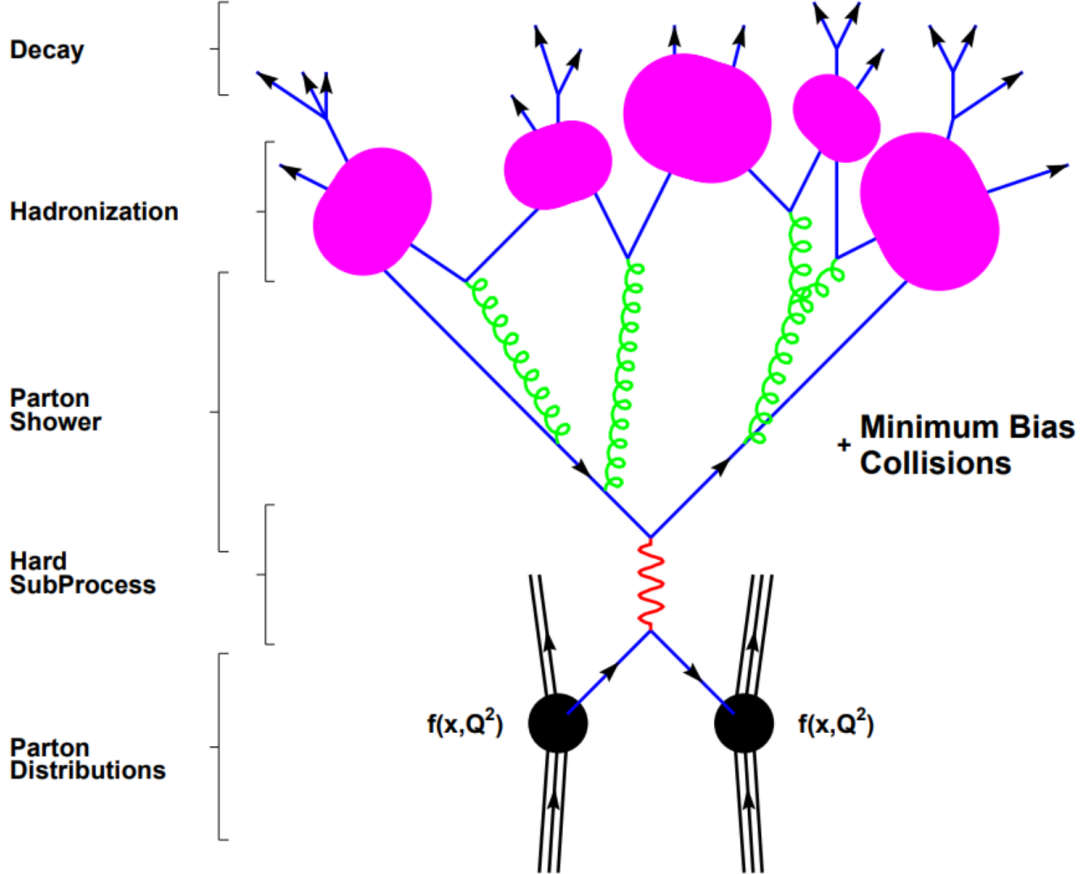


Figure 2.3: Diagram showing the different stages of jet formation. Taken from [22].

2.6 Top Quark and Top-Higgs Associated Processes

This thesis presents three measurements of top quarks in multilepton final states with the two measurements in Sec. 5 and 6 focusing specifically on $t\bar{t}H$ and tH production. As such, the top quark and processes where a H boson is produced in association with one or two top quarks will be introduced more thoroughly in this section.

2.6.1 Top Quark

The top quark was discovered at the Tevatron experiment in 1995 [23, 24] and since its discovery many studies have been performed to study its properties. It is the most massive particle in the SM and the only particle with a Yukawa coupling of order one [10]. The high mass of the top quark makes it especially interesting to study new physics. In the SM, we observed that

heavier particles tend to prefer to decay into more heavy particles. Assuming new particles to be heavier than the SM particles would make the top quark a significant decay product and as such it may prove vital in the search for new physics.

At the LHC, most top quarks are produced in the production of a $t\bar{t}$ pair via gluon fusion (90% BR) or via quark-antiquark annihilation (10% BR). Rarely, also single top quark production occurs via the weak interaction from a W and b boson but it is significantly less likely to occur due to the weak interaction being less prevalent than the strong interaction.

The Feynman diagrams for $t\bar{t}$ and top quark production can be seen in Fig. 2.4.

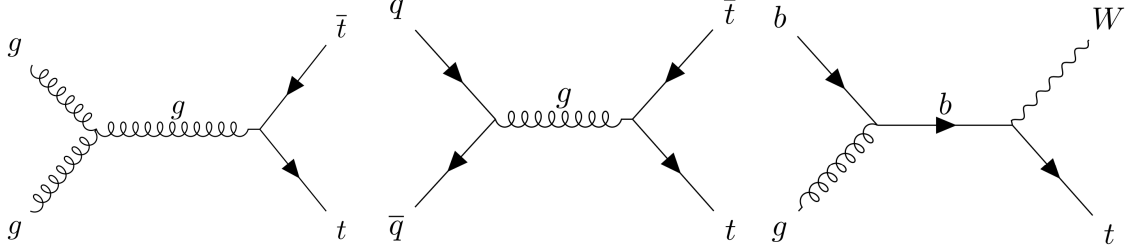


Figure 2.4: Representative Feynman diagrams for the top quark production process. From left to right, in decreasing order of likelihood at LHC: gluon fusion, quark-antiquark annihilation, bW interaction.

Each top quark of the $t\bar{t}$ pair decays rapidly and independently into a $W^\pm b$. Depending on how the $W^\pm$ decays afterwards, we differentiate different topologies.

Most frequently (46% BR), both $W^\pm$ decay fully hadronically into a pair of quarks resulting in a total of 6 jets in the final state. With the highest branching ratio and the events being fully reconstructable due to the absence of neutrinos in the final state, this decay channel offers many interesting advantages. However, at the same time the hadronic decay channel is limited by large backgrounds and the complexity of reconstructing and identifying the produced jets.

Second most frequent is the semileptonic decay mode (45% BR), where only one $W^\pm$ boson decays into a quark-antiquark pair, while the other one decays into leptons. This results in electrons, muons or taus (with their respective neutrinos) in the final state, where each lepton flavor has the same BR. It offers a more limited background compared to the fully hadronic decay mode while also featuring a high branching ratio and a reduced final state multiplicity.

Lastly, both W bosons can decay dileptonically (9% BR), where both $W^\pm$ decay into leptons. Due to having the least background, it is the easiest process to study at the LHC due to detectors like the CMS and ATLAS detector, which are able to detect and reconstruct leptons with high precision. It is mainly limited by its low branching ratio and the presence of two neutrinos in the final state.

The measurements presented in Sec. 4, 5 and 6 all target leptonic final states due to their clean signatures with relatively low background. The dominant SM contributions to these signatures arise from processes in which one or more top quarks are produced in association with a heavy boson or other top quarks. These processes include $t\bar{t}H$ [25], $t\bar{t}W$ [26], $t\bar{t}Z$ [27], tZq [28], tHq [25], $t\bar{t}t\bar{t}$ [29].

2.6.2 Top Associated Higgs Production Processes

As shown in Sec. 2.3, the Yukawa coupling of the Higgs boson to fermions is proportional to the fermion mass. The top quark features the largest mass of the SM [23, 24] particles and as a result it is the only particle with a H Yukawa coupling y_t of roughly order one [10].

Consequently, the production of a H in association with top quarks (tH and t $\bar{t}$ H) represents a significant mode of H boson generation at the LHC, as documented in Ref. [30]. In Run 2 of the LHC, the CMS collaboration has measured the ratio of y_t to its SM expectation, $\kappa_t := y_t/y_t^{\text{SM}}$, to be within $-0.9 < \kappa_t < -0.7$ or $0.7 < \kappa_t < 1.1$, at 95% confidence level (CL) [25] by probing H boson production in association with one or two top quarks in leptonic final states. This measurement has been improved via including more decay modes in Ref. [31], yielding the following best fit: $\kappa_t = 1.01^{+0.11}_{-0.10}$. Fig. 2.5 shows a comprehensive overview of the Yukawa couplings measured so far.

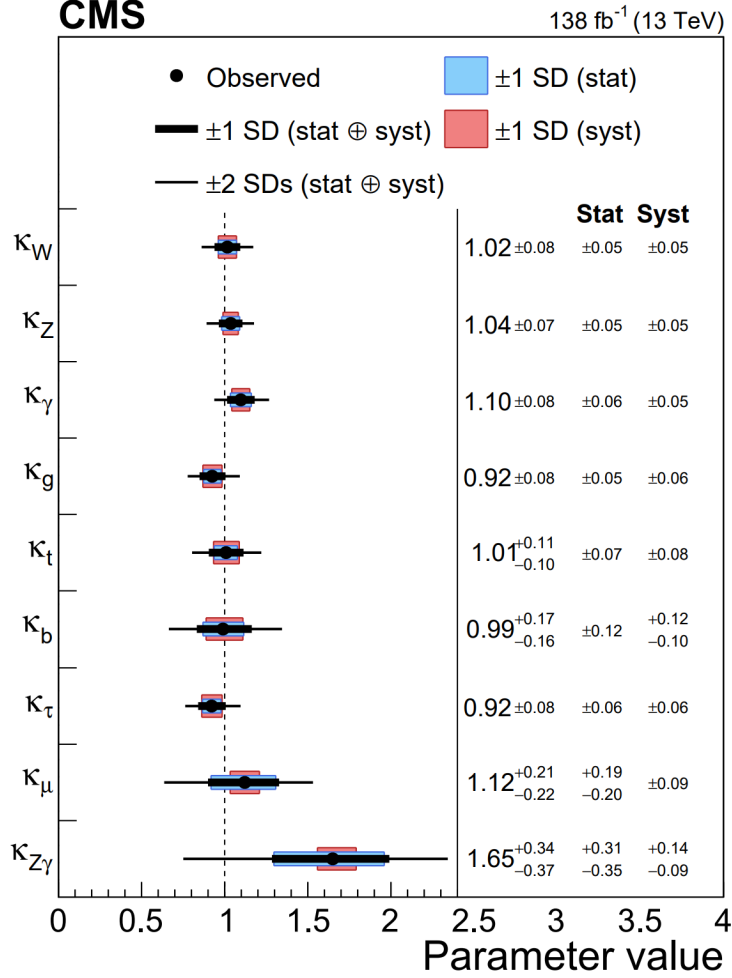


Figure 2.5: Yukawa couplings to various fermions and bosons. Taken from Ref. [31].

The SM² predicts a cross section of 506.5 fb [32] t $\bar{t}$ H production at $\sqrt{s} = 13$ TeV at a H boson mass of $m_H = 125.38$ GeV with the corresponding Feynman diagrams shown in Fig. 2.6. For tH production, we observe three main production modes. The dominant production mode occurs via the t-channel (tHq) with a cross section of 74.3 fb [32], which can be seen in Fig. 2.7. The tW (tHW) associated channel features the second highest cross section with 15.2 fb [32]. The representative Feynman diagrams for tW associated production are shown in Fig. 2.8. Lastly, tH production also occurs via the s-channel at a cross section of 2.9 fb [32] and can be seen in Fig. 2.9.

²This value is computed at next-to-leading accuracy in QCD together with EWK corrections computed at the same order in perturbation theory.

Due to destructive interference occurring between the tHq and tHW diagrams where the H boson couples either to the top quark (left-side diagrams of Fig. 2.7 and 2.8) or to the W boson (right-side diagrams of Fig. 2.7 and 2.8) according to the SM prediction, the cross sections of their production modes are rather small. However, their rates are altered significantly if the value of y_t were to differ from its SM prediction. Assuming a negative y_t , often also referred to as the inverted top coupling (ITC) scenario, we would see a large enhancement of the tH production rate. In this case, the negative sign of y_t changes the destructive interference described before into a constructive interference, which in the largest case changes the cross section of tH production from 74.3 fb to 848.0 fb [32]. As a consequence, measuring the tH production rate allows us a determination of the relative sign of y_t with respect to the W-H coupling on top of a model independent determination of the magnitude of y_t .

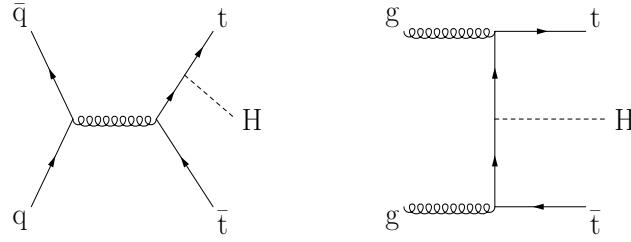


Figure 2.6: Representative Feynman diagrams for the $t\bar{t}H$ production processes.

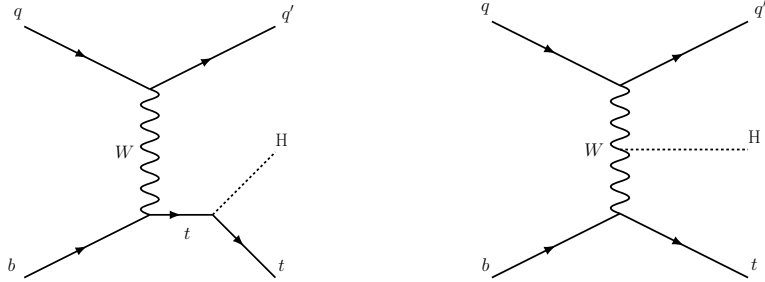


Figure 2.7: Representative Feynman diagrams for the t-channel tH production processes.

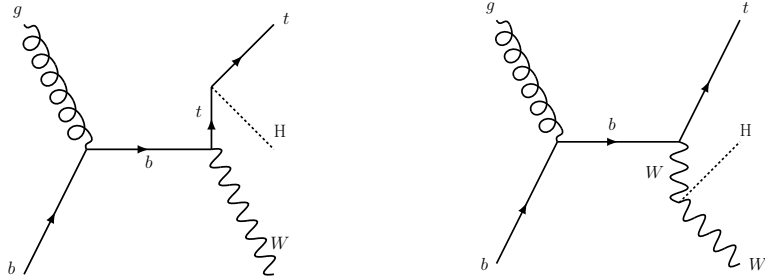


Figure 2.8: Representative Feynman diagrams for the tW-associated tH production processes.

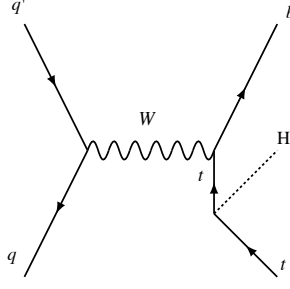


Figure 2.9: Representative Feynman diagram for the s-channel tH production processes.

2.7 Physics Beyond the Standard Model

2.7.1 Open Topics in the Standard Model

Although, the SM describes many processes with great accuracy, there are still phenomena that it cannot explain. This section introduces some of these open problems.

Naturalness

The open problem of naturalness within the SM [33] revolves around the question of why certain fundamental parameters, such as the mass of the H boson, seem to be finely tuned to maintain the stability of the universe at quantum scales. In the case of the H boson mass, loop corrections from the fermions and bosons to the H boson propagator, like the ones on Fig. 2.10, have a significant effect. These corrections are dominated by the top quark which couples the strongest to the H boson due to it being the particle with the largest mass.

$$\Delta m_H^2 = \text{---} \text{H} \text{---} \text{---} \text{H} \text{---} + \text{---} \text{H} \text{---} \text{---} \text{H} \text{---} + \dots$$

Figure 2.10: Relevant corrections to the H boson propagator due to top quark loops (left) and top squark loops (right)

Since the mass of the H boson is highly sensitive to the quantum corrections from virtual particles, this leads to an apparent discrepancy between its observed mass and the mass predicted by these corrections. A large amount of fine-tuning is required to reconcile these values. This in turn raises concerns about the SM itself, since physical constants and masses should not require excessive fine-tuning to produce the observed results. Resolving the problem of naturalness could lead to a more complete description of the universe and provide a more satisfying explanation for the observed hierarchy masses and interactions in the SM. Alternatively, it might also be that this is only a perceived issue as these values just happen to naturally occur in this way and we overvalue their importance.

Neutrino Masses

Unlike other elementary particles, neutrinos have no natural mechanism for acquiring mass in the SM. However, experimental evidence from neutron oscillation experiments [34, 35] suggests that neutrinos are indeed massive. As such, neutrinos oscillate between different states as they propagate through space. The inability of the Higgs mechanism to generate neutrino masses as well as the absence of right-handed neutrinos in the SM raises questions about the underlying nature of neutrinos as they could imply new particles or interactions beyond the SM.

Lepton Flavor Universality

Lepton flavor universality (LFU) is a fundamental principle in the SM. It states that the three lepton families (electron, muon, and tau) interact with the EWK force identically, except for mass-induced differences. However, recent experimental data has raised questions about LFU, particularly in the decay of B mesons. Both the LHCb and Belle II experiments have measured the ratios of R_K , R_{K^*} , $R(D)$ and $R(D^*)$ [36–47] and put tension on the SM prediction of LFU.

Gravity

Although general relativity and the SM are both very successful theories, scientists have not yet been able to unify them into one theory. Several theories attempt to introduce gravity via a spin 2 mediator, called the graviton [48]. The SM does not include a description of gravity as a QFT. However, compared to the other fundamental forces, the effects of gravity are negligible in the accessible energy range. Only at the Planck scale, which is 15 orders of magnitude higher than the TeV scale at which the LHC currently operates, are the effects of gravity assumed to be relevant. This immense difference in scale sheds light on parts of the hierarchy problem, since the SM does not propose a natural reason for such a large discrepancy between the weak and the Planck scale.

Dark Matter

Many astrophysical and cosmological observations, such as galactic rotation curves, gravitational lensing, and the cosmic microwave background, suggest the presence of a non-luminous, invisible form of matter that exerts a gravitational influence on visible matter. However, the SM has no particles that can account for the observed gravitational effects, motivating the search for new particles that make up dark matter. Several candidates have been proposed with two prominent ones being Weakly Interacting Massive Particles (WIMPs) [49] and axions [50–52]. Both require new theoretical extensions of the SM to be fully integrated.

2.7.2 CP Violation and the Strong CP Problem

CP symmetry is a fundamental principle in particle physics that posits, that laws of physics should remain unchanged if a particle is replaced by its antiparticle (Charge conjugation, C) and then spatial coordinates are inverted (Parity, P). Observations indicate that there is a significant imbalance between matter and antimatter in the observable universe, with matter overwhelmingly predominating, often called the baryon asymmetry of the universe [53]. As a result, there is a strong motivation to look for CP violating processes as they provide a mechanism to generate this imbalance by favoring processes that produce matter over antimatter.

As the SM allows for CP violation in the strong sector, extensive searches have been performed measuring the level of CP violation in the strong sector [50–52, 54–58]. However, CP violation has been observed to be markedly absent in strong interactions. This non-observation of CP violation despite its allowance is called the strong CP problem [12, 13].

Searches for CP violation in the strong sector are closely related to searches for a neutron Electric Dipole Moment (EDM), which so far shows no signs of CP violation [57, 58]. Many theoretical attempts to resolve this discrepancy include the Peccei-Quinn theory [59], which posits an additional U(1) symmetry and predicts the existence of an axion, a hypothetical particle that could also account for dark matter. However, so far no axion has been found [50–52, 54–56].

CP violation is also observed in the SM through the CKM matrix in the electroweak sector. Specifically, CP violation can be observed in processes involving the decay of K mesons and B mesons, where the weak force allows for a quark to change its flavor in a manner, that does not treat matter and antimatter symmetrically [60–63]. However, the amount of CP violation observed so far cannot account for all of the baryon asymmetry of the universe, indicating that there must be other CP violating processes as well.

The top quark’s strong coupling to the H boson and its large mass make it an excellent probe for potential CP-violating effects within the Higgs sector. The SM H boson is purely CP-even. This means that any experimental observation compatible with the presence of a CP-odd term in the H boson Lagrangian would be a direct indication of the presence of new physics.

The ATLAS and CMS Collaborations have studied the couplings of the H boson to Vector gauge bosons (V) and also tested such interactions for CP violation [64–80]. All studies showed no signs of pure CP-odd couplings of the H boson to any gauge boson and were compatible with a pure CP-even H boson Lagrangian. Overall, these CP-odd contributions are expected to only yield a minor contribution to the coupling.

In couplings to V bosons, CP-odd contributions may only enter via nonrenormalizable higher-order operators that are suppressed by powers of $1/\Lambda^2$ [81], where Λ is the scale of the physics beyond the SM in an effective field theory, or via nonrenormalizable interaction terms [82, 83].

In couplings between the H boson and fermions however a renormalizable CP-violating coupling can occur at tree level providing a stronger theoretical motivation for CP violating effects to appear compared to couplings to V bosons. As a result, the top-Higgs Yukawa coupling is a great candidate to study the CP structure of couplings between the Higgs boson and fermions in proton-proton collisions [84].

Several searches for CP violation in the coupling of the H boson to fermions have been performed by the ATLAS and CMS Collaborations. So far, no deviations from the SM prediction of a purely CP-even scenario have been observed.

The coupling of the H boson to tau leptons was studied in Ref. [85]. Additionally, measurements of the CP structure of the coupling of the H boson to the top quark were performed using $t\bar{t}H$ and tH production modes with different final states. Measurements with the final states of two photons [77, 78] or four leptons [79] have been performed, which all were in agreement with the SM prediction. Lastly, the CP measurements in the gluon-gluon fusion production mode can also be interpreted in terms of fermionic couplings [79, 86, 87].

In Sec. 5 a measurement of the CP structure top-Higgs Yukawa coupling is presented targeting $t\bar{t}H$ and tH production in multilepton final states.

2.7.3 Standard Model Effective Field Theory

There are two ways to look for new physics. The first way is to search for new physics directly via the production of new particles. The second, more indirect approach, consists of looking for novel interactions of known particles in the SM. In the following explanation, as well as in the analyses covered in this thesis, I will focus in the latter. Generally, to extend the SM, we expand it via an Effective Field Theory (EFT) [88–90].

A desirable feature for any description of non SM interactions is to be model independent. This allows us to search for new physics without committing to a particular extension of the SM. Also, if no new physics are observed, it allows us to quantify at which accuracy we are able to exclude new Physics.

There are several features we want to be included in an extension of the SM.

1. Any extension of the SM needs to satisfy the S-matrix axioms of unitarity, analyticity and relativity.
2. The symmetries of the SM (Lorentz-invariance and $SU(3)_c \times SU(2)_L \times U(1)_\gamma$ gauge symmetry) need to be respected.
3. We need to be able to recover the SM in an appropriate limit.
4. It needs to be general enough to be able to capture any physics beyond the SM, while also giving us guidance as to where new physics are more likely to appear.
5. We need to be able to calculate radiative corrections at any order in SM and new interactions in the extended theory.

The SM itself is the most general theory of quark and lepton fields together with a single Higgs doublet field interacting via a $SU(3)_c \times SU(2)_L \times U(1)_\gamma$ gauge symmetry. All operators in the Lagrangian of the SM are restricted to be of mass dimension four³.

We can extend this theory by adding operators of higher dimensions. A dimensional analysis tells us, that these operators have coefficients of inverse powers of mass. This means, that they are suppressed if the mass is large compared to the experimentally accessible energies. As a result, lower dimensions will generally be dominant. Also, we exclude odd dimensional operators, as they violate both lepton and baryon number [88]. Another feature is, that only a few of these operators contribute to a given physical process [91, 92].

The Lagrangian then becomes:

$$\mathcal{L} = \mathcal{L}_{\text{SM}} + \sum_i \frac{c_i}{\Lambda^2} \mathcal{O}_i + \dots \quad (2.19)$$

Where $\mathcal{L}_{\text{SM}}$ is the SM Lagrangian and $\mathcal{O}_i$ corresponds to the dimension 6 operators. c_i are dimensionless coefficients to parameterize the strength at which the new physics operators couples to the SM. Dimension 8 operators are also allowed but more suppressed than dimension 6 operators. Hence, we expect the dimension 6 operators to be dominant. As a result, often only dimension 6 operators are considered, as it is done for example in the measurement presented in Sec. 4. This new Lagrangian also fulfills the requirement to recover the SM at the limit $\Lambda \rightarrow \infty$. Also, this expansion allows us to calculate radiative corrections at any order in SM and new interactions.

³Besides the quadratic term of the Higgs potential are all of dimension four.

432 Lastly, we need to specify the particle content of the theory. This means, we need to specify
433 which fields are constructed from the operators $\mathcal{O}_i$ and present at low energies (below Λ). The
434 included fields are the SM fields including the Higgs doublet field and nothing else.

435 Any minimal, non-redundant set of operators is called a basis. As such, there are an infinite
436 amount of bases to choose and several distinct constructions might offer different advantages
437 depending on the use-case. Generally, the choice of basis depends on which one is more con-
438 venient for the specific application as one can always transform one basis into another. The
439 measurement presented in Chap. 4 uses the Warsaw basis, which is a common choice for many
440 analyses. A construction of the Warsaw basis for one generation of SM fermions can be found
441 in Ref. [93], which was later extended to three generations of fermions in Ref. [94]. It includes a
442 complete basis of dimension 6 operators and is characterized by 2499 independent parameters.

3 The LHC and the CMS experiment

3.1 Large Hadron Collider

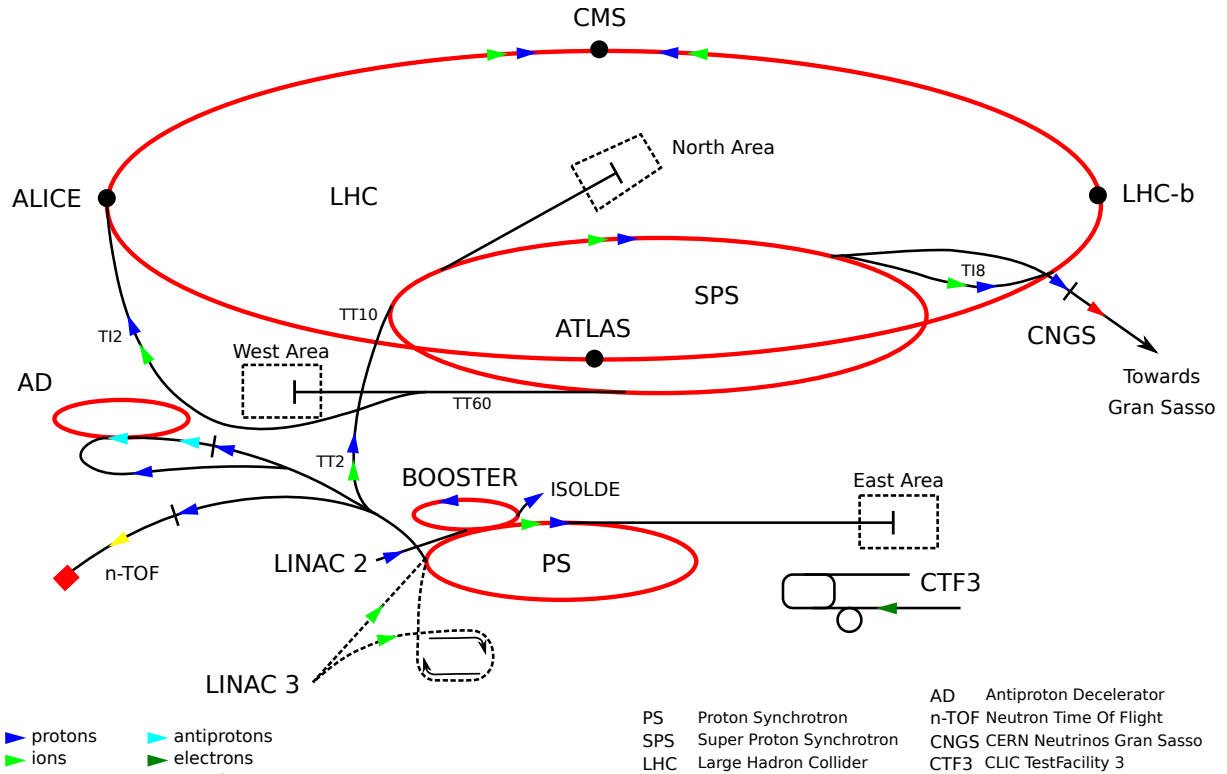


Figure 3.1: The full LHC accelerator chain including the LHC. Figure originally from [95].

The Large Hadron Collider (LHC) is a circular proton-proton collider located in an underground tunnel on the Swiss-French border near Geneva. With a diameter of 27 km, it is the largest physics experiment in the world.

The collider itself accelerates two beams of hadrons to a centre-of-mass energy of $\sqrt{s} = 13$ TeV and then collides the two beams in opposite directions inside the circular collider. In the subsequent collisions, the available energy is used to create new particles.

The LHC was designed to study the properties of the SM of particle physics. A major focus has been on the potential discovery of the H boson, which was subsequently discovered in 2012 by the CMS [1, 3] and ATLAS [2] collaborations, and on the search for physics beyond the SM. This is done by either looking for inconsistencies between measurements and the SM, or even by means of direct searches for new physics.

To accelerate the protons, the LHC uses an accelerator chain, in which the protons pass through several stages using earlier CERN accelerators as boosters. In the first stage, protons are created by ionising hydrogen gas and stripping the hydrogen nucleus of its valence electron. The protons are then injected into a radio-frequency quadrupole, which bundles and accelerates them

into beams. Following this step, the protons are accelerated to 50 MeV in the linear accelerator LINAC2 [96]. In the next step, they are injected into the Proton Synchrotron Booster [97], which accelerates them to 1.4 GeV. They then enter the Proton Synchrotron [98], which boosts them further to 26 GeV. In this special step, the bunch structure is set, which groups the protons into discrete bunches. From there, the protons enter the Super Proton Synchrotron [99], where they are accelerated to 450 GeV. After this final stage, the protons are injected into the LHC. Here they reach their final centre-of-mass energy of 13.6 TeV.

Inside the LHC, the energy of the protons is increased by a set of 16 superconducting radio frequency cavities operating at a frequency of 400 MHz. Each of these cavities further accelerates the protons with an acceleration voltage of 2 MeV. To keep the structure of the bunches intact and prevent them from smearing out over time, the voltage is synchronised with the proton bunches so that earlier arriving protons are accelerated less and later arriving protons are accelerated more, effectively focusing and narrowing the bunches.

To keep the protons on their circular trajectory, the LHC uses a set of superconducting niobium-titanium dipole magnets. To preserve the superconducting properties of these magnets, they are cooled down to 1.9 K using a liquid helium circuit. In addition to the dipole magnets used for bending, there are also sets of quadrupole magnets located between the bending magnets. They allow the beam to be focused perpendicular to the direction of motion, helping to reduce beam losses.

There are a total of four collision points along the LHC, where additional magnets are placed to further focus the beam and direct it to the collision points. Several experiments are hosted along the LHC ring, each with their own areas of operation. An important consideration, was the instantaneous luminosity for each of the experiments, translating roughly to the collision rate. The ATLAS [100] and CMS [7, 8] experiments are designed for a high instantaneous luminosity $\mathcal{L} = 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$. Additionally, there are two experiments designed for a lower luminosity. The LHCb experiment [101] focuses on b-quark physics and aims for a luminosity of $\mathcal{L} = 10^{32} \text{ cm}^{-2} \text{ s}^{-1}$, while the TOTEM experiment [102] focuses on proton scattering at small angles and aims for a luminosity of $\mathcal{L} = 2 \cdot 10^{29} \text{ cm}^{-2} \text{ s}^{-1}$.

Alternatively, the LHC can also be filled with heavy ions, typically Pb, allowing for a wide range of additional studies. The ALICE experiment [103] focuses exclusively on heavy ion Pb-Pb collisions with a target luminosity of $\mathcal{L} = 10^{27} \text{ cm}^{-2} \text{ s}^{-1}$.

As already mentioned above, instantaneous luminosity is an important figure of merit besides the center-of-mass energy. It defines the relation between the event rate and the cross section of a process with a given cross section σ .

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

The instantaneous luminosity only depends on the experimental setup and is process independent. It can be approximated by

$$\mathcal{L} = \frac{n_b N_p^2 f}{4\pi\sigma_x\sigma_y} R \quad (3.2)$$

where N_p corresponds to the number of protons per bunch, n_b to the number of colliding bunches, f to the beam revolution frequency, $\sigma_{x,y}$ to the beam sizes along the transverse directions of the beam and R to a geometric reduction factor to account for the crossing angle at the

interaction point.

Additionally, some measurements not only measure the cross section of processes but also something called a differential cross section. This compares certain observable distributions, such as particle momentum or energy, with their theoretical expectations, allowing an even more detailed comparison as a further way of testing the SM or searching for new physics.

Closely related to the instantaneous luminosity is the integrated luminosity L , which will be referred to in this paper as the luminosity alone. As the name suggests, the integrated luminosity is the integral over time of the instantaneous luminosity.

$$L = \int \mathcal{L} dt \quad (3.3)$$

For Run 2 of the LHC, data was taken in the years of 2016, 2017 and 2018 by the CMS experiment with the integrated luminosity shown in Fig. 3.2.

To achieve such high luminosity, the protons are collimated into bunches, as explained above. As a result, multiple collisions occur at each bunch crossing, leading to overlapping collisions inside the detector, a phenomenon known as Pile-Up (PU), which is one of the many challenges the LHC experiments face. Experiments such as the CMS must then try to extract and distinguish the particles from a single collision (often the most energetic). The PU levels during the LHC's Run 2 [104] can be seen in Fig. 3.2 with the average number of PU interactions being 27, 38 and 37 during its operation in 2016, 2017 and 2018.

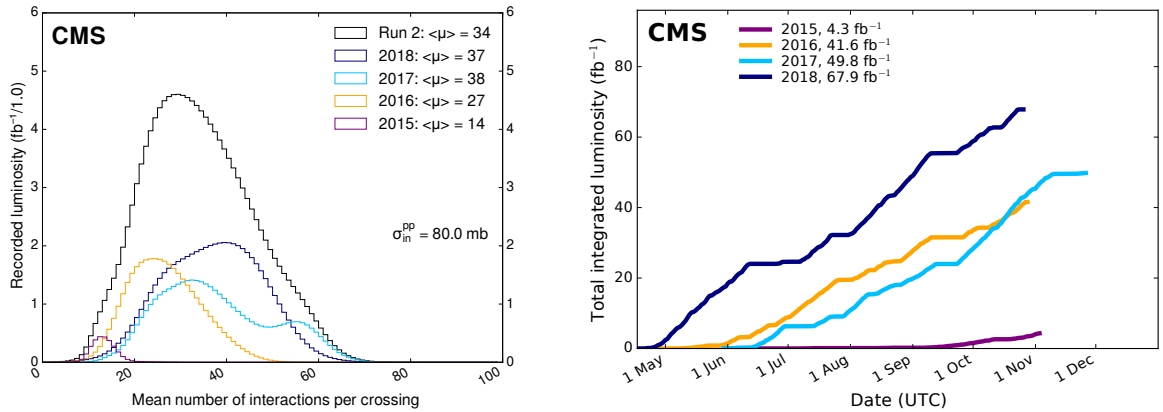


Figure 3.2: Left: Distributions of the number of interactions per bunch crossing representing the number of pile-up interactions. Right: Integrated luminosity of the LHC during Run 2. Note, that the actual integrated luminosity measured by the CMS detector might be slightly lower due to the inactive periods of the detector. Taken from [105].

3.2 CMS Experiment

The CMS experiment is one of the LHC's general-purpose high-luminosity detectors, the other being ATLAS. As such, it aims to measure a wide range of processes. As its name suggests, it was designed with a particular focus on muon detection. A central feature of the CMS detector is its superconducting solenoid with an inner diameter of 6 m and a length of 14 m, which generates a magnetic field of 3.8 T and allows a good resolution of muons. In addition, the CMS detector

includes a granular tracking detector and hermetic calorimeters.

A general sketch of the CMS detector and its components can be seen in Fig. 3.3. It also shows how the subdetectors are usually divided into two parts. The first part is the central part surrounding the beam pipe, which is usually called the barrel. The second one are the endcaps located at the side of the barrel, which help to increase the acceptance.

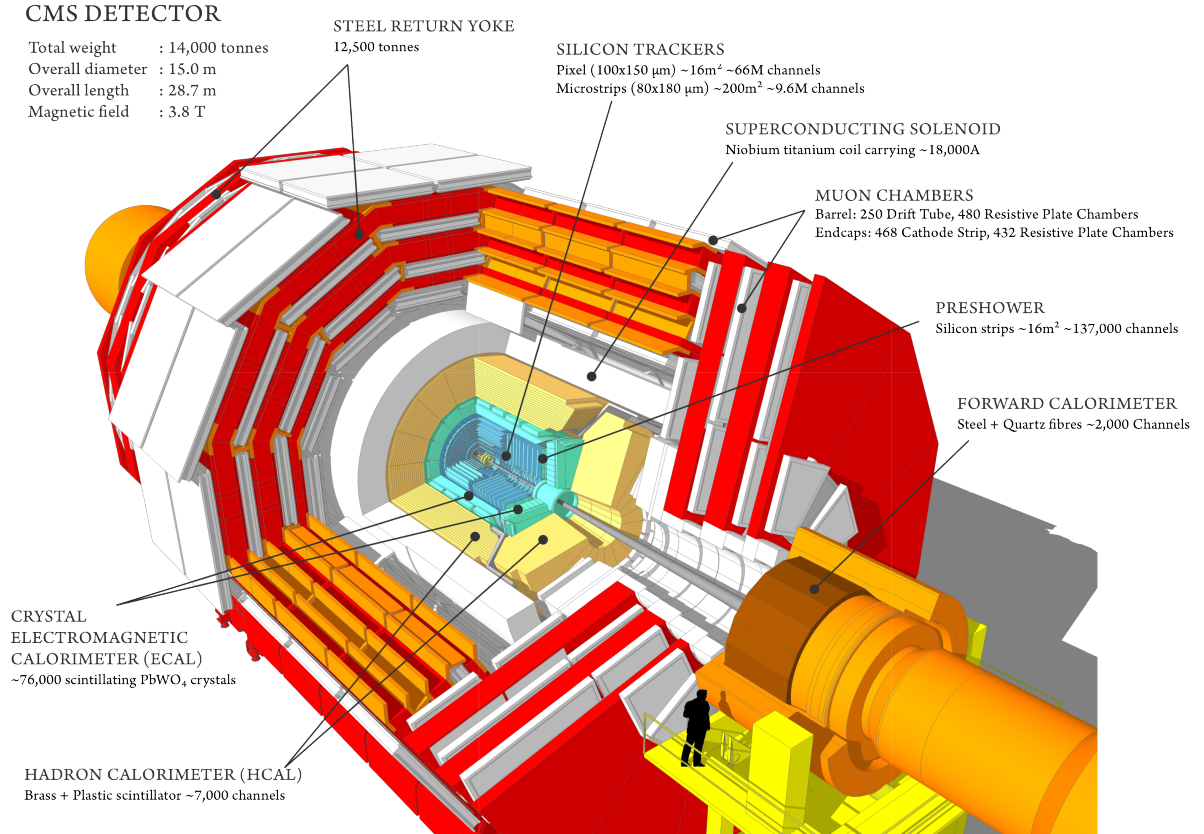


Figure 3.3: Layout of the CMS detector and its main components. Taken from [106].

The general behaviour of different particles travelling through the CMS detector is shown in Fig. 3.4. Details, on how the individual components work, can be found in their corresponding subsections.

3.2.1 Coordinate System and Notation

The origin of the coordinate system used in CMS is at the collision point in the centre of the detector. The z -axis points into the direction of the beams, while the x and y -axes are perpendicular to the beam direction. The y -axis points upwards, while the x -axis points inwards at the centre of the LHC ring. We can then define a radial coordinate r in the x - y -plane. Together with the azimuthal angle ϕ , measured in the x - y -plane from the y -axis, and the polar angle θ , measured from the z -axis, they form a complete set of polar coordinates. Often however, θ is discarded in favor of the pseudorapidity η , defined as

$$\eta = \ln \tan \left(\frac{\theta}{2} \right) \quad (3.4)$$

This is due to the fact, that the difference in pseudorapidity between two particles is Lorentz

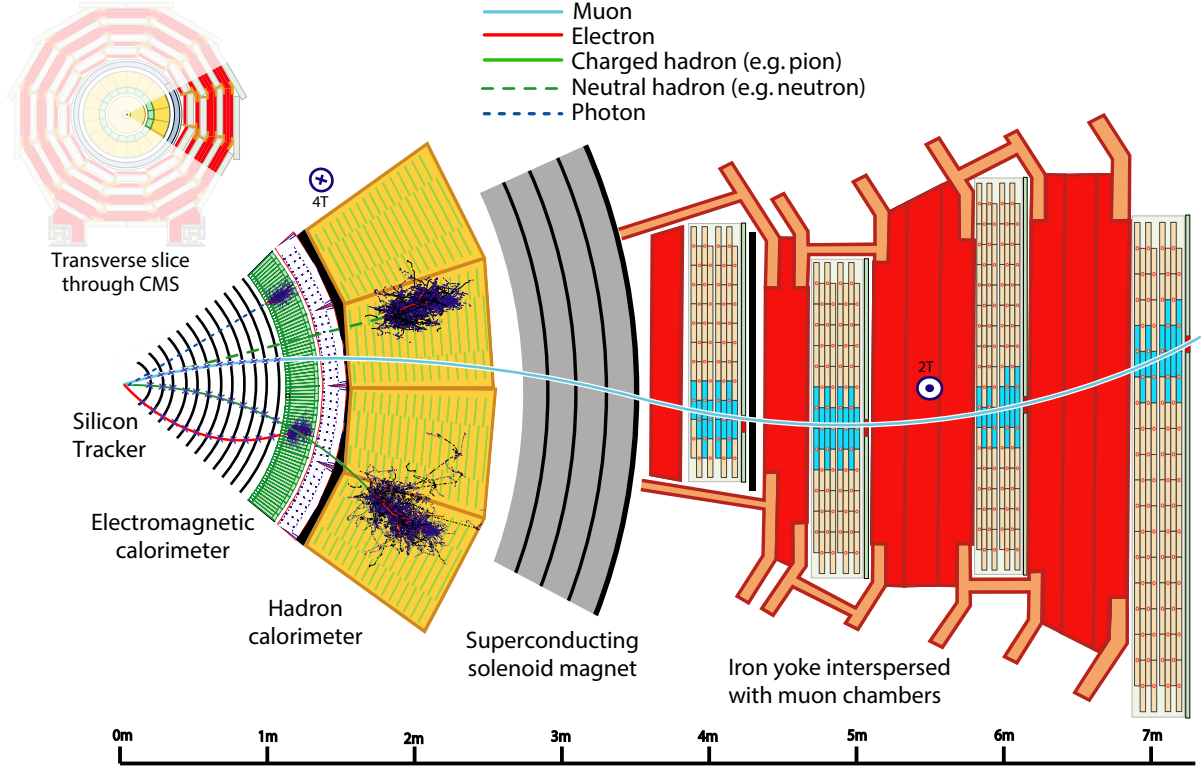


Figure 3.4: Showcase of a slice of the CMS detector showing its components and the behaviour of different particles. Taken from [107].

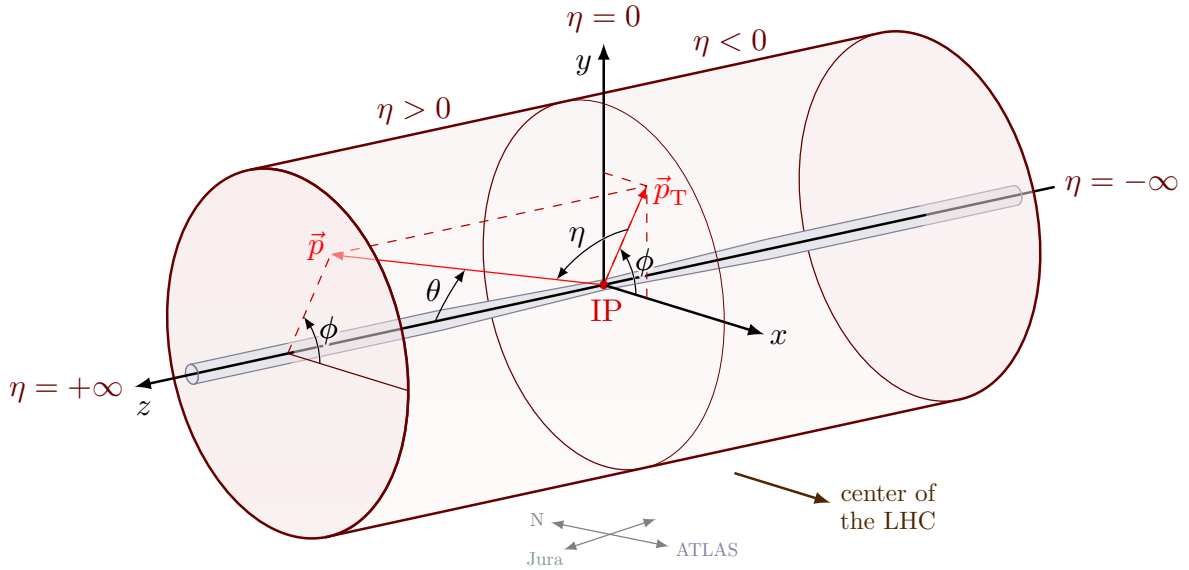


Figure 3.5: Scheme of the CMS coordinate system. Taken from [108]

invariant for boosts along the beam direction. Although Lorentz invariance only applies to massless particles, it proves to be an accurate approximation for massive particles due to their high energies. Thus, angular differences between particles are usually measured as ΔR , defined as

$$\Delta R = \sqrt{\Delta\phi^2 + \Delta\eta^2} \quad (3.5)$$

Finally we define the momentum transverse to the beam direction as p_T . Fig. 3.5 shows the

544 CMS coordinate system with the information discussed above.

545 3.2.2 Tracker

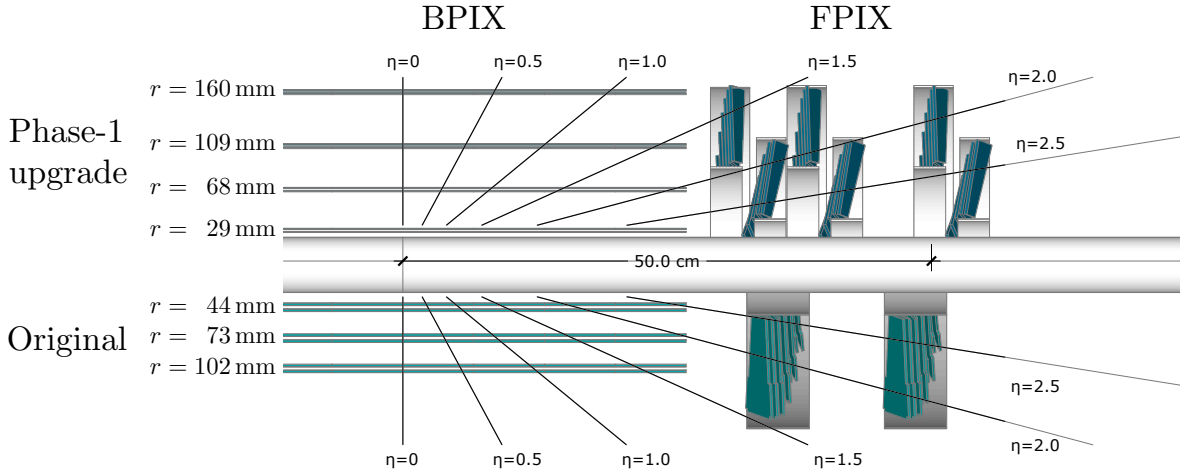


Figure 3.6: Schematic view of the IT and the changes made during the phase-1 upgrade during the extended year-end technical stop of the LHC in 2016/2017. Taken from [109].

546 The tracker consists of the Inner Tracker (IT), which is the part of the detector closest to the
547 interaction point, and the Outer Tracker (OT).

548 Moving outwards from the interaction point, particles first encounter the IT of the CMS
549 detector [110, 111]. Its task is to precisely track the path, momentum, and impact parameter of
550 charged particles produced in the high-energy proton-proton collisions. The electrically charged
551 high-energy particles produced in the central collision, leave ionized traces as they pass through
552 the silicon material, which are then used to reconstruct the particle tracks. With its current
553 design, it is able to reconstruct high p_T tracks with an efficiency of more than 95% for isolated
554 tracks with an efficiency reaching 90% in the $|\eta| < 2.5$ range for tracks contained within jets.
555 Like other components of the CMS detector, the tracker is also split into a barrel section covering
556 the pseudorapidity range of up to $|\eta| \leq 1.8$, and an endcap section covering the range of $1.8 < |\eta| < 2.5$.
557 Due the proximity of the IT to the interaction point, its occupancy is very high, which
558 raises the need for a very granular and fast readout. Not only does the high occupancy increase
559 the need for very fine spatial resolution, but a fine granularity is also required to reconstruct
560 particle tracks with sufficient precision. Thus, the IT, often referred to as a pixel detector,
561 consists of 3(4) layers in the barrel region and 2(3) disks in the endcap (from 2017) made of very
562 granular silicon pixel detector with a spacial resolution between 10 to 15 μm .

563 The OT on the other hand consists of silicon strip detectors, which allow for a 2D spatial
564 resolution and is located 20 to 116 cm away from the interaction point. Being further away from
565 the interaction point, they experience a lower occupancy. There, silicon strip detectors provide
566 sufficient radiation hardness and resolution, while simultaneously being a cheaper alternative
567 to the pixel detectors and requiring less power and readout channels, making them a perfect
568 candidate for the OT.

569 Each charged particle leaves a series of hits in the tracker which can then be used to recon-
570 struct various parameters. The reconstructed parameters include the particle tracks, impact
571 parameters, momentum and even the charge of the particles, which is reconstructed from the

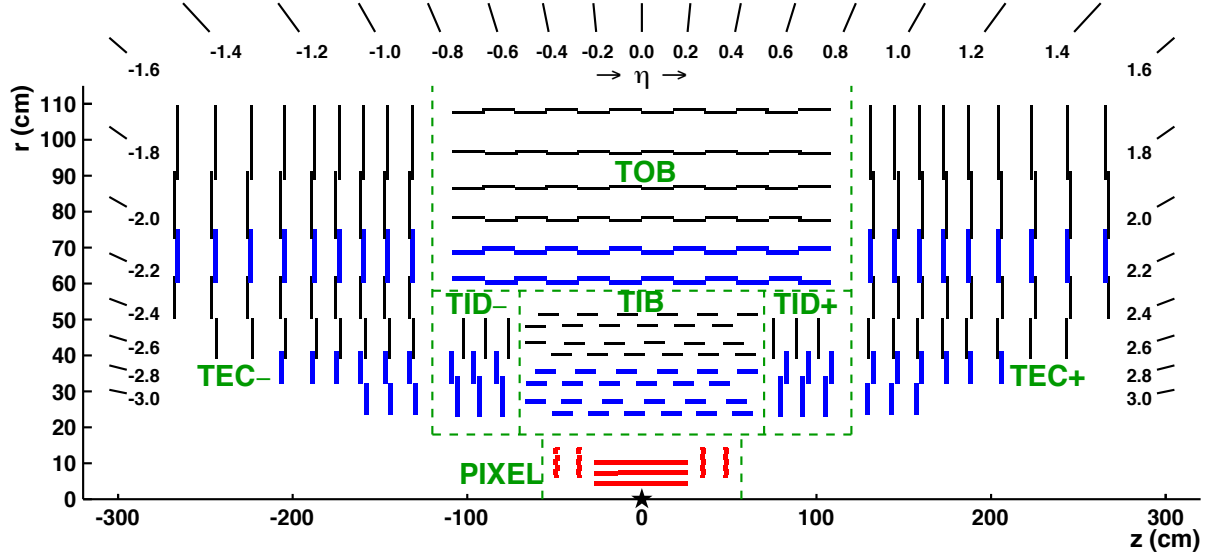


Figure 3.7: Schematic view of the tracker. The red part shows the IT while everything else belongs to the OT. Taken from [112].

curvature of their tracks due to the magnetic field provided by the solenoid magnet.

3.2.3 Calorimeters

Situated in between the tracker and the solenoid are the calorimeters. Their task is to measure the energy of the particles produced in the collision. On the side closer to the interaction point lies the Electromagnetic Calorimeter (ECAL) [113, 114]. With the ECAL targeting electrons, positrons and photons, these particles deposit all their energy in the ECAL. Outside of the ECAL lies the Hadronic Calorimeter (HCAL) [115, 116]. Due to the limited space between the ECAL and the solenoid, parts of the HCAL are actually located outside of the solenoid.

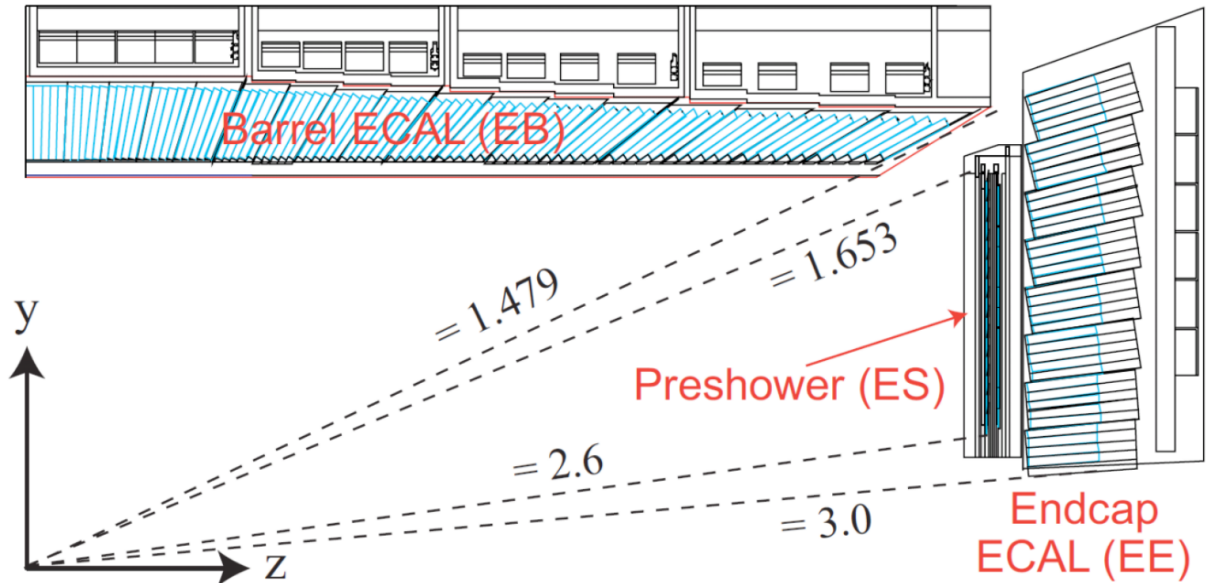


Figure 3.8: Schematic view of the ECAL, showing the barrel section, as well as the endcap section with the preshower detectors. Taken from [114].

The ECAL is a scintillation calorimeter made with lead tungstate ($PbWO_4$) crystals. These crystals provide good radiation hardness, a very high density and therefore a very short radi-

tion length. Another advantage is their small Moliere radius. The scintillation light then gets captured with specialized photodetectors to compensate for their comparatively low light yield. It consists out of a barrel section, which covers the pseudorapidity range of $\eta \leq 1.48$, and an endcap section, which covers the pseudorapidity range of $1.65 \leq \eta \leq 2.6$, as shown in Fig. 3.8. Compared to the barrel section, the endcap section has a reduced granularity. However, to compensate for this, it incorporates preshower detectors installed before the lead tungstate crystals. They help to increase the granularity to the level necessary to be able to distinguish between similar looking classes of processes, such as the decay of a neutral pion which has a similar signature than a high-energy photon.

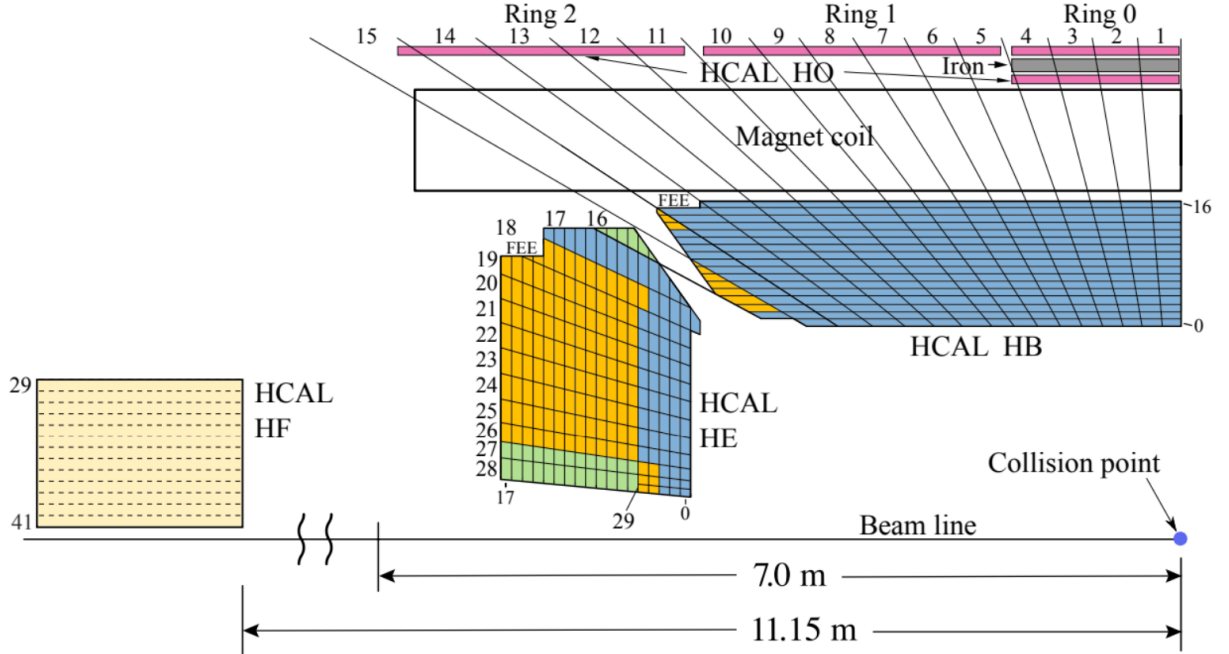


Figure 3.9: Schematic view of the HCAL, showing the barrel section, as well as the endcap section. Taken from [116].

Since the HCAL targets hadrons, it is designed in a way that hadrons deposit all their energy in the HCAL. However, since hadrons have to pass through the ECAL before reaching the HCAL, the ECAL is designed, so that hadrons deposit only a small amount of energy in the ECAL. The HCAL is the only part of the detector allowing us to measure the energy of neutral hadrons and provides a complimentary measurement to the charged hadron measurement of the tracker. Its high energy resolution and hermeticity also help to accurately measure the energy of neutral particles, and as such, with its extensive coverage of the outgoing particles, is crucial to measure the missing transverse energy.

As already mentioned above, the HCAL surrounds the ECAL and can be seen in Fig. 3.9. It is a sampling calorimeter with brass layers, chosen for their short interaction length, interspersed with plastic scintillators. Similar to the ECAL, the HCAL consists of a barrel section, covering the range of $\eta \leq 3$ and an endcap section. The endcap section is split between the HCAL cover and the very forward calorimeter, which extends the coverage of the entire endcap section up to $3 \leq \eta \leq 5$. Unlike the rest of the HCAL, the very forward calorimeter is made out of steel and quartz fibres. This has the advantage of shorter hadronic showers which provide better absorption of very forward hadron showers.

3.2.4 Solenoid Magnet

The superconducting magnet is one of the main features of the CMS detector and is located between the calorimeters and the muon system. It consists of niobium-titanium ($NbTi$) cables which are cooled to 1.9 K to achieve superconductivity. A special cooling system using liquid helium is used to cool the magnet to this temperature. It has a length of about 13 m and a diameter of about 6 m, creating a magnetic field of 3.8 T inside the magnet and 2 T on the outside.

The strong magnetic field is crucial in identifying particles as they pass through the detector. The stronger the magnetic field, the greater the curvature of charged particles passing through it. This allows to infer the charge and the p_T of particles from the curvature of their trajectory.

3.2.5 Muon Spectrometer

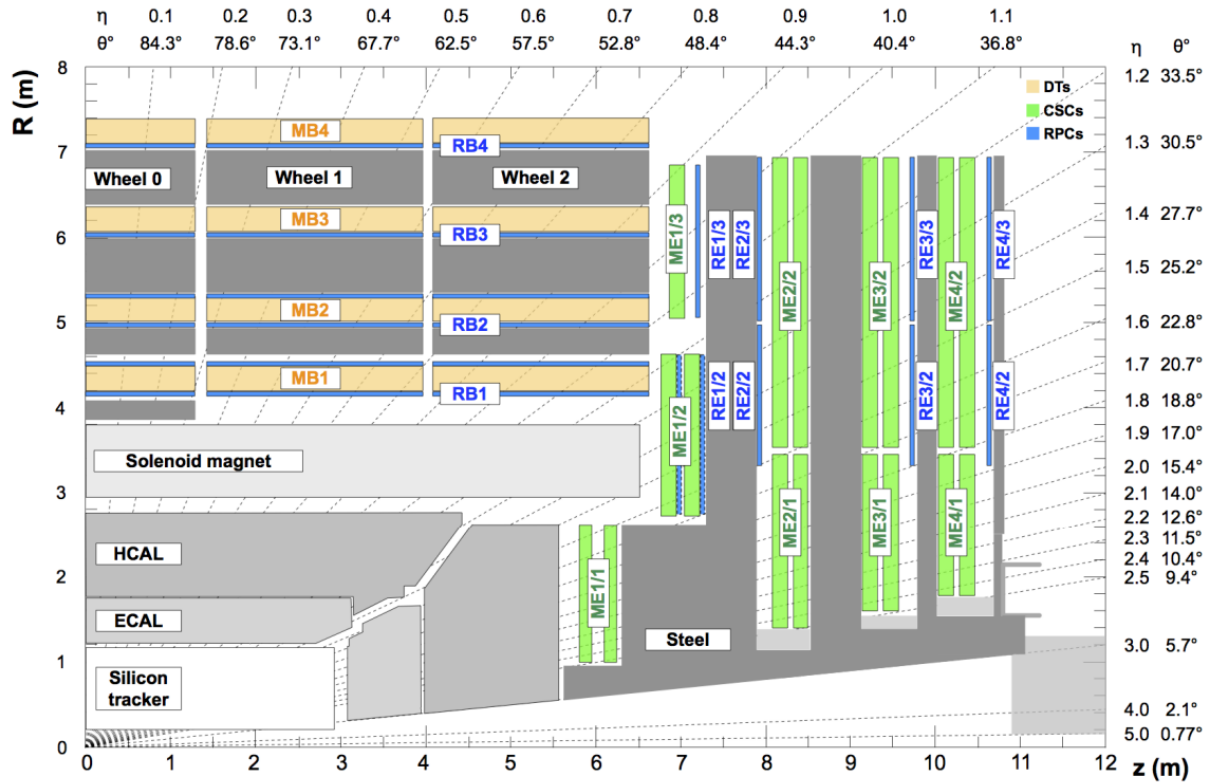


Figure 3.10: Schematic view of a quadrant of the CMS muon spectrometer displaying its muon systems. Taken from [117].

While all particles other than muons and neutrinos are stopped in the calorimeters, muons pass through the calorimeters without depositing much energy and pass through the solenoid into the muon spectrometer. Muons are measured and identified in the range $|\eta| < 2.4$ by gaseous detectors embedded in the steel flux-return yoke outside the solenoid muon spectrometer shown in Fig. 3.10. The identification of muons is crucial, as they provide clear signatures for a wide array of physics processes, helping with the identification of processes at high luminosities. The muon system not only detects and measures muons, it is also designed to trigger based on their presence.

The muon spectrometer features three kinds of gaseous detectors: Drift Tubes (DT), Resistive Plate Chambers (RPC) and Cathode Strip Chambers (CSC). Each of these type of detectors

have their own distinctive features and are used in a complementary way to form the muon spectrometer of the CMS detector.

The barrel region is divided into five wheels perpendicular to the z -axis and populated with DTs (up to $|\eta| \leq 1.2$). Each wheel is further split into four muon chambers interspersed with the sections of the saturated iron yoke of the magnet system. The three inner rings of the DT are able to measure the muon trajectory in the z direction as well as the r - ϕ bending angle, while the outermost ring only measures the bending angle. Drift chambers work by having so called drift cells filled with gas. When a muon passes through these cells, it ionizes the gas inside. By measuring the drift time of the ionized gas to an anode wire, the position of the muon can be determined.

The components in the endcap section experience quite different conditions compared to those in the barrel region. Here, the magnetic field is very inhomogeneous and a larger background contribution is expected. The endcap section of the muon spectrometer features four concentric layers of CSCs, which are situated in the pseudorapidity range of $0.9 < |\eta| < 2.4$. CSCs can handle non-uniform magnetic fields well and as such are a good fit for the endcap detector system. They are multi-wire proportional chambers with finely segmented cathode strips with the wires themselves pointing radially. This allows for a precise measurement of the ϕ component of the muon track.

The endcap section also features five layers of RPC detectors, which are interlaced with five layers of iron magnet yoke. The RPCs cover a pseudorapidity range of $|\eta| < 1.9$. They consist of gaseous parallel-plate detectors and have very good timing resolution. Due to its fast timing resolution of less than 25 ns it complements the CSC and makes for a very good trigger.

In summary, the muon system provides great coverage of the pseudorapidity range of $|\eta| < 2.4$. It provides accurate transverse momentum resolution, especially in combination with the other systems, and a precise muon trigger with specific p_T thresholds.

3.2.6 Trigger System

With a high collision rate of up to 40 MHz, the CMS detector generates petabytes of data every second. However, it is not feasible to store and analyse such vast amounts of information, resulting in the need of a system which reduces the amount of data in real time by only selecting the most promising events. For this purpose, the trigger system was developed.

The trigger system consists of two stages: the Level-1 (L1) trigger and the High-Level Trigger (HLT). The L1 trigger is composed of custom hardware processors using information from calorimeters and muon detectors, designed for low latency decisions with a buffer of up to 4 μ s. The readout of the CMS detector imposes an upper limit of 100 kHz on the acceptance rate of the L1 trigger. To achieve this, it uses basic information from the calorimeters and muon system, as it is not feasible to read out the tracking system at every bunch crossing.

Several algorithms are running in parallel in L1, all of them implemented in hardware for additional processing speed. Each subdetector is equipped with its own local trigger, which promptly reconstructs the muon hits in the muon spectrometer and the energy deposited in the calorimeters. It is followed by another trigger which reconstructs electrons, jets and hadronic taus (τ_h) from the calorimeter information. Simultaneously, three track finders construct muon candidates using information from the muon spectrometer. In the end, a global L1 trigger makes the final decision based on the gathered and reconstructed information, focusing primarily on high-energy particles.

Once the L1 trigger gives a positive result, the HLT reads out the full event information including the tracker information that was excluded in the L1 trigger step. It is a software-based system, performing a much more elaborate analysis of the event data. The analysis utilizes complex algorithms to reconstruct the full event information like particle tracks and their energies. The HLT then looks for specific topologies that promise the most interesting physics. Finally, it further reduces the event rate down to around 1 kHz. The remaining events are then stored for later analysis.

3.2.7 Object Identification and Selection

The global event reconstruction (also called particle-flow event reconstruction [118]) aims to reconstruct and identify each individual particle in an event with an optimized combination of all subdetector information. In this process, particles get identified, assigned a particle type (photon (γ), electron, muon, charged hadron, neutral hadron) and their direction and energy gets determined.

The energy of photons is determined via the energy deposited in the ECAL. If a photon can be linked to any charged particle trajectories in the ECAL, they get assigned to the corresponding charged particle. The energy of electrons is determined by combining information of the track momentum at the main interaction vertex, the corresponding energy deposited in the ECAL, and the energy of the photons attached to the track that have been emitted via bremsstrahlung. The momentum is estimated by using information from the energy measurement of the ECAL together with the momentum measurement of the tracker and electrons are required to have pseudorapidity $|\eta| < 2.5$. The momentum resolution also depends on the bremsstrahlung energy emitted by the electron as it traverses the material in front of the ECAL [119, 120].

The muon energy is obtained from the momentum of the corresponding track and are measured in the pseudorapidity range $|\eta| < 2.4$. By matching the muons to tracks of the silicon tracker, a measurement of the transverse momentum and its resolution is obtained.

To determine the energy of hadrons, a combination of the track momentum and the corresponding ECAL and HCAL energies corrected for the response function of the calorimeters to hadronic showers, is used. The energy of neutral hadrons is obtained from the corresponding corrected ECAL and HCAL energies.

In the measurements presented in Chap. 4, 5 and 6 reconstructed electrons and muons are required to satisfy additional selection criteria to select prompt leptons in the decays of W and Z bosons. This lepton selection is performed via a dedicated BDT classifier [121] trained to select prompt leptons while rejecting leptons from other sources like detector mismeasurements or the decay of heavy-flavor hadrons. Three increasingly tight selection criteria based on the classifier output are used to select leptons. Leptons that fulfil the tightest selection of the three (tight leptons) are used to define the Signal Regions (SR) of the two analysis, aiming for a high purity in prompt leptons. The fakeable object definition is used in the fake-factor method described in Ref. [25], which is a data-driven background estimation method to estimate nonprompt leptons that are falsely identified as prompt leptons. As a result, the fakeable object definition aims to be enriched in nonprompt leptons. Finally, the loose definition is used to veto leptons in the SR definitions.

Hadronic tau leptons (τ_h) are reconstructed using the hadron-plus-strips algorithm. Like in the selection of light leptons and with the same purposes, different levels of selection criteria based on the output of the “Deep Tau v2.1” discriminator [122], which are described in detail in

Ref. [25].

Hadronic jets are clustered using candidates compatible with the infrared and collinear safe anti-kt algorithm [123, 124] with a distance parameter of 0.4. The momentum of a jet is determined as the vectorial sum of all particle momenta in the jet and several corrections are applied. To account for contributions originating from PU, which can contribute additional tracks and energy depositions to the jet momentum, charged particles originating from PU vertices are discarded and an offset contribution is applied [125]. Additionally, corrections to the jet energy are applied, which are derived from simulations to match the measured response of jets to that of particle level jets. Any remaining differences to the Jet Energy Scale (JES) between data and simulations are accounted for by measurements of the momentum balance in dijet, $\gamma + \text{jet}$, $Z + \text{jet}$, and multijet events [126]. Finally, corrections to the Jet Energy Resolution (JER) are applied [126] as well as additional selection criteria to remove jets potentially dominated by anomalous contributions from various subdetector components or reconstruction failures.

To discriminate jets produced from b decays (b jets) from jets coming from light-flavour quarks and gluons, the DeepJet discriminator [127–129] is used. Similar, to the lepton and τ_h reconstruction, different working points are used. The loose working point is defined to correctly identify b jets with an efficiency of around 85% while the medium working point aims for 70%.

3.2.8 Experimental Systematic Uncertainties

Various imprecisely-known or simulated effects may alter the event yield of signal and background processes as well as the shape of the distributions in the discriminating observables that are used for the signal extraction in any analysis. These effects are usually called systematic uncertainties and modelled as nuisance parameters in the Maximum-Likelihood (ML) fit of the signal extraction. These nuisance parameters are able to modify the event yield and may cause migration of events among regions and different bins in the fitted distributions.

Usually, we broadly classify nuisance parameters into two types: Ones that only affect the yield in a category (rate uncertainties), which are assigned a log-normal probability density function, and nuisance parameters that also affect the shape of the distributions (shape uncertainties), which are modelled via polynomial interpolation with a Gaussian constraint and are also allowed to modify the event yield.

Generally, systematic uncertainties can either be traced back to experimental or theoretical uncertainties. Theoretical uncertainties are usually dependent on how well the signal and backgrounds are modelled, which includes for example up to which order the samples used for the analysis are modelled to. Experimental uncertainties are a collection of the uncertainties of individual components like the trigger efficiency, energy reconstruction or misidentification rates. As the theoretical uncertainties often differ for each analysis, they will be discussed individually for each of the analysis presented in Chap. 4, 5 and 6. However, as all of these three analyses use data collected by the CMS experiment during Run 2 of the LHC, a comprehensive list of the most important experimental systematic uncertainties that are relevant for these analyses is presented here.

Integrated Luminosity: The integrated luminosities for the 2016, 2017, and 2018 data-taking years have 1.2-2.5% individual uncertainties [130–132], while the overall uncertainty for the 2016-2018 period is 1.6%. These effects are applied as rate uncertainties.

Instantaneous Luminosity: The event yields of the signal and background processes may be

affected by uncertainties in the instantaneous luminosity and in the pp inelastic cross section as different PU conditions may modify the efficiency to pass the event selection criteria. To account for that, generally, the product of the instantaneous luminosity and the pp inelastic cross section, which is used to calculate the number of PU interactions, is varied by 1σ [104] and applied to the event yields.

L1 ECAL Trigger Efficiency: During the 2016 and 2017 data-taking periods, a gradual shift in the timing of the inputs of the ECAL L1 trigger in the region at $|\eta| > 2.0$ occurred. To account for that, additional corrections [133] to the ECAL measurements are applied which are computed from data and applied to the acceptance evaluated by simulations. The uncertainty in these corrections is taken as shape uncertainty, uncorrelated across data-taking periods.

Trigger Efficiency: The uncertainty on the efficiencies of the triggers are propagated to the event yields and usually treated as uncorrelated across years.

Identification and Isolation Efficiency for e and μ : The analyses presented use two different strategies to estimate the identification and isolation efficiencies for e and μ . The analysis in Chap. 4 follows the “tag-and-probe” method [117, 119, 134] to estimate the lepton scale factors, which are propagated to the final fitting variable distributions. The two analyses in Chap. 5 and 6 estimate the efficiencies as a function of the lepton p_T and η in a dedicated way for the different lepton selections following the strategy of Ref. [25]. In both cases, the uncertainty is taken as a shape uncertainty.

Identification Efficiency for τ_h : The uncertainty of the τ_h identification efficiency is dominated by statistical effects and is therefore usually treated as uncorrelated across years and decay modes. The uncertainty is taken as a shape uncertainty.

Energy Scale of e, μ and τ_h : The energy scales of electrons and muons are known with an uncertainty of less than 1% and are neglected in the analysis. The uncertainties associated to the energy scale of τ_h are obtained by varying the corresponding scale factor by its uncertainties, which are lower than 1.1%. The total uncertainty in the τ_h energy scale is taken as shape uncertainty and is treated as uncorrelated across years.

Jet Energy Corrections: These systematic uncertainties involve the uncertainty in the Jet Energy Scale (JES) and the uncertainty in the Jet Energy Resolution (JER), which are evaluated by shifting the scale and resolution applied to the reconstructed jets by $\pm 1\sigma$ after which the events are reanalyzed [135]. They are usually taken as shape uncertainties.

b-tag Efficiency and Mistag Rate: Uncertainties in the b tagging efficiencies and mistag rates are propagated to the event yields as function of the jet p_T and η . The purity and statistics of the control sample used to derive the data-to-MC correction factors as well as the effect of the JES uncertainties is considered.

MET Resolution and Response: To account for the uncertainties of the MET resolution and response, the JES and JER are varied within their respective uncertainties after which MET and all variables related to MET are recomputed. The resulting total uncertainty is taken as shape uncertainty and is treated as correlated across years.

799 **Other:** The uncertainty in the normalization of the charge flip background, which is present
800 in the $2\ell ss$ categories, amounts to 30%. The uncertainties associated to the nonprompt
801 background estimation techniques are treated as uncorrelated across the years, while the
802 ones associated to the charge flips and conversions are treated as correlated.

4 Search for Physics Beyond the Standard Model in Top Quark Production with Additional Leptons in the Context of Effective Field Theory

This chapter corresponds to the studies presented in Ref. [136] as well as some additional studies. The analysis was performed in collaboration with the involvement of researchers from all the universities listed below:

- University of Zurich, Switzerland
- University of Notre Dame, USA
- University of Nebraska-Lincoln, USA
- The Ohio State University, USA
- University of Oviedo, Spain

Besides several smaller contributions, my main contributions to this analysis can be broadly summarized in the following two points:

Signal Region Four-heavy-quark Operators: I developed and implemented a new dedicated signal region in the $2\ell ss$ channel specifically targeting the four four-heavy-quark operators. This signal region is derived by implementing cuts on the b-jet multiplicity to separate the $t\bar{t}t\bar{t}$ signal from other processes and represents a dominant force of sensitivity for the four four-heavy quark operators.

Conceptual Introduction of a $t\bar{t}$ Control Region: I performed qualitative studies on introducing a $t\bar{t}$ control region to better constrain the “fakes” background from misidentified nonprompt leptons. The fakes background is derived from the data-driven fake factor method, which requires well-defined control regions to estimate fake rates, and mostly consists of $t\bar{t}$ events in the multilepton final states. If these regions have contamination from signal or other background processes not accounted for, like changed in the $t\bar{t}$ cross section due to BSM contributions, it can lead to incorrect fake factor estimates, thereby affecting the EFT search. The introduction of a $t\bar{t}$ control region helps to better constrain the $t\bar{t}$ contribution in the analysis and as such to also ensure correct estimates on the fake rate.

4.1 Introduction

This chapter presents a measurement of Effective Field Theory (EFT) operators from SM extensions that couple the top quark to leptons, bosons, and other heavy (top or bottom) quarks and builds on the SM EFT extension of Sec. 2.7.3.

A search for new physics in the top quark sector is motivated by the large mass of the top quark which results in a top Higgs (H) Yukawa coupling of roughly order of one, with a more detailed description in Sec. 2.6.1. So far, besides the measurement in Ref. [137], processes associated to top quark production in leptonic final states ($t\bar{t}H$ [25], $t\bar{t}W$ [26], $t\bar{t}Z$ [27], tZq [28], tHq [25], $t\bar{t}t\bar{t}$ [29]) have not yet been studied simultaneously using an EFT framework to probe for potential effects of new physics impacting these associated top quark processes.

The measurement presented in this chapter builds on the approach developed in Ref. [137], which studied 16 dimension 6 EFT operators (in the Warsaw basis) using the data collected in 2017 by the CMS experiment amounting to 41.5fb^{-1} . In this approach, EFT effects are included by means of event weights that are applied to the simulated samples, which uses the SM EFT expansion described in Sec. 2.7.3 and allows for detector-level predictions accounting for all relevant interference effects and correlations among the Wilson Coefficients¹ (WCs). The same approach has also been used to study $t\bar{t}Z$ tZq and tWZ processes [138], which probes five WCs at the same time, as well as $t\bar{t}H$ and $t\bar{t}Z$ processes in which the Higgs or Z boson is boosted [139], which study eight WCs simultaneously. Building on all these previous analyses, the analysis presented in this chapter studies 26 different WCs adding an additional 10 WCs compared to the previous approach so that it incorporates all the relevant signatures in the multilepton final state. Also, the full Run 2 dataset of the CMS experiment is used, increasing the total integrated luminosity to 137fb^{-1} . As a result, this measurement thus represents the most global detector-level EFT analysis to date.

This chapter is organized as follows.

Sec. 4.2 discusses the data samples used and how the various EFT contributions were introduced into the samples.

The event selection is described in Sec. 4.3, with a special focus on how the sensitivity to the four four-heavy quark operators has been improved.

Sec. 4.4 describes the background estimation and also features additional studies to constrain the fakes background via a dedicated $t\bar{t}$ control region, which is not included in the published paper but is planned to be included in future iterations of the measurement.

The systematic uncertainties are detailed in Sec. 4.5.

Sec. 4.6 presents the results.

4.2 Data Samples and Signal Simulation

This analysis uses the data collected in the Run 2 of the CMS experiment during 2016-2018 from proton-proton collisions at $\sqrt{s} = 13\text{ TeV}$ with a combination of single-, double-, and triple-lepton triggers.

The analysis targets leptonic final states from top quark production ($t\bar{t}H$, $t\bar{t}\ell\bar{\ell}$, $t\bar{t}\ell\nu$, $t\bar{t}\ell q$, tHq , and $t\bar{t}t\bar{t}$) and aims to measure dimension-six EFT effects. Processes with the same leptonic

¹Even though effects among dimension 6 operators are suppressed with the same power as effects between dimension 8 operators and the SM, only dimension 6 operators were included for technical reasons.

final states, that are not impacted by these EFT operators, are considered as backgrounds for this analysis. To estimate these backgrounds, a combination of simulated samples and control samples in data are used and described in Sec. 4.4.

The signal contribution is simulated at Leading Order (LO) with the MADGRAPH5_aMC@NLO event generator (version 2.6.5) [140–142]. This simulation incorporates the DIM6TOP model [143] to include EFT effects. Using the Warsaw basis described in Sec. 2.7.3 of gauge-invariant dimension-six operators, the model focuses on operators involving one or more top quarks. Additionally, we assume that EFT effects are the same for all lepton generations even though the DIM6TOP model allows for independent EFT effects for each generation of leptons.

Including all operators included in the DIM6TOP model that significantly affect top quark processes with leptonic final states amounts to 26 operators in total which are listed in Tab. 4.1.

The 26 operators fall into four main categories: operators involving four heavy quarks (4hq), operators involving two heavy quarks and two light quarks (2hq2lq), operators involving two heavy quarks and two leptons (2hq2 ℓ) and operators involving two heavy quarks and bosons (2hqV).

Leptons affected by the 2hq2 ℓ operators may be either charged or neutral and the bosons in the 2hqV operators include both gauge bosons and the Higgs boson. In Fig. 4.1, examples of how these WCs can affect top associated processes.

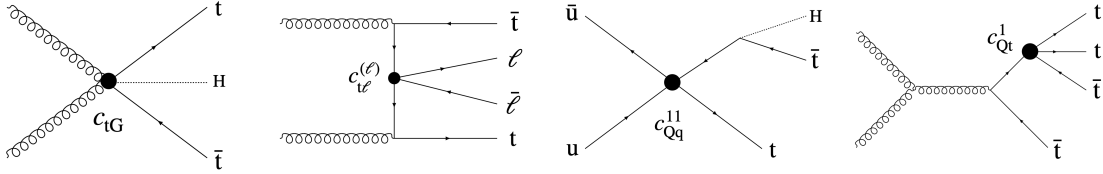


Figure 4.1: Example Feynman diagrams illustrating WCs from each of the categories listed in Tab. 4.1. From left to right, the diagrams show vertices associated with the c_{tG} , $c_{t\ell}^{(\ell)}$, c_{Qq}^{11} , and c_{Qt}^1 .

Table 4.1: List of WCs included in this analysis grouped according to the categories of WCs defined in [143]. The abbreviations for the WCs categories used in this paper are noted parenthetically.

Operator category	Wilson coefficients
Two-heavy (2hqV)	$c_{t\varphi}, c_{\varphi Q}^-, c_{\varphi Q}^3, c_{\varphi t}, c_{\varphi tb}, c_{tW}, c_{tZ}, c_{bW}, c_{tG}$
Two-heavy-two-lepton (2hq2 ℓ)	$c_{Q\ell}^{3(\ell)}, c_{Q\ell}^{- (\ell)}, c_{Qe}^{(\ell)}, c_{t\ell}^{(\ell)}, c_{te}^{(\ell)}, c_t^{S(\ell)}, c_t^{T(\ell)}$
Two-heavy-two-light (2hq2lq)	$c_{Qq}^{31}, c_{Qq}^{38}, c_{Qq}^{11}, c_{Qq}^{18}, c_{tq}^1, c_{tq}^8$
Four-heavy (4hq)	$c_{QQ}^1, c_{Qt}^1, c_{Qt}^8, c_{tt}^1$

Diagrams with zero EFT vertices (SM) and diagrams with one EFT vertex (new physics) are considered for each of the six signal processes. Consequently, the amplitude of each process depends linearly on the WCs and the cross section depends quadratically on the WCs. Using MADGRAPH5_aMC@NLO event reweighting, the 26 dimensional quadratic parametrization is determined for each event, which is used to determine the dependence of any observable bin on the WCs. The procedure is described in detail in Ref. [137].

4.3 Event Selection and Categorization

The analysis targets events in which top quarks are produced in association with additional charged leptons. The event selection is defined based on the multiplicity of charged leptons, jets and b jets. The goal is to separate subsamples of the broader multilepton data set into categories containing different admixtures of the contributing signal processes as it is not possible to isolate individual processes. This results in 43 categories, each binned in terms of a kinematical variable which is described in Sec. 4.3.5.

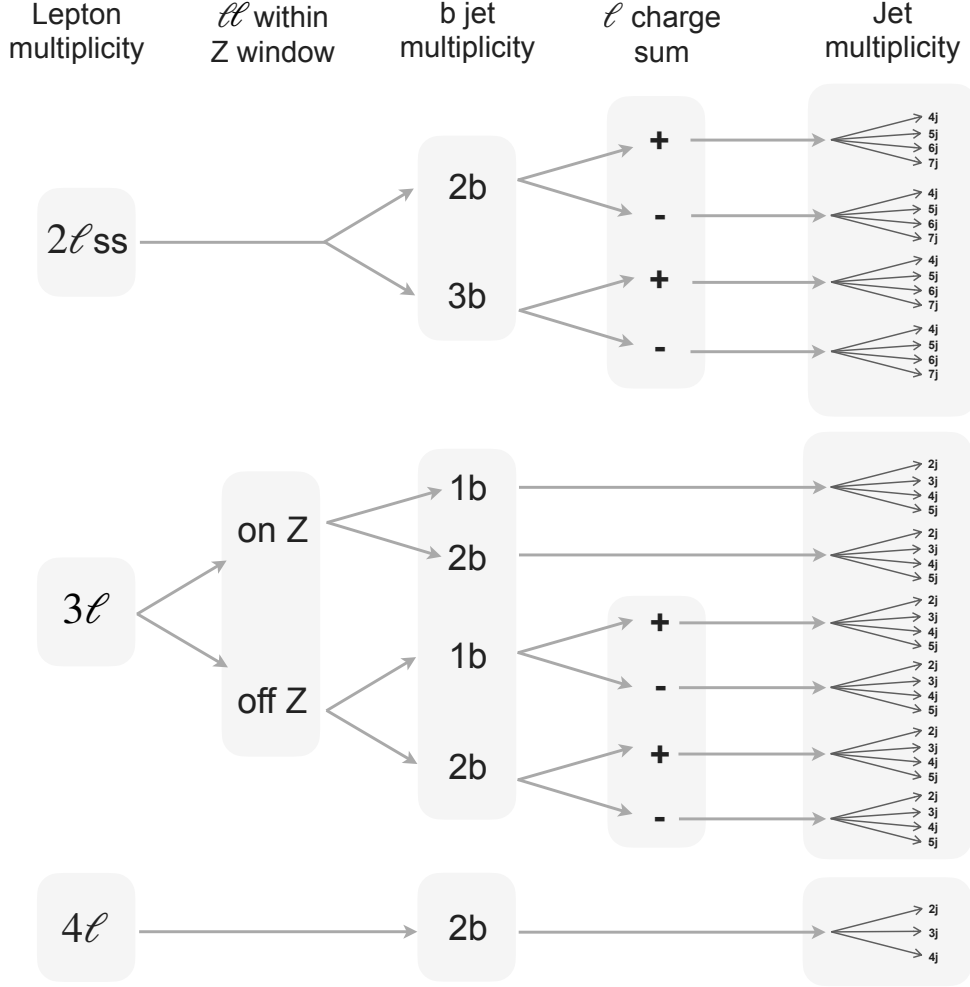


Figure 4.2: Summary of the event selection categorization. The details for the selection requirements are described in Sec. 4.3.2–4.3.4.

Events are required to have either two same-sign leptons ($2\ell_{ss}$), three leptons (3ℓ), or four or more leptons (4ℓ). The 3ℓ event category features an additional cut to separate events with and without on-shell Z boson decays (pair of same-flavor and opposite-sign leptons with an invariant mass within 10 GeV of the Z boson mass) which are referred to as the on-Z and off-Z subcategories. Events in the $2\ell_{ss}$ and 3ℓ off-Z category are further divided based on the sum of the lepton charges. Fig. 4.2 and Tab. 4.2 show a summary of the event selection.

To avoid backgrounds from light resonances, events featuring a pair of leptons with an invariant of less than 12 GeV are rejected. Also, events need to have at least two jets with $p_T > 30$ GeV and $|\eta| < 2.4$. As it can also be seen in Fig. 4.2, all events are also required to have at least one or more b tagged jets. τ leptons only enter our event selections via their $\tau \rightarrow e$ and $\tau \rightarrow \mu$ decay modes.

Table 4.2: Object requirements for the 43 event selection categories. Requirements separated by commas indicate a division into subcategories. The kinematical variable that is used in the event category is also listed. Sec. 4.3.5 provides further details regarding the kinematical distributions.

Event category	Leptons	$m_{\ell\ell}$	b tags	Lepton charge sum	Jets	Kinematical variable
2 ℓ ss 2b	2	No requirement	2	>0, <0	4, 5, 6, ≥ 7	$p_T(\ell_j)_{\max}$
2 ℓ ss 3b	2	No requirement	≥ 3	>0, <0	4, 5, 6, ≥ 7	$p_T(\ell_j)_{\max}$
3 ℓ off-Z 1b	3	$ m_Z - m_{\ell\ell} > 10 \text{ GeV}$	1	>0, <0	2, 3, 4, ≥ 5	$p_T(\ell_j)_{\max}$
3 ℓ off-Z 2b	3	$ m_Z - m_{\ell\ell} > 10 \text{ GeV}$	≥ 2	>0, <0	2, 3, 4, ≥ 5	$p_T(\ell_j)_{\max}$
3 ℓ on-Z 1b	3	$ m_Z - m_{\ell\ell} < 10 \text{ GeV}$	1	No requirement	2, 3, 4, ≥ 5	$p_T(Z)$
3 ℓ on-Z 2b	3	$ m_Z - m_{\ell\ell} < 10 \text{ GeV}$	≥ 2	No requirement	2, 3, 4, ≥ 5	$p_T(Z)$ or $p_T(\ell_j)_{\max}$
4 ℓ	≥ 4	No requirement	≥ 2	No requirement	2, 3, ≥ 4	$p_T(\ell_j)_{\max}$

4.3.1 Event Selection to Target the 4hq Operators

The 4hq operators mainly affect $t\bar{t}t\bar{t}$ processes and as a result, our ability to constrain the 4hq operators is directly coupled to how well we can isolate the rare $t\bar{t}t\bar{t}$ signal from other processes. Even though the $t\bar{t}t\bar{t}$ signal can be found in all three event categories, its largest contribution is found in the 2 ℓ ss category. This means, that in the 2 ℓ ss category, a good separation of $t\bar{t}t\bar{t}$ from other processes will have the largest effect.

A natural choice to isolate the $t\bar{t}t\bar{t}$ signal from other processes and create a region enriched in $t\bar{t}t\bar{t}$ is the number of b jets present in the final state as it is the only signal process featuring more than two top quarks. Ideally, assuming a perfect reconstruction one would expect four b jets in the final state. However, as the medium b jet working point only features an efficiency of 70%, often only three b jets will be identified in the final state. As a result, dividing the 2 ℓ ss category into events with three or more and two medium b jets lets us efficiently separate the $t\bar{t}t\bar{t}$ signal from other processes which can be seen in Fig. 4.3.

Applying this cut on the b jet multiplicity improves the sensitivity to the 4hq operators by around 20% due to the better isolation of the $t\bar{t}t\bar{t}$ events while not affecting the sensitivity to operators not in the 4hq group.

Even though, the 2 ℓ ss features most of the $t\bar{t}t\bar{t}$ events, they are also found in the 3 ℓ category. Motivated by the success of applying a cut on three or more b jets in the 2 ℓ ss region, studies applying the same cut in the 3 ℓ category have been performed. However, after implementing the cut on the b jet multiplicity in the 2 ℓ ss category, no further improvement is observed when applying the same cut in the 3 ℓ region. Similarly, applying a cut on three b jets in the 3 ℓ category without applying it in the 2 ℓ ss category, results in an improved sensitivity to the 4hq due to the improved separation of $t\bar{t}t\bar{t}$ events. However, the improvement is smaller than the improvement provided by applying the cut in the 2 ℓ ss category. Consequently, as applying a cut on three b jets in the 3 ℓ category yields no improvement, it is not present in the final measurement.

Finally, additional studies showed, that the sensitivity to the 4hq operators is provided primarily by the dedicated region described in this section in the 2 ℓ ss category. This is expected, as the region was designed to primarily increase the sensitivity to the 4hq operators. To obtain a quantitative characterization of the sensitivity provided by these bins, a fit with only these bins included was performed. The resulting 2σ CIs are only degraded by about 4-6% (with respect to a fit with all bins included), showing that this region is indeed a the dominant source of sensitivity to the 4hq operators.

threshold of 25, 15, and 10 GeV, respectively. If the third lepton is an electron, the threshold is $p_T > 15$ GeV, which suppresses the contributions from nonprompt electrons and helps stay above trigger thresholds. We also require at least two jets with $p_T > 30$ GeV. Events, which contain a same-flavor opposite-sign pair of leptons with a mass within 10 GeV of m_Z (91.2 GeV), are separated to isolate an enhanced contribution from the on-shell Z boson decay, primarily from the $t\bar{t}Z$ process. If events are not in this region, they are further separated based on whether the sum of the lepton charges is positive or negative to again exploit the difference in cross section between $t\bar{t}W^+$ and $t\bar{t}W^-$. All 3ℓ events are also categorized by the number of b jets passing the medium working point, where we either require them to have exactly one b jet (enhances $t\bar{t}\ell\bar{\ell}q$) or two or more b jets (separates $t\bar{t}\ell\bar{\ell}q$ from $t\bar{t}\ell\bar{\ell}\bar{\ell}$).

4.3.4 The 4ℓ Event Category

The 4ℓ event category targets $t\bar{t}\ell\bar{\ell}$ and $t\bar{t}H$ events, requiring at least four leptons passing the specific selection criteria. The first through fourth leptons must be above the p_T threshold of 25, 15, 10, and 10 GeV, respectively. If the last two leptons are electrons, the requirement becomes $p_T > 15$ GeV for both because of the same reasons described in the 3ℓ event category. The events must have at least two jets with $p_T > 30$ GeV and $|\eta| < 2.4$. At least two of these jets must be b jets, where one of them is required to pass medium working point, while the second is allowed to pass the loose working point.

4.3.5 Kinematic Variables

The selections described in Sec. 4.3.2-4.3.4 result in 43 unique categories of events. Each of these 43 categories is binned in terms of a kinematic variable to gain additional sensitivity to EFT effects.

Besides the 3ℓ on-Z categories, all categories are binned in terms of $p_T(\ell j)_{\max}$. It is defined as the combination with the largest p_T of the vectorial sum of the momenta of all possible pairs of objects in the collections of leptons and jets. As such, it can be any combination of the transverse momenta of two leptons, two jets, or a lepton and a jet and provides good sensitivity to a broad range of EFT effect that grow with energy.

The presence of the Z boson in the 3ℓ on-Z categories motivates to choose variables that provide sensitivity to EFT operators involving the Z boson. In these categories, the variable $p_T(Z)$ is chosen, which corresponds to the p_T of the same-flavor opposite-sign lepton pair associated with the Z boson. The only exception in the 3ℓ on-Z category are events in the categories with two or three jets and two or more b jets. There, the more general variable $p_T(\ell j)_{\max}$ is used as it provides better sensitivity to the c_{Qq}^{31} and c_{Qq}^{38} vertices, which do not have a Z boson in the EFT vertex but can still contribute to these final states. An example of such a process is shown in Fig. 4.4.

In summary, the $p_T(Z)$ variable is used for all of the on-shell Z categories, except for the two and three jet categories with two b-tagged jets; the $p_T(Z)$ variable is thus used in a total of six event categories. In the remaining 37 event categories, the $p_T(\ell j)_{\max}$ variable is used. For the categories that are binned in $p_T(\ell j)_{\max}$, four bins are used. For the categories that are binned in $p_T(Z)$ (which generally have larger numbers of selected events), five bins are used. This results in 178 total analysis bins. Binning the 43 analysis categories in terms of the $p_T(\ell j)_{\max}$ and $p_T(Z)$ variables provides an improvement in sensitivity of up to a factor of about two, compared to the

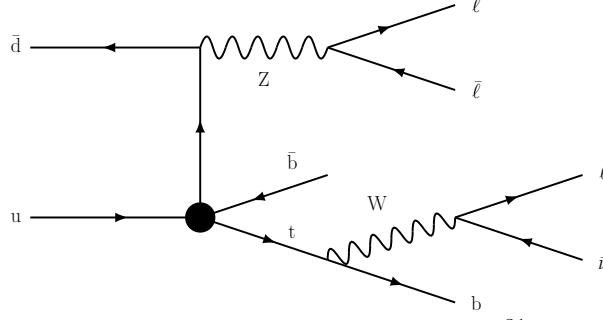


Figure 4.4: Example Feynman diagram illustrating how the c_{Qq}^{31} and c_{Qq}^{38} WCs can impact the processes in 3ℓ categories with two b quarks and an on-shell Z boson. These two WCs are a part of the $2hq2lq$ group, but unlike the other WCs in this group, these two WCs are associated with operators that have vertices involving a top and bottom quark pair, as pictured in the figure.

case where the 43 analysis categories are not further subdivided.

4.4 Background Estimation

Backgrounds are classified as either reducible or irreducible depending on the source of the reconstructed leptons passing the tight object selection criteria. A background is considered reducible when one or more of the reconstructed leptons passing the tight object selection criteria do not correspond to a lepton originating from the prompt decay of a W or Z boson or a τ lepton decay. Otherwise, the background is considered irreducible.

Diboson WZ and ZZ production make up the main contribution of irreducible backgrounds, but also a subleading contribution from triboson and tWZ production processes is expected. The latter would in principle be affected by some of the WCs studied in this analysis, however, as tWZ production does not have a strong sensitivity to these WCs and is only making up around 3% of the total expected yield, it is categorized as background. Irreducible backgrounds are estimated via simulations of these processes².

We differentiate between three main types of reducible backgrounds. The first one is called “misidentified leptons” (often also referred to as “fakes”), which means that either at least one of the reconstructed electrons or muons stem from a non-prompt lepton or hadron, or that at least one of the reconstructed τ_h originates from the misidentification of a quark or gluon jet. The main contribution to this background arises from $t\bar{t} + \text{jets}$ production, due to the large cross section of this process and the presence of b jets in the final state. The contribution of misidentified leptons is estimated via the Misidentification Probability (MP) method described in Ref. [25], which uses the fakeable object definition of leptons.

Another reducible background contribution comes from “asymmetric photon conversions”, which entails the conversion of a photon into electrons. It is possible that the electron produced in a photon conversion carries almost all the energy of the original converted photon, while the other electron carries too little energy to be detected. The contribution of these backgrounds is typically dominated by $t\bar{t}\gamma$ production is significantly suppressed by the electron reconstruction and identification algorithms, since we require electron tracks to have hits in the innermost layers of the silicon tracker and we veto electron candidates that are matched to a reconstructed photon conversion vertex. We estimate this contribution using $t\bar{t}\gamma$ simulation (similar to Ref. [149]) at LO.

²Using MADGRAPH5_amc@NLO, POWHEG [144–147] and MCFM [148].

“Charge flips” pose another reducible background. It stems from a mismeasurement of the lepton charge and contributes mainly to the $2\ell ss$ SR. This contribution is dominated by $t\bar{t}$ events and is estimated by selecting events passing the same selection as the $2\ell ss$ SR, but inverting the same-sign requirement on the dilepton system. Events in this region are weighted by the probability of each of the leptons to have their charge measured with the wrong sign that is determined via simulations. The electron charge mismeasurement rate is very small ($< 1\%$), however, since the backgrounds yielding to opposite-sign lepton pairs have much higher cross section than signal, this corresponds to a significant background. The charge misidentification rate is negligible in muons. Complementing the prediction of the simulation, we compare it to observation of a region enriched in $Z \rightarrow ee$, where the charge of one of the electrons has been measured with the incorrect sign. Even though both agree withing the applied uncertainties of 30%, a constant scale factor to apply for residual differences in our prediction is applied.

4.4.1 Prospects of Introducing a $t\bar{t}$ Control Region

The background coming from misidentified leptons is dominated by $t\bar{t}$ production. This means that if new physics, that alter the $t\bar{t}$ production rate, would be present in data, the change in $t\bar{t}$ production would directly lead to a change in the misidentified lepton background. As a result, part of the change in $t\bar{t}$ production rate would be absorbed into the fakes background, which in turn decreases our sensitivity to operators that affect $t\bar{t}$ production.

To mitigate this negative effect, which decreases our sensitivity, a dedicated $t\bar{t}$ Control Region (CR) is proposed to better constrain EFT operators affected by $t\bar{t}$ processes. In this section, a study about the potential of introducing such a $t\bar{t}$ CR³ is presented by showing the impact on the constraints of the c_{tG} operator.

The $t\bar{t}$ CR uses the event selection described in the analysis note of the inclusive $t\bar{t}H$ measurement [150]. Most importantly, we require electrons or muons in the final state and at least two jets out of whom at least one is classified as a b tagged jet. The datacard does not account for all correlations of nuisances. However, given that this study primarily serves as a proof of concept, this is sufficient.

The parametrization of the EFT processes is taken from [143]. As c_{tG} is one of the operators which is the most affected by $t\bar{t}$ processes, this study is performed evaluating the effects of such a CR on said operator.

Four scenarios are analyzed by performing a scan of the negative log likelihood for three values of c_{tG} (0.0, 0.5 and 1.0).

Scenario 1: This scenario represents the baseline scenario, corresponding to the analysis presented in this chapter as is. This means that EFT effects are scaled as in Ref. [137] and no $t\bar{t}$ CR is present.

Scenario 2: In this scenario, no $t\bar{t}$ CR is present and EFT effects are scaled as in Ref. [137]. However, the misidentified leptons background gets scaled according to the changes of the $t\bar{t}$ cross section due to EFT effects. This is motivated, as the primary source of the misidentified leptons background stems from $t\bar{t}$ production. Effectively, this lets us compare how well the assumption, that the misidentified leptons background comes from mostly $t\bar{t}$ events and scales according to $t\bar{t}$ production, holds up.

³In the published version of the analysis, no such $t\bar{t}$ CR is present. However, due to the promising results of this study, it is planned to include such a $t\bar{t}$ CR in the Run 3 iteration of this analysis.

Scenario 3: This scenario corresponds to the baseline scenario (scenario 1) with an additional $t\bar{t}$ CR included.

Scenario 4: Scenario 4 corresponds to scenario 2, where the misidentified leptons background is scaled according to $t\bar{t}$ production with an additional $t\bar{t}$ CR included.

Evaluating the four scenarios above allows us to make several comparisons.

Scenario 1 vs 2: Comparing the baseline of the analysis to the version, where the misidentified leptons background is scaled according to $t\bar{t}$ production, lets us test if the assumption made in scenario 2 works. Comparing the plots in Fig. 4.5 shows, that our assumption works.

Scenario 3 vs 4: This comparison corresponds to the comparison of scenarios 1 and 2 with the only change, that now a $t\bar{t}$ CR is included. This lets us test, if our assumption that the misidentified leptons background scales according to $t\bar{t}$ production still holds up after the inclusion of a $t\bar{t}$ CR. The plots in Fig. 4.6 show, that the assumption still holds after introducing a $t\bar{t}$ CR.

Scenario 1 vs 3: Comparing the baseline version of the analysis against the analysis with a $t\bar{t}$ CR included allows us to estimate, how much better we can constrain EFT parameters like c_{tG} that are sensitive to $t\bar{t}$ processes. The plots shown in Fig. 4.7 show the potential improvements in constraining operators sensitive to $t\bar{t}$ processes by introducing a $t\bar{t}$ CR. Event tough not all systematics and nuisances are considered and other operators that are less sensitive to $t\bar{t}$ processes might see less of an improvement after including a $t\bar{t}$ CR, these plots still provide a clear qualitative motivation to include such a $t\bar{t}$ CR in future iterations of the analysis.

The results of these studies strongly motivate the inclusion of a $t\bar{t}$ CR in future iterations of this analysis, as it helps to significantly improve the sensitivity to operators affecting $t\bar{t}$ production.

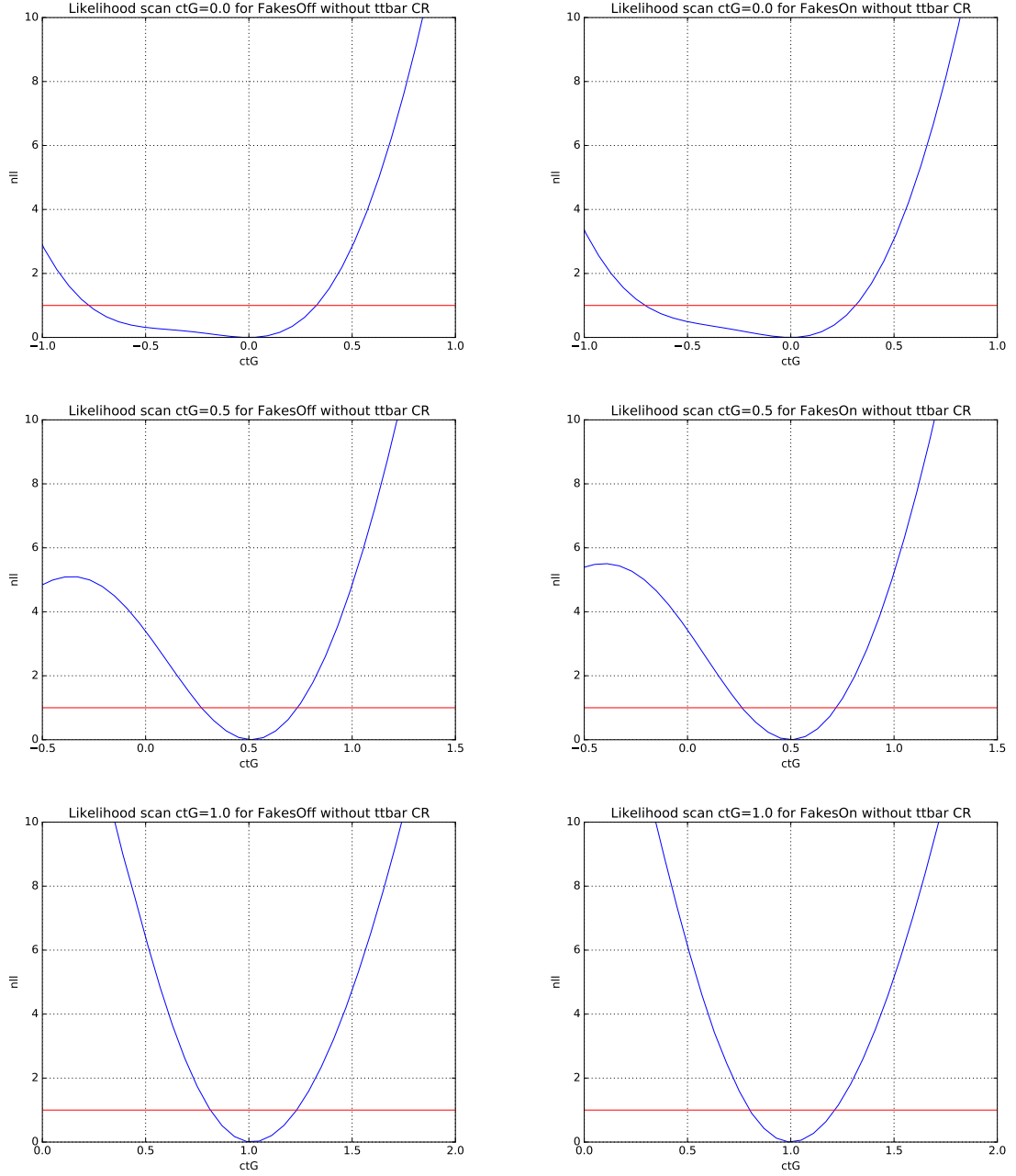


Figure 4.5: Comparison of scenario 1 (left) to scenario 2 (right). The top row assumes $c_{tG} = 0.0$, the center row $c_{tG} = 0.5$ and the bottom row $c_{tG} = 1.0$.

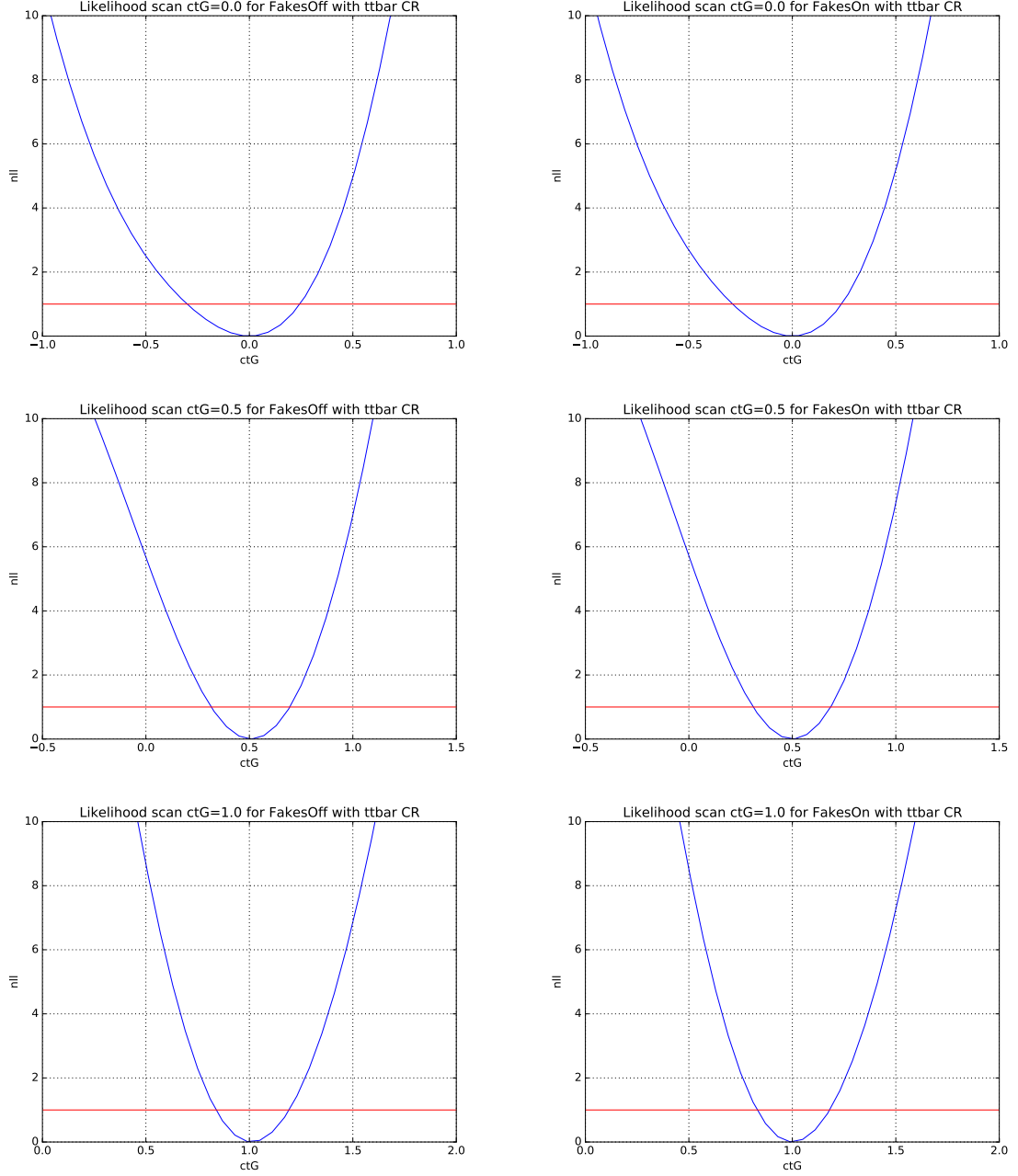


Figure 4.6: Comparison of scenario 3 (left) to scenario 4 (right). The top row assumes $c_{tG} = 0.0$, the center row $c_{tG} = 0.5$ and the bottom row $c_{tG} = 1.0$.

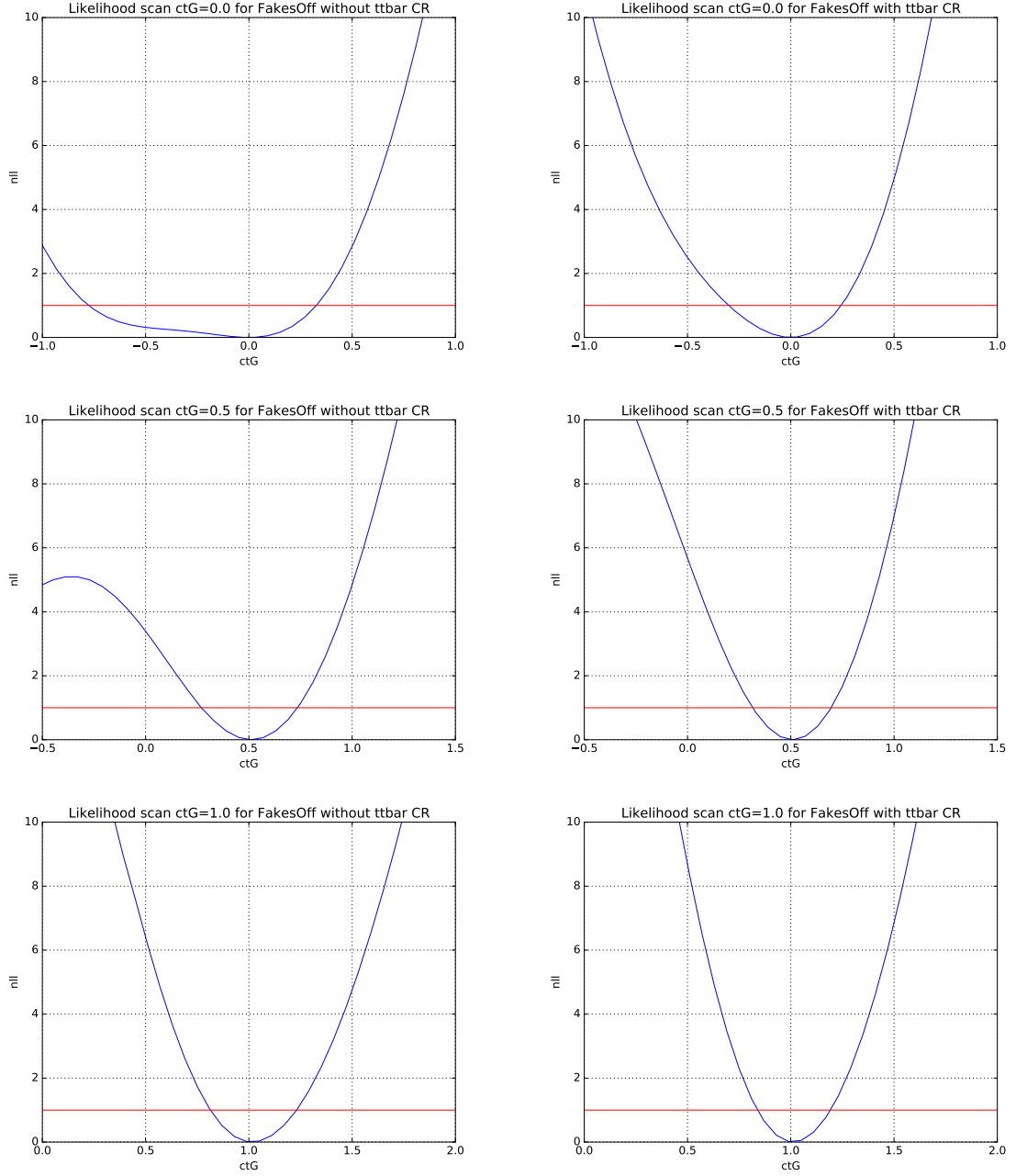


Figure 4.7: Comparison of scenario 1 (left) to scenario 3 (right). The top row assumes $c_{tG} = 0.0$, the center row $c_{tG} = 0.5$ and the bottom row $c_{tG} = 1.0$.

4.5 Systematic Uncertainties

The various experimental systematic uncertainties have already been discussed in Sec. 3.2.8 and will not be discussed in detail here. However, below the most important theoretical systematic uncertainties are discussed. Overall, this analysis considers the following systematic uncertainties: integrated luminosity, JES and JER, b jet tagging scale factors, theoretical cross section, renormalization (μ_R) and refactorization scales (μ_F), parton shower, additional radiation, e and μ identification and isolation, trigger efficiency, pileup, L1 ECAL trigger efficiency corrections, misidentified lepton rate and charge misconstruction rate.

Theoretical cross section: Excluding $t\bar{t}\gamma$, which is calculated at LO, the predicted yields of all signal and background processes are normalized to their theoretical cross section values which are at least calculated at NLO. The theoretical uncertainties stem from the choice of the QCD scale (μ_R and μ_F) as well as the choice of the Parton Distribution Scale (PDF), which result in an overall uncertainty of 1-4%.

Renormalization and Factorization Scales: The μ_R and μ_F scales are independently shifted by a factor of two (up and down) to measure the uncertainties in the matrix element generators. This allows to measure the change in shape due to the variations. However, since the simulated samples are normalized to their NLO predictions, whose uncertainty is already accounted for in via the theoretical cross section uncertainties, they uncertainties on the μ_R and μ_F scales are not allowed to change the inclusive cross section and are only allowed to change kinematic shapes.

Parton Shower: To estimate the uncertainty due to Initial- and Final-State Radiation (ISR and FSR) in the parton-shower simulation, the scale is varied by a factor of two (up and down), similar to the strategy employed for μ_R and μ_F .

Additional Radiation: Due to constraints in incorporating additional partons within the MADGRAPH5_aMC@NLO generator, it's not feasible to include extra partons in the single t ($t\bar{\ell}\bar{\ell}q$ and tHq) LO EFT samples. Consequently, the $t\bar{\ell}\bar{\ell}q$ LO sample is compared to the NLO tZq sample. For each jet bin, discrepancies that are not accounted for by systematic uncertainties are attributed to an extra radiation uncertainty. This uncertainty stems from challenges in MADGRAPH5_aMC@NLO t -channel simulations, and therefore, it is also applied to the tHq sample.

4.6 Results

Fig. 4.8, 4.9, and 4.10 show the postfit plots in the different signal regions, where all 26 WCs and all NPs are fitted simultaneously by minimizing the Negative Log Likelihood (NLL). The hatched regions in the stacked plot and shaded regions in the ratio plot correspond to the total systematic uncertainty. No significant discrepancy between the SM hypothesis and the data is observed, which shows a p-value of 0.18 using a saturated model.

Fig. 4.11 shows the resulting 1 and 2σ Confidence Intervals (CIs) from the likelihood fits, where either the other WCs are fixed to their SM value of zero (dashed red) or are profiled (solid black). Additionally, the 1 and 2σ CIs for each WC are listed in Tab. 4.3 and 4.4. All CIs are in agreement with the SM.

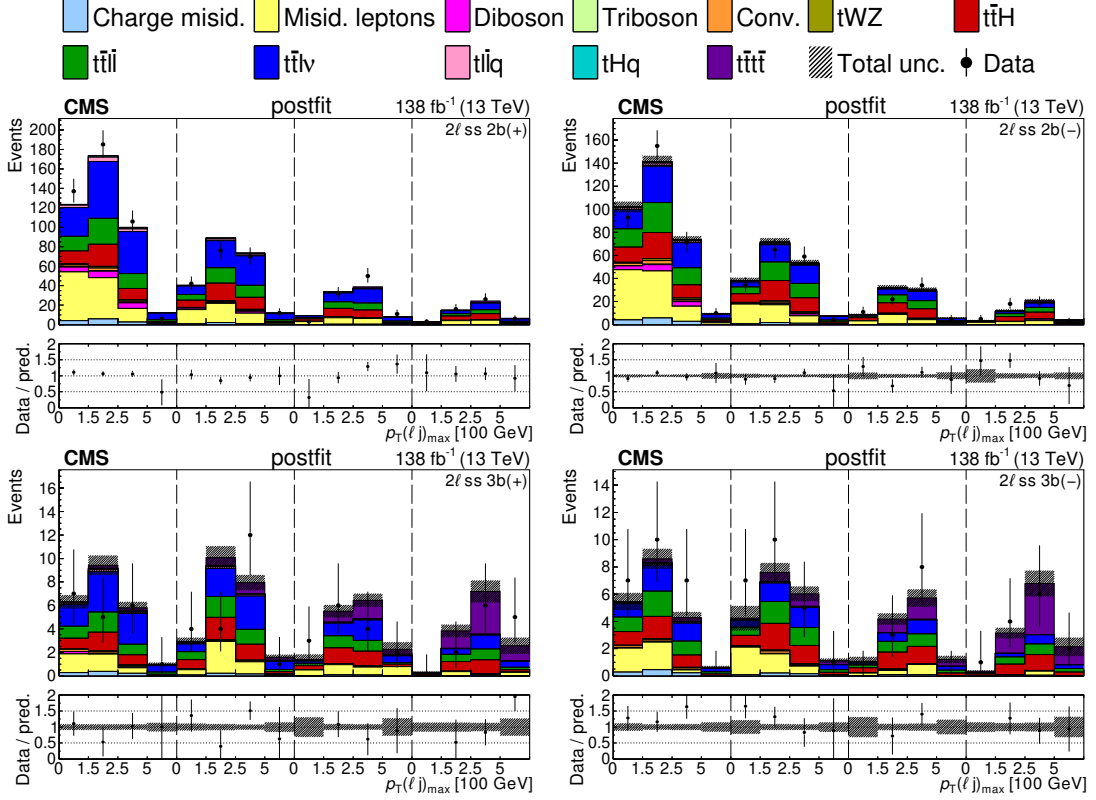


Figure 4.8: These plots show the $2lss\ 2b$ and $2lss\ 3b$ categories. The differential distribution in the plots is $p_T(\ell)_\text{max}$. The jet subcategories are arranged from low jet multiplicity to high jet multiplicity from left to right for each individual plot. For example, in the $2lss\ 2b\ (+)$ plot, the first four bins are the $p_T(\ell)_\text{max}$ variable for $2lss\ 2b\ (+)\ 4j$, the next four bins are for $2lss\ 2b\ (+)\ 5j$, etc. The process labeled “Conv.” corresponds to the photon conversion background, “Misid. leptons” corresponds to misidentified leptons, and “Charge misid.” corresponds to leptons with a mismeasured charge.

The scans of some WCs, with the other 25 WCs set to zero as illustrated in Fig. 4.11, exhibit disjoint 1σ intervals. This phenomenon arises from the quadratic structure of the EFT parametrization. While this degeneracy is theoretically possible for all WCs, it can be broken when contributions from other processes result in one of the two minima having significantly better agreement with the data. Notably, this degeneracy is only significant enough to cause disjoint CIs in the scans of the $4hq$ WCs.

However, when the other WCs are profiled in the fit, these double minima disappear since interferences between the WCs can compensate for each others effects, which results in a single extended, flat minimum rather than two separate ones. Even in cases where individual scans show shallow double minima—ones that don’t create disjoint CIs, the CIs can be wider than those derived from profiled scans, which is a phenomenon detailed in Ref. [137].

This study, encompassing a simultaneous fit of all 26 WCs, supersedes Ref. [137] as the most comprehensive detector-level EFT analysis to date. It extends the scope by incorporating 10 additional WCs not covered in Ref. [137] and achieves substantially tighter constraints on the WCs. The WCs included in both analyses show an improvement by a factor of 2 to 6 depending on the specific WC, which can largely be traced back to the differential approach combined with the larger data set.

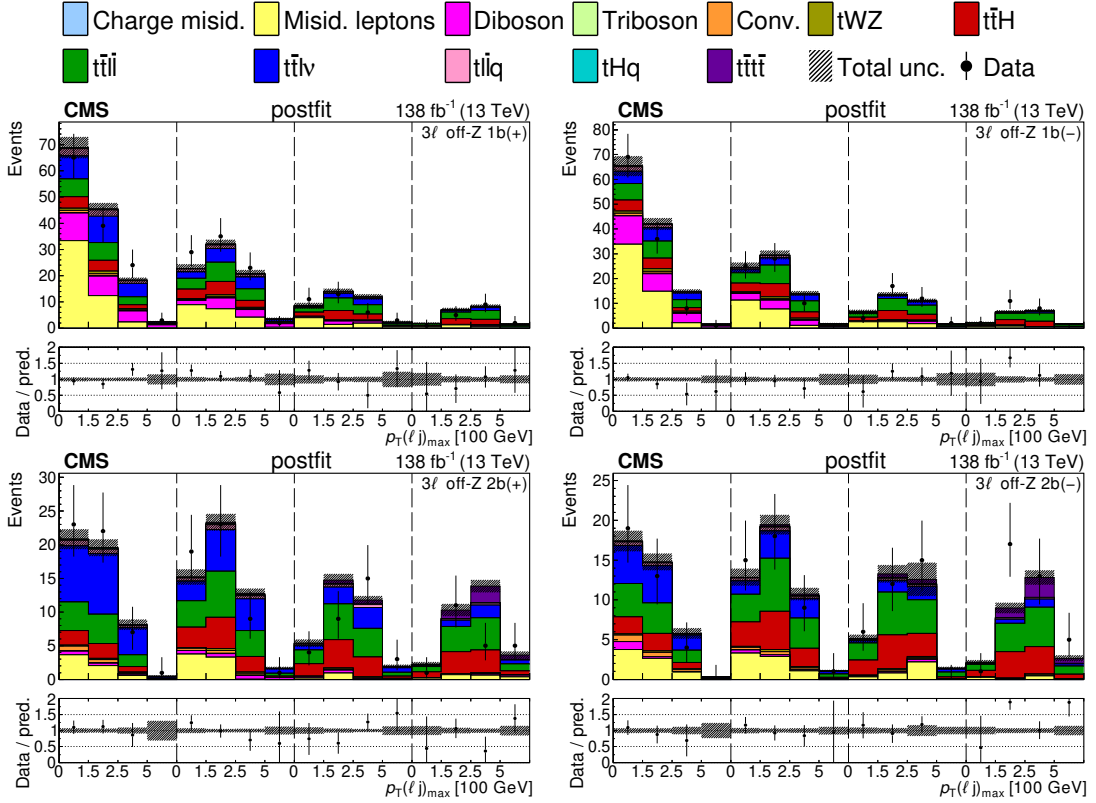


Figure 4.9: The categories shown in these plots are 3ℓ off-Z 1b and 3ℓ off-Z 2b. The differential distribution in the plots is $p_T(\ell)_{\max}$. The jet subcategories are arranged from low jet multiplicity to high jet multiplicity from left to right for each individual plot. For example, in the 3ℓ off-Z 1b (+) plot, the first four bins are the $p_T(\ell)_{\max}$ variable for 3ℓ off-Z 1b (+) 2j, the next four bins are for 3ℓ off-Z 1b (+) 3j, etc.

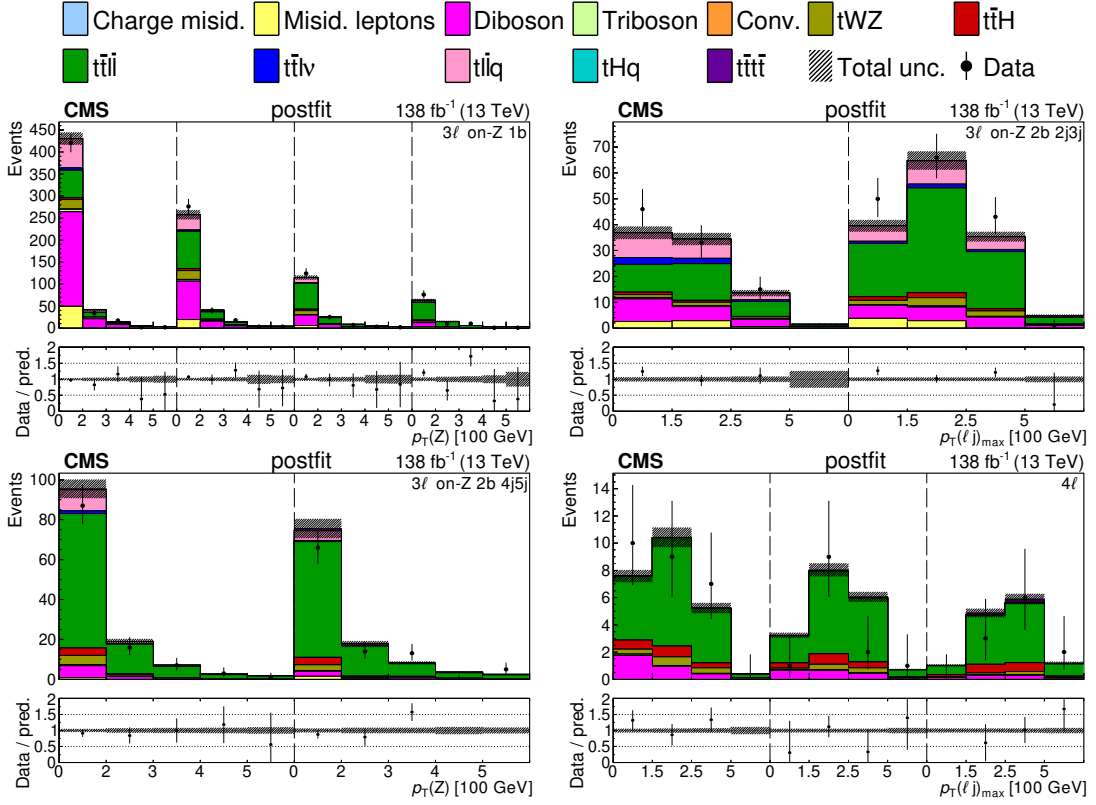


Figure 4.10: The categories shown in these plots are 3ℓ on-Z 1b, 3ℓ on-Z 2b, and 4ℓ. The differential distribution is $p_T(Z)$ in the plots of 3ℓ on-Z 1b and 3ℓ on-Z 2b (4j and 5j), and $p_T(\ell)_\text{max}$ in the plots of 3ℓ on-Z 2b (2j and 3j) and 4ℓ. The jet subcategories are arranged from low jet multiplicity to high jet multiplicity from left to right for each individual plot. For example, in the 3ℓ on-Z 1b plot, the first five bins are the $p_T(Z)$ variable for 3ℓ on-Z 2b 2j, the next five bins are for 3ℓ on-Z 2b 3j, etc.

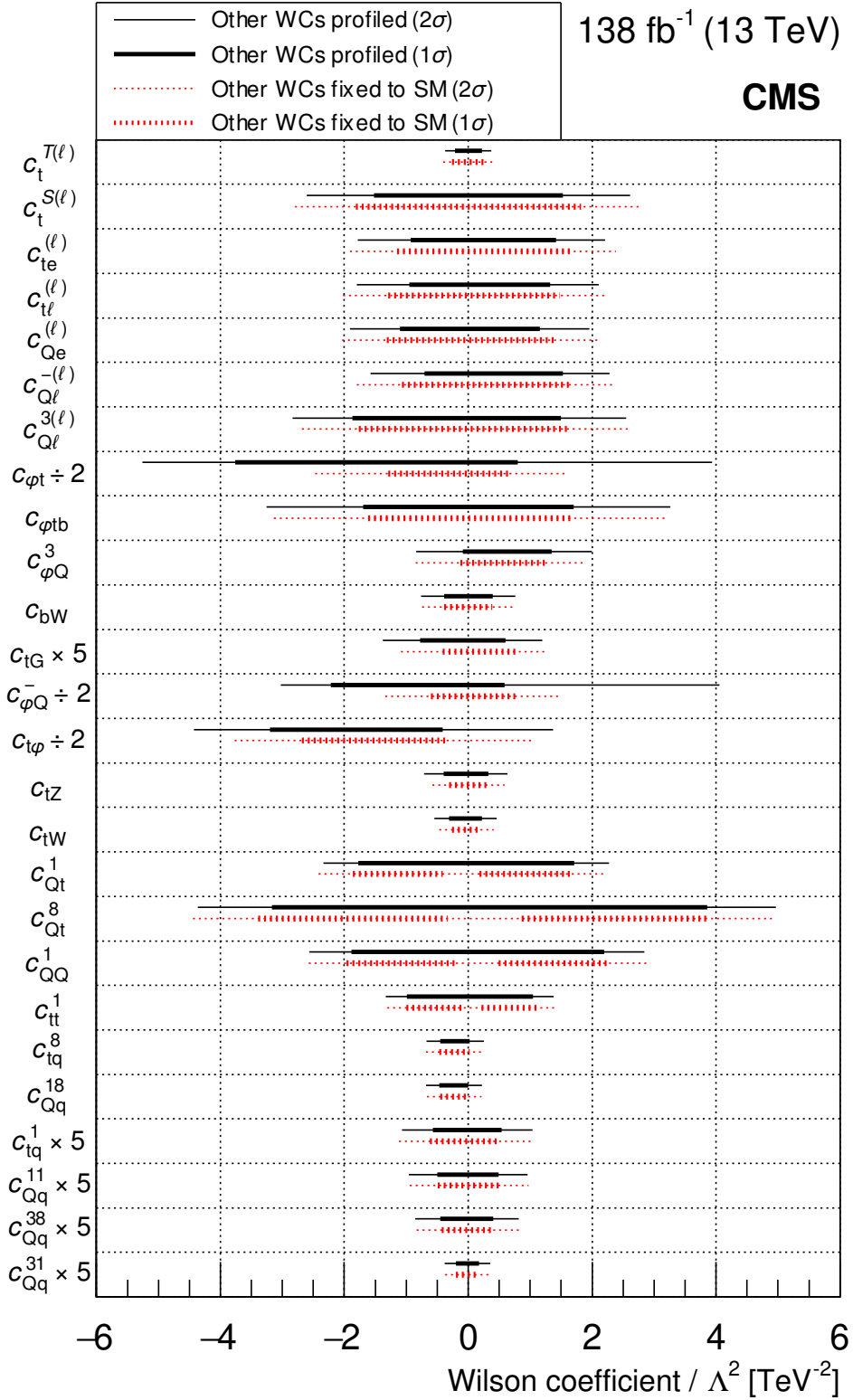


Figure 4.11: Summary of CIs extracted from the likelihood fits. The WC 1σ (thick line) and 2σ (thin line) CIs are shown for the case where the other WCs are profiled (in solid black), and the case where the other WCs are fixed to their SM values of zero (in dashed red). To make the figure more readable, the intervals for $c_{t\varphi}$, $c_{\varphi t}$, and $c_{\varphi Q}^-$ were scaled by 0.5, and the intervals for c_{tG} , c_{tq}^1 , c_{Qq}^{11} , c_{Qq}^{38} , and c_{Qq}^{31} were scaled by 5.

Table 4.3: The 1σ uncertainty intervals extracted from the likelihood fits. The intervals are shown for the case where the other WCs are profiled, and the case where the other WCs are fixed to their SM values of zero.

WC/ Λ^2 [TeV $^{-2}$]	1σ CI (other WCs profiled)	1σ CI (other WCs fixed to SM)
WC category 2hq2 ℓ		
$c_t^{T(\ell)}$	[−0.22, 0.22]	[−0.26, 0.26]
$c_t^{S(\ell)}$	[−1.52, 1.53]	[−1.81, 1.82]
$c_{te}^{(\ell)}$	[−0.93, 1.41]	[−1.15, 1.68]
$c_{t\ell}^{(\ell)}$	[−0.95, 1.32]	[−1.29, 1.47]
$c_{Qe}^{(\ell)}$	[−1.10, 1.16]	[−1.32, 1.40]
$c_{Q\ell}^{-(\ell)}$	[−0.71, 1.53]	[−1.07, 1.64]
$c_{Q\ell}^{3(\ell)}$	[−1.87, 1.50]	[−1.76, 1.63]
WC category 2hqV		
$c_{\varphi t}$	[−7.52, 1.59]	[−2.59, 1.32]
$c_{\varphi tb}$	[−1.69, 1.70]	[−1.61, 1.67]
$c_{\varphi Q}^3$	[−0.09, 1.35]	[−0.13, 1.25]
c_{bW}	[−0.39, 0.40]	[−0.39, 0.39]
c_{tG}	[−0.15, 0.12]	[−0.08, 0.15]
$c_{\varphi Q}^-$	[−4.44, 1.17]	[−1.20, 1.57]
$c_{t\varphi}$	[−6.40, −0.82]	[−5.37, −0.64]
c_{tZ}	[−0.40, 0.32]	[−0.31, 0.32]
c_{tW}	[−0.31, 0.22]	[−0.26, 0.21]
WC category 4hq		
c_{Qt}^1	[−1.77, 1.71]	[−1.86, −0.41] $\cup$ [0.19, 1.70]
c_{Qt}^8	[−3.17, 3.86]	[−3.39, −0.34] $\cup$ [0.86, 3.87]
c_{QQ}^1	[−1.89, 2.19]	[−1.96, −0.16] $\cup$ [0.49, 2.25]
c_{tt}^1	[−0.99, 1.05]	[−1.00, −0.08] $\cup$ [0.21, 1.11]
WC category 2hq2lq		
c_{tq}^8	[−0.45, 0.03]	[−0.46, 0.02]
c_{Qq}^{18}	[−0.47, −0.00]	[−0.45, 0.00]
c_{tq}^1	[−0.11, 0.11]	[−0.12, 0.10]
c_{Qq}^{11}	[−0.10, 0.10]	[−0.10, 0.10]
c_{Qq}^{38}	[−0.09, 0.08]	[−0.09, 0.08]
c_{Qq}^{31}	[−0.04, 0.03]	[−0.04, 0.03]

Table 4.4: The 2σ uncertainty intervals extracted from the likelihood fits. The intervals are shown for the case where the other WCs are profiled, and the case where the other WCs are fixed to their SM values of zero.

WC/ Λ^2 [TeV $^{-2}$]	2σ CI (other WCs profiled)	2σ CI (other WCs fixed to SM)
WC category 2hq2 ℓ		
$c_t^{T(\ell)}$	[−0.37, 0.37]	[−0.40, 0.40]
$c_t^{S(\ell)}$	[−2.60, 2.62]	[−2.80, 2.80]
$c_{te}^{(\ell)}$	[−1.78, 2.21]	[−1.91, 2.39]
$c_{t\ell}^{(\ell)}$	[−1.80, 2.11]	[−2.02, 2.20]
$c_{Qe}^{(\ell)}$	[−1.91, 1.96]	[−2.04, 2.12]
$c_{Q\ell}^{- (\ell)}$	[−1.58, 2.28]	[−1.80, 2.33]
$c_{Q\ell}^{3(\ell)}$	[−2.84, 2.55]	[−2.69, 2.58]
WC category 2hqV		
$c_{\varphi t}$	[−10.52, 7.87]	[−4.93, 3.18]
$c_{\varphi tb}$	[−3.25, 3.26]	[−3.14, 3.18]
$c_{\varphi Q}^3$	[−0.84, 2.00]	[−0.85, 1.89]
c_{bW}	[−0.76, 0.76]	[−0.75, 0.75]
c_{tG}	[−0.28, 0.24]	[−0.22, 0.25]
$c_{\varphi Q}^-$	[−6.06, 8.12]	[−2.68, 2.94]
$c_{t\varphi}$	[−8.85, 2.75]	[−7.54, 2.11]
c_{tZ}	[−0.71, 0.64]	[−0.58, 0.59]
c_{tW}	[−0.55, 0.46]	[−0.47, 0.41]
WC category 4hq		
c_{Qt}^1	[−2.34, 2.27]	[−2.41, 2.22]
c_{Qt}^8	[−4.37, 4.97]	[−4.45, 4.96]
c_{QQ}^1	[−2.56, 2.84]	[−2.57, 2.89]
c_{tt}^1	[−1.33, 1.38]	[−1.31, 1.43]
WC category 2hq2lq		
c_{tq}^8	[−0.68, 0.25]	[−0.68, 0.24]
c_{Qq}^{18}	[−0.68, 0.22]	[−0.67, 0.21]
c_{tq}^1	[−0.21, 0.21]	[−0.22, 0.20]
c_{Qq}^{11}	[−0.19, 0.19]	[−0.19, 0.20]
c_{Qq}^{38}	[−0.17, 0.16]	[−0.17, 0.16]
c_{Qq}^{31}	[−0.08, 0.07]	[−0.08, 0.07]

4.7 Summary

This chapter shows a search for new physics in top quark production in leptonic final states in the context of EFT. The events are from proton-proton collisions collected by the CMS experiment at a center-of-mass energy of 13.7 TeV corresponding to an integrated luminosity of 138 fb^{-1} . EFT effects are included via event weights of simulated samples, which allow for detector-level predictions that include correlations and interference effects among EFT operators and between EFT operators and SM processes. The optimization to increase the sensitivity to operators including vertexes with four heavy quarks is presented in detail and a new $t\bar{t}$ CR to improve the sensitivity to operators sensitive to said process is motivated. The WCs of 26 EFT operators were simultaneously fit to the data and confidence intervals of the WCs were extracted with the other WCs either profiled or fixed to their SM value of zero. In all cases, the data are found to be consistent with the SM expectations.

5 Search for CP Violation in $t\bar{t}H$ and tH Production in Multilepton Channels at $\sqrt{s} = 13 \text{ TeV}$

The chapter that follows corresponds to the studies presented in Ref. [151]. The analysis was performed in collaboration with the involvement of researchers from all the universities listed below:

- University of Zurich, Switzerland
- Universidad de Oviedo, Principado de Asturias, Spain
- Universite Catholique de Louvain, Belgium
- Institute of High Energy Physics, CAS, Beijing, China
- Cornell University, Ithaca, USA
- Vilnius University, Lithuania

Besides several smaller contributions, my main contributions to this analysis can be broadly summarized in the following points:

Development of CP Discrimination: I have successfully developed and trained the Boosted Decision Trees (BDTs) that are instrumental in differentiating between CP-even and CP-odd events, in turn improving the sensitivity to the CP structure of the top Yukawa coupling.

Validation: I was heavily involved in validating our data in the corresponding validation and control regions.

Additionally, I have had the privilege of representing the analysis at the preapproval talk and the chance to present this analysis at the yearly SPS conference in Freiburg, Switzerland in 2022.

5.1 Introduction

With a measurement of the Charge-Parity (CP) structure of the top-Higgs Yukawa coupling already motivated in Sec. 2.7.2. This section presents a measurement of the CP structure of the H boson at tree level by studying the $t\bar{t}H$ and tH processes in final states with multiple electrons, muons, and hadronically decaying tau leptons (τ_h). The cross section measurement published by the CMS Collaboration [25] is extended by interpreting the results in terms of the spin-parity of the H. Additional machine learning techniques are used to maximise the separation between different H CP scenarios.

The measurement is based on data recorded by the CMS experiment in pp collisions at $\sqrt{s} = 13 \text{ TeV}$ during the LHC Run 2, corresponding to an integrated luminosity of 138 fb^{-1} , with an in-depth description of the CMS detector to be found in Sec. 3. The search for CP violation in the $t\bar{t}H$ and tH production modes using multilepton final states follows other CMS measurements where the CP structure of the coupling y_t of the observed boson to the top quark was studied finding no deviation with respect to the SM prediction of CP-even scenario [77].

This analysis includes the signatures $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$, and $3\ell + 0\tau_h$, which account for the H decay modes $H \rightarrow WW$ and $H \rightarrow \tau\tau$ targeting events in which at least one top quark decays leptonically and providing the highest sensitivity to possible CP violation effects. The symbol ℓ denotes light leptons (e, μ), and “ss” means “same-sign”. The symbol τ_h denotes hadronically decaying tau leptons. As in previous analyses [77], the separation of the $t\bar{t}H$ and tH signals from backgrounds is improved with machine learning techniques, mainly BDTs and artificial Deep Neural Networks (DNNs), as well as with matrix element methods [152, 153]. In particular, machine learning methods are employed to improve the separation between CP-odd and CP-even scenarios, both pure and mixed, for the $t\bar{t}H$ and tH signals.

5.2 Phenomenology

The phenomenology discussed in this section expands on the discussion in Sec. 2.7.2. The Lagrangian for the fermions-Higgs interaction can be written as a superposition of amplitudes with a CP-even and a CP-odd phase, where any deviation from the SM prediction of a purely CP-even H boson would indicate new physics and hence be described as a Beyond the SM (BSM) phenomenon.

Assuming that the spin-0 H boson is a mass eigenstate, the $t\bar{t}H$ Lagrangian can be parameterized as follows:

$$\mathcal{L}_{t\bar{t}H} = \frac{m_t}{v} \bar{\psi}_t (\kappa_t + i\gamma_5 \tilde{\kappa}_t) \psi_t H, \quad (5.1)$$

where $\bar{\psi}_t$ and ψ_t represent Dirac spinors, v denotes the vacuum expectation value of the SM H field, and κ_t and $\tilde{\kappa}_t$ correspond to the CP-even and CP-odd top-Higgs Yukawa coupling modifiers. The parameter κ_t is proportional to $\cos(\alpha)$, while $\tilde{\kappa}_t$ is proportional to $\sin(\alpha)$, where α is the mixing angle. As there is no CP violation according to the SM, α needs to be either 0° or 180° .

The specific values chosen for κ_t and $\tilde{\kappa}_t$ influence the coupling, impacting the cross section and kinematic properties of both the $t\bar{t}H$ and tH processes. As derived in Ref. [154], variations in the differential cross section of the $t\bar{t}H$ and tH processes depending on the choice of α are used to determine the CP structure. Depending on the chosen α , we can identify three distinct

scenarios, as outlined in Tab. 5.1.

Kinematic differences between the purely CP-even, the purely CP-odd, and the mixed scenario can be exploited to discriminate between them and examine the exact CP scenario that is favoured by nature. It is important to note that the cross section of the $t\bar{t}H$ process is symmetric around $\alpha = 90^\circ$ and is therefore not sensitive to the difference between the SM coupling ($\alpha = 0^\circ$) and the inverse coupling ($\alpha = 180^\circ$).

Table 5.1: Possible CP scenarios

Scenario	α
Purely CP-even	0° or 180°
Purely CP-odd	90° or 270°
Mixed	$\neq 0^\circ, \neq 90^\circ, \neq 180^\circ$

5.3 Data Samples

The data and simulated samples used in this analysis are those used in the inclusive measurement of the $t\bar{t}H$ and tH cross sections performed by the CMS Collaboration [25]. The most important highlights are listed here for completeness.

This analysis uses pp collision data recorded at $\sqrt{s} = 13$ TeV at the LHC during 2016-2018. Data-taking periods during which the CMS detector was not fully operational are excluded from the analysis. The total integrated luminosity of the analyzed data set amounts to 137 fb^{-1} , of which 36.3 [130], 41.5 [131], and 59.8 fb^{-1} [132] have been recorded in 2016, 2017, and 2018, respectively.

The SM cross sections for the $t\bar{t}H$ and tH signals and for the most relevant background processes estimated from simulation are reported in Tab. 5.2. The backgrounds arising from nonprompt or misidentified leptons (collectively labelled “nonprompt” in the figures of this chapter) and from lepton charge mismeasurement are described in Sec. 5.5; regardless of the processes that originated them, they are fully determined from data. All the other background contributions are determined from simulation.

The $t\bar{t}H$ and tH signals as well as $t\bar{t}\gamma$, $t\bar{t}x$, tZ , $t\bar{t}WW$, W +jets, Drell-Yan (DY), $W\gamma$, and $Z\gamma$ backgrounds are simulated at LO. Other processes like the backgrounds arising from $t\bar{t}$ production in association with W and Z bosons ($t\bar{t}W$, $t\bar{t}Z$), from triboson (WWW , WWZ , WZZ , ZZZ , and $WZ\gamma$) production, as well as from the production of four top quarks ($t\bar{t}t\bar{t}$) are generated at Next to LO (NLO) accuracy.

The $t\bar{t}H$ and tH samples are produced assuming all couplings of the H boson have the values expected in the ITC scenario. To account for variations in the kinematic properties of $t\bar{t}H$ and tH signal events, signal events are reweighted according to the method recommended in Refs. [155, 156] by using κ_t and $\tilde{\kappa}_t$.

The simulation also incorporates the effect of Pileup (PU), which are simultaneous pp collisions occurring in the same or nearby bunch crossings. This is achieved by overlaying inelastic pp interactions onto all Monte Carlo (MC) events. Simulated events are weighed so that the PU distribution of simulated samples matches the one observed in the data.

All MC events are passed through a detailed simulation of the CMS detector using GEANT4 [157, 158] and are processed with the same CMS event reconstruction software as the data.

To bridge residual discrepancies between data and simulation, simulated events are corrected

either through weights or by varying relevant metrics. These adjustments account for differences in various aspects: trigger efficiencies; reconstruction and identification efficiencies for e , μ , and τ_h ; the energy scale for τ_h and jets; the efficiency of identifying jets from b quark hadronization and the misidentification rates for light-quark and gluon jets; and the resolution in missing transverse momentum (p_T^{miss}). These corrections, usually a few percent, are derived from various SM processes like DY ($Z/\gamma^* \rightarrow ee$, $Z/\gamma^* \rightarrow \mu\mu$, and $Z/\gamma^* \rightarrow \tau\tau$), $t\bar{t}$, and γ +jets production, as cited in Ref. [126, 129, 134, 159, 160].

Table 5.2: Standard model cross sections for the $t\bar{t}H$ and tH signals as well as for the most relevant background processes estimated from simulation. The cross sections are quoted for pp collisions at $\sqrt{s} = 13$ TeV.

Process	Cross section [fb]	Process	Cross section [fb]
$t\bar{t}H$	507 [32]	$t\bar{t}Z$	839 [32]
tHq	74.3 [32]	$t\bar{t}W$	650 [32, 162, 163]
tHW	15.2 [161]	$t\bar{t}WW$	6.98 [140]
ggH	4.86×10^4 [32]	WZ	4.50×10^4 [164]
qqH	3.78×10^3 [32]	ZZ	1.69×10^4 [164]
WH	1.37×10^3 [32]		
ZH	884 [32]		

5.4 Event Selection

The event selection criteria follow closely that of the $t\bar{t}H$ inclusive analysis in the multilepton channel, which are described in full detail in Ref. [25]. Nonetheless, a summary is shown here for completeness.

The event selection in this analysis is designed to detect the rare $t\bar{t}H$ and tH (tHq and tHW) signals in multilepton final states despite the presence of other SM processes with larger cross section also yielding to leptons in the final state. More specifically, the H boson decays where H decays into a pair of W bosons or τ leptons are targeted. The W subsequently decay either hadronically or into electrons or muons, while the τ can decay to electrons, muons or τ_h . Events with a pair of loose leptons with an invariant mass smaller than 12 GeV are rejected, as they are not well modeled by the simulation. Moreover, events are required to contain at least one jet of $p_T > 25$ GeV. Events are collected by a set of single, double, and triple lepton triggers that are designed to maximize the efficiency of the trigger set. The thresholds on the lepton p_T range from 8 to 24 GeV (from 12 to 27 GeV) for muons (electrons).

The events are analyzed in mutually exclusive categories, also referred to as “channels”, based on the multiplicity of light leptons and τ_h , with requirements on the charge of the light leptons in some cases. The three different channels covered in this analysis are $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$ and $3\ell + 0\tau_h$, where ℓ refers to an electron or muon and the τ_h refers to a hadronic τ , while the “ss” (“os”) refers to same-sign (opposite-sign) electrons or muons. They correspond to the three most sensitive channels in the inclusive $t\bar{t}H$ multilepton measurement at CMS [25] out of the ten channels used (see Fig. 5.1) and contain enough $t\bar{t}H$ events to be sensitive to signal kinematic properties.

Details on the selections applied to each channel are discussed in detail in the following sections. Additionally, a summary can be found in Tab. 5.3.

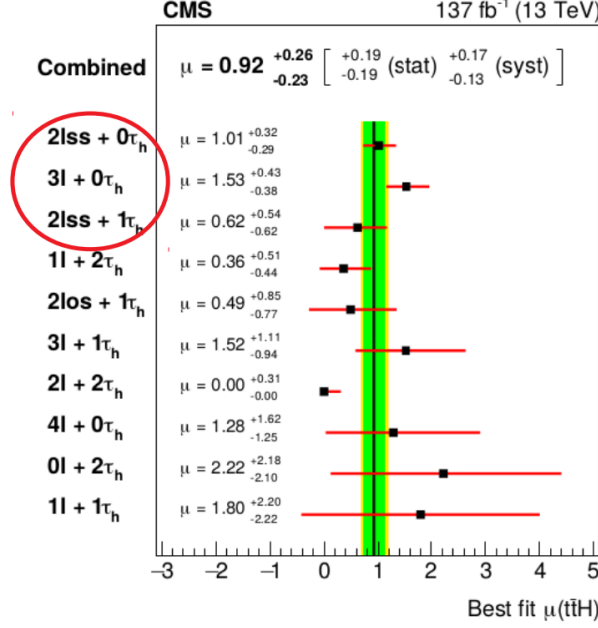


Figure 5.1: Sensitivity in all ten channels used in the inclusive $t\bar{t}H$ multilepton measurement at CMS [25] with the three most sensitive channels highlighted.

5.4.1 $2\ell ss + 0\tau_h$ Category

The $2\ell ss + 0\tau_h$ category targets $t\bar{t}H$ signal events in which the H boson decays into a pair of W bosons, one of which decays leptonically while the other decays hadronically. Simultaneously, one of the top quarks decays to leptons while the other one decays to hadrons. We also require the lepton from the W boson and the lepton from the top quark to have the same sign. Selected events are therefore required to contain two leptons of the same charge and which are both passing the tight object selection criteria. Additionally, the lepton of highest (lowest) p_T is required to have $p_T > 25$ GeV (> 15 GeV). Due to the large background from $t\bar{t}+\text{jets}$ the same charge requirement on the two leptons gets introduced. Even though this cut removes half of the $t\bar{t}H$ signal events, it removes almost all of the $t\bar{t}+\text{jets}$. Residual $t\bar{t}+\text{jets}$ background contributions are further suppressed by requiring the charge of all fakeable electrons and muons in the event to be well measured. Electrons must satisfy two conditions which test the consistency between the independent measurements of the electron charge obtained from the position of the ECAL cluster and from its track, while muons must satisfy the condition that the estimated uncertainty on the p_T of the muon track is below 0.2 times its p_T . The latter is equivalent to requiring that the sign of the curvature of the muon track, which determines its charge, is measured with a significance of 5σ . After applying these conditions, the charge misidentification rate is on the per-mille level for electrons and negligible for muons [165]. The background from $t\bar{t}Z$ production is suppressed by requiring that the event contains no pair of same-flavor opposite-sign loose leptons with mass close to the mass of the Z boson, i.e. $|m_{\ell\ell} - m_Z| < 10$ GeV, where $m_Z = 91.2$ GeV [166].

For what concerns the jet multiplicity, we select events that have at least three jets of $p_T > 25$ GeV and $|\eta| < 2.4$, among which at least two satisfy the loose Working Point (WP) of the b -tagging discriminator or that at least one satisfies the medium WP.

Events containing more than two tight leptons or a loose τ_h passing the very-loose WP of the τ_h identification discriminator are vetoed. The former avoids overlap with the $3\ell + 0\tau_h$ category, while the latter avoids overlap with the $2\ell ss + 1\tau_h$ category.

5.4.2 $2\ell ss + 1\tau_h$ Category

The $2\ell ss + 1\tau_h$ category targets $t\bar{t}H$ signal events in which the H boson decays into a pair of τ leptons, where one decays leptonically while the other decays into a τ_h . In the $t\bar{t}H$ case, one top quark decays to leptons and the other one decays to hadrons, while in the tH case, the single top quark decays leptonically. Additionally, the lepton from the τ decay and the lepton from the top quark decay have the same sign. The event selection criteria applied in the $2\ell ss + 1\tau_h$ category are identical to those applied in the $2\ell ss + 0\tau_h$ category, except that events selected in this category are required to contain one τ_h passing the very-loose WP of the τ_h identification discriminant, and there is no requirement on the mass of the selected electron pair m_{ee} . Also, if the second highest p_T lepton is a muon, the p_T requirement is relaxed to $p_T > 10$ GeV. The charge of the τ_h is required to be opposite to the charge of the leptons. Overlap with the $2\ell + 2\tau_h$ category is avoided by applying a modified τ_h veto requiring that the events selected in the $2\ell ss + 1\tau_h$ category do not contain two loose τ_h passing the medium WP of the τ_h identification discriminant.

5.4.3 $3\ell + 0\tau_h$ Category

The $3\ell ss + 0\tau_h$ category targets $t\bar{t}H$ signal events in which the H boson decays into a pair of W bosons. Two final states are covered: those where only one top quark and the two W bosons decay leptonically, and those where both top quarks but only one W boson decays leptonically.

Selected events are required to contain exactly three leptons passing the tight object selection criteria. The lepton of highest, second-, and third-highest p_T is required to have $p_T > 25$ GeV, > 15 GeV and > 10 GeV, respectively. The charge sum of the leptons is required to be either $+1$ or -1 . The background from $t\bar{t}Z$ production is suppressed by vetoing events containing a pair of loose leptons of the same flavor and opposite charge with invariant mass $|m_{\ell\ell} - m_Z| < 10$ GeV.

For what concerns the jet multiplicity, we select events that have at least two jets, among which at least two satisfy the loose WP of the b-tagging discriminant or at least one satisfies the medium WP. Events containing less than four jets are required to satisfy the condition $E_T^{miss} LD > 45$ GeV in case the event contains a pair of loose leptons of the same flavor and opposite charge, and $E_T^{miss} LD > 30$ GeV if the event does not contain such lepton pair. If the event contains four or more jets, no requirement on $E_T^{miss} LD$ is applied, as the contributions of background processes are negligible in this case.

Events containing a loose τ_h passing the very-loose WP of the τ_h identification discriminant are vetoed, as are events containing two pairs of loose leptons of the same flavor and opposite charge which satisfy the condition $m_{\ell\ell\ell\ell} < 140$ GeV. While the first condition avoids overlap with the $3\ell + 1\tau_h$ category, the second condition avoids overlap with the $t\bar{t}H$ -tagged category of the $H \rightarrow ZZ^* \rightarrow 4\ell$ analysis [167].

5.4.4 Further Event Classification in the Categories

Despite the selection mentioned above, the regions are still dominated by background events. We therefore use multivariate methods DNNs to separate the contribution from the various signal and background species. These discriminators were developed for the inclusive measurement [25] and take as an input variables related to the event kinematics. The neural networks have 3 (4) output nodes in the $2\ell ss + 1\tau_h$ and $3\ell + 0\tau_h$ ($2\ell ss + 0\tau_h$) categories, which estimate the probability for each event to correspond to $t\bar{t}H$, tHq or another background (to $t\bar{t}H$, tHq , $t\bar{t}W$

Table 5.3: Event selections applied in the $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$, $3\ell + 0\tau_h$.

Selection	$2\ell ss + 0\tau_h$	$2\ell ss + 1\tau_h$	$3\ell + 0\tau_h$
Trigger	Single- and double-lepton triggers		Single-, double- and triple-lepton triggers
Lepton p_T	$p_T > 25 / 15 \text{ GeV}$	$p_T > 25 / 15 \text{ (e) or } 10 \text{ GeV (}\mu\text{)}$	$p_T > 25 / 15 / 10 \text{ GeV}$
Lepton η	$ \eta < 2.5 \text{ (e) or } 2.4 \text{ (}\mu\text{)}$		$ \eta < 2.5 \text{ (e) or } 2.4 \text{ (}\mu\text{)}$
$\tau_h p_T$	—	$p_T > 20 \text{ GeV}$	—
$\tau_h \eta$	—	$ \eta < 2.3$	—
Charge requirements	2 same-sign leptons and charge quality requirements		—
	$\sum_{\ell, \tau_h} q = \pm 1$		$\sum_{\ell} q = \pm 1$
Jet multiplicity**	≥ 3 jets		≥ 2 jets
b tagging requirements**	≥ 1 medium b-tagged jet or ≥ 2 loose b-tagged jets		≥ 2 loose b-tagged jets
Light jet and b-tag***	≥ 1 light jets, ≥ 1 medium b-tagged jet		
Missing transverse momentum	$E_T^{\text{miss}} LD > 30 \text{ GeV}^{**}$		$p_T^{\text{miss}} LD > 45 \text{ GeV}^{\dagger}$
Dilepton mass	$m_{\ell\ell} > 12 \text{ GeV}^*$, $ m_{\ell\ell} - m_Z > 10 \text{ GeV}$		

* Applied on all pairs of leptons that pass loose selection.

** If events do not pass these cuts, *** is required.

$\dagger$ If the event contains a SFOS lepton pair and $N_{\text{jet}} \leq 3$. If the $N_{\text{jet}} \leq 3$ but there is no SFOS lepton pair, the cut is 30 GeV.

$\ddagger$ Applied to all SFOS lepton pairs.

or other background). The extra node is added in the $2\ell ss + 0\tau_h$ category to gain sensitivity to the irreducible $t\bar{t}W$ background.

Events are then classified according to its most-probable node. In the $2\ell ss + 0\tau_h$ and $3\ell + 0\tau_h$ an additional subcategorization is performed in the lepton flavor and b-tagged jet multiplicity to gain sensitivity to signal.

The number of events in the $2\ell ss + 0\tau_h$ and $3\ell + 0\tau_h$ categories is high enough to allow for sub-categorisation. This is used to enhance the signal and background separation. This choice of subcategorization improves the expected limits and helps validate the data-driven fake background estimation. The sub-categorisation is done as follows:

$2\ell ss + 0\tau_h$: In the $2\ell ss + 0\tau_h$ category, events are sub-categorised depending on the flavour of the leptons ($ee/e\mu/\mu\mu$). Except in the $t\bar{t}H$ node, as in that node an additional classification in bins of the CP discriminant is applied. This flavour categorization exploits the fact that the identification efficiencies are lower and misidentification rates are higher for electrons compared to muons, and the charge misidentification rates are sizeable for electrons and negligible for muons. It is intended to separate further the $t\bar{t}W$ component of the background from the $t\bar{t}H$ and $t\bar{t}Z$ components.

$2\ell ss + 1\tau_h$: The $2\ell ss + 1\tau_h$ category, events are separated only depending on the output of the DNN classifier.

$3\ell + 0\tau_h$: In the $3\ell + 0\tau_h$ category, events on the tH -region and $t\bar{t}H$ -region are separated according to the number of jets that pass the medium WP of the b-tagging discriminant (2b and 1b). In the background region we further separate events according to the lepton flavour ($eee/ee\mu/e\mu\mu/\mu\mu\mu$), for the same reasons outlined before.

To build the final distributions in each of the subcategories, we categorize according to the score of the most probable node. Then, we bin the discriminants constructing quantiles in the quantity of backgrounds. The number of bins is then decided upon the achieved expected limit and keeping also the total statistics high enough.

This selection allows to gain sensitivity to the inclusive $t\bar{t}H$ and tH production. We additionally make use of multivariate discriminators to capture the shape differences between the $t\bar{t}H$

CP-even component and a potential $t\bar{t}H$ CP-odd component. A dedicated BDT is trained for each category to distinguish between these two components, as described in Sec. 5.7, and that we label as BDT_{CP} . Events in the $t\bar{t}H$ node of each category are then classified according to the score of BDT_{CP} .

5.5 Background Estimation

Like in the measurement presented in Chap. 4, backgrounds are classified as either reducible or irreducible depending on the source of the reconstructed leptons passing the tight object selection criteria. A background is considered reducible when one or more of the reconstructed leptons passing the tight object selection criteria do not correspond to a lepton originating from the prompt decay of a W or Z boson or a τ lepton decay. Otherwise, the background is considered irreducible.

The same three reducible backgrounds (misidentified leptons, asymmetric photon conversions and charge flips) as in the measurement presented in Chap. 4 are considered. As they have already been described in detail in Sec. 4.4, a detailed description is skipped here.

However, as different processes are considered signal, we also consider a different selection of processes as irreducible background. Most of the irreducible background is made up by $t\bar{t}W(W)$, $t\bar{t}Z$ and diboson backgrounds, from SM H boson production via the processes ggH , qqH , WH , $t\bar{t}WH$ and $t\bar{t}ZH$ and so-called “rare” backgrounds. Rare backgrounds include processes as tZ production, the production of same-sign WW pairs, triboson and $t\bar{t}t\bar{t}$ production.

Irreducible backgrounds are modeled using samples of simulated events with the highest precision available. The full list of samples is shown in [150]. We use NLO samples for the main backgrounds: $t\bar{t}Z$, $t\bar{t}W$, and WZ . We also make use of dedicated $t\bar{t}W$ samples including α^3 terms and their NLO corrections in pQCD, proportional $\alpha^3\alpha_s$, which are found to have a significant effect [162, 163]. The normalization of $t\bar{t}Z$, $t\bar{t}W$ and WZ is parameterized as freely-floating nuisance parameters that are profiled in the signal extraction fit.

To validate the modelling of the $t\bar{t}W(W)$, $t\bar{t}Z$, WZ and ZZ backgrounds, we use dedicated CR, which will be further evaluated in Sec. 5.6.

Table 5.4: Summary of the reducible backgrounds for all channels. The dagger symbol † denotes, when a background is estimated with data driven methods, while otherwise they are estimated using MC simulations.

Process	$2\ell ss + 0\tau_h$	$2\ell ss + 1\tau_h$	$3\ell + 0\tau_h$
Misidentified leptons †	✓	✓	✓
Flips †	✓	✓	—
Conversions	✓	✓	✓

5.6 Background Control Regions

To constrain the irreducible background contributions from WZ and ZZ processes, we define two CR. They are defined in the 3ℓ and 4ℓ categories and are included in the signal extraction fits.

In order to check the validity of our objects and background samples as well as our data driven background estimation, three additional regions called Validation Regions (VR) are defined. For completeness, a short description on their selection and purpose is discussed in Sec. 5.6.3.

5.6.1 Trilepton Control Region

The three lepton CR is defined by inverting the Z boson veto present in the $3\ell + 0\tau_h$ SR defined in Sec. 5.4. The selection criteria on jets and b tagged jets are dropped in this region. Besides, the $E_T^{miss} LD > 45$ GeV criteria is applied in case the event contains a pair of loose leptons of the same flavor and opposite charge, if the event does not contain such lepton pair the criteria is $E_T^{miss} LD > 30$ GeV and no requirement on $E_T^{miss} LD > 30$ is applied at all if the event contains four or more jets.

Events are then classified as the number of jets and b tagged jets in 12 bins: 0 b tagged jets with 1, 2, 3 or more than 3 jets; 1 b tagged jet with 2, 3, 4 or more than 4 jets, and more than 1 b tagged jets with 2, 3, 4 or more than 4 jets. This allows to separate the $t\bar{t}Z$ and WZ backgrounds. Additionally, events are categorized according to the flavor of the leptons and can be seen in in Fig. 5.2.

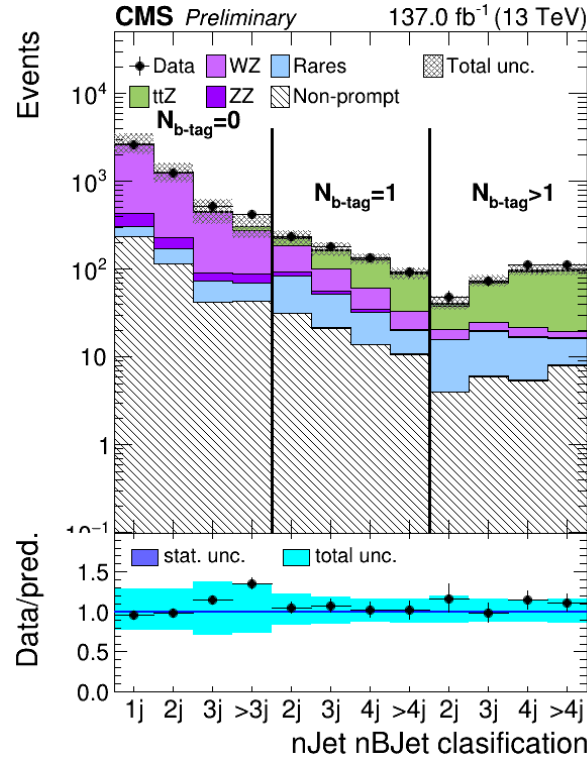


Figure 5.2: 3 lepton CR distribution for all years combined

5.6.2 Four-lepton Control Region

A four lepton CR is defined by events with four leptons, two of which form a Z boson candidate. Moreover, the jet and b tagging discriminator selections are not applied in this case. Events in this region are classified according to the number of Z boson candidates and the jet and b tagged jet multiplicity, four categories are created using that information:

- Events with two pairs of opposite-sign same flavor leptons with masses compatible with the Z boson.
- Events with exactly one pair of opposite-sign same flavor leptons with a mass compatible with the Z boson and no jets.

- Events with exactly one pair of opposite-sign same flavor leptons with a mass compatible with the Z boson and exactly 1 medium WP b tagged jet.
- Events with exactly one pair of opposite-sign same flavor leptons with a mass compatible with the Z boson and more than one medium WP b tagged jet.

The obtained distribution is shown in Fig. 5.3.

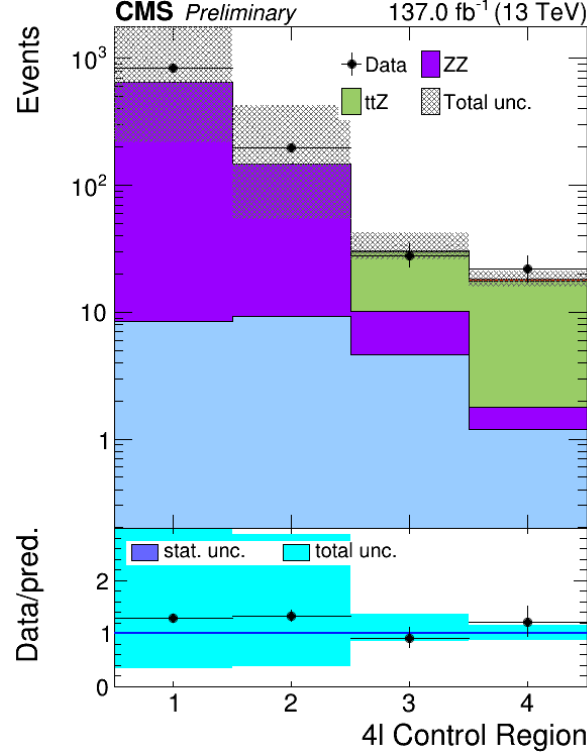


Figure 5.3: 4 lepton CR distribution for all years combined

The sensitivity to $t\bar{t}Z$ and ZZ background processes is driven by the 3ℓ CR, however, the 4ℓ CR provides a reasonably sensitive alternative measurement and is enriched in ZZ events.

5.6.3 Validation Regions

Three Jet Validation Region The Three Jet ($3j$) VR is built by selecting events in the $2\ell ss + 0\tau_h$ region that contain exactly three jets, including forward jets. It is used to check the estimation of the misidentified lepton background and allows us to check our variables and objects. Additionally, the enlargement of the acceptance allows us to check the modeling of the variables and objects in the forward region, that is relevant for the measurement of tHq production. Such a region is enriched in $t\bar{t}W$ and WZ production and events with misidentified leptons, mostly due to $\tau\tau$ events. The corresponding plots can be seen in Fig. 5.4 and show a good agreement.

$t\bar{t}Z$ Validation Region This VR is defined by reversing the Z veto in the $3\ell + 0\tau_h$ region and selecting only events with at least two central jets. Like the other VR it is used to validate the modelling of our variables and our objects. It is also enriched in $t\bar{t}Z$, one of our main backgrounds, and as such lets us check the modelling of this background. The corresponding plots can be seen in Fig. 5.5 and show a good agreement.

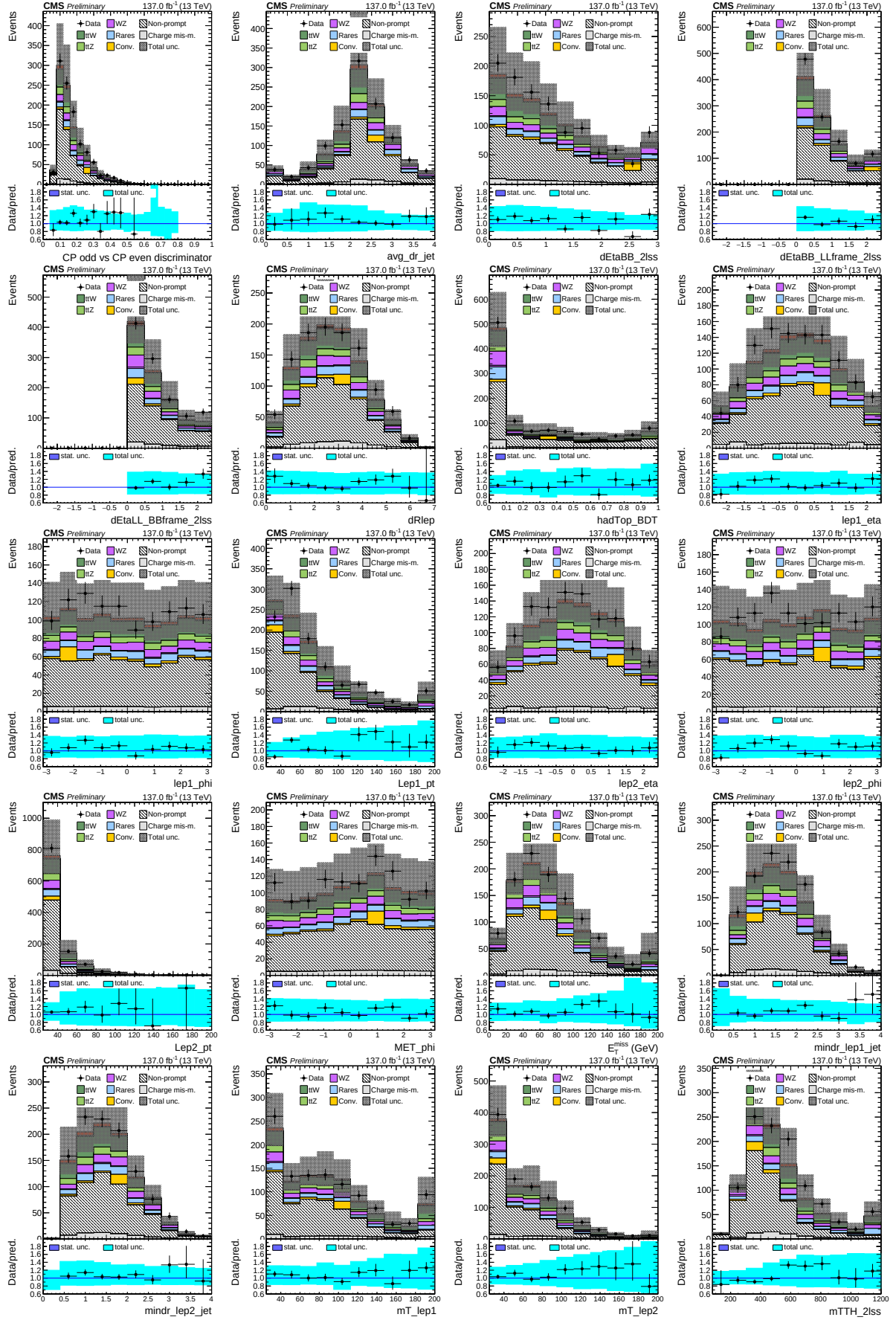


Figure 5.4: Plots for the 3j VR

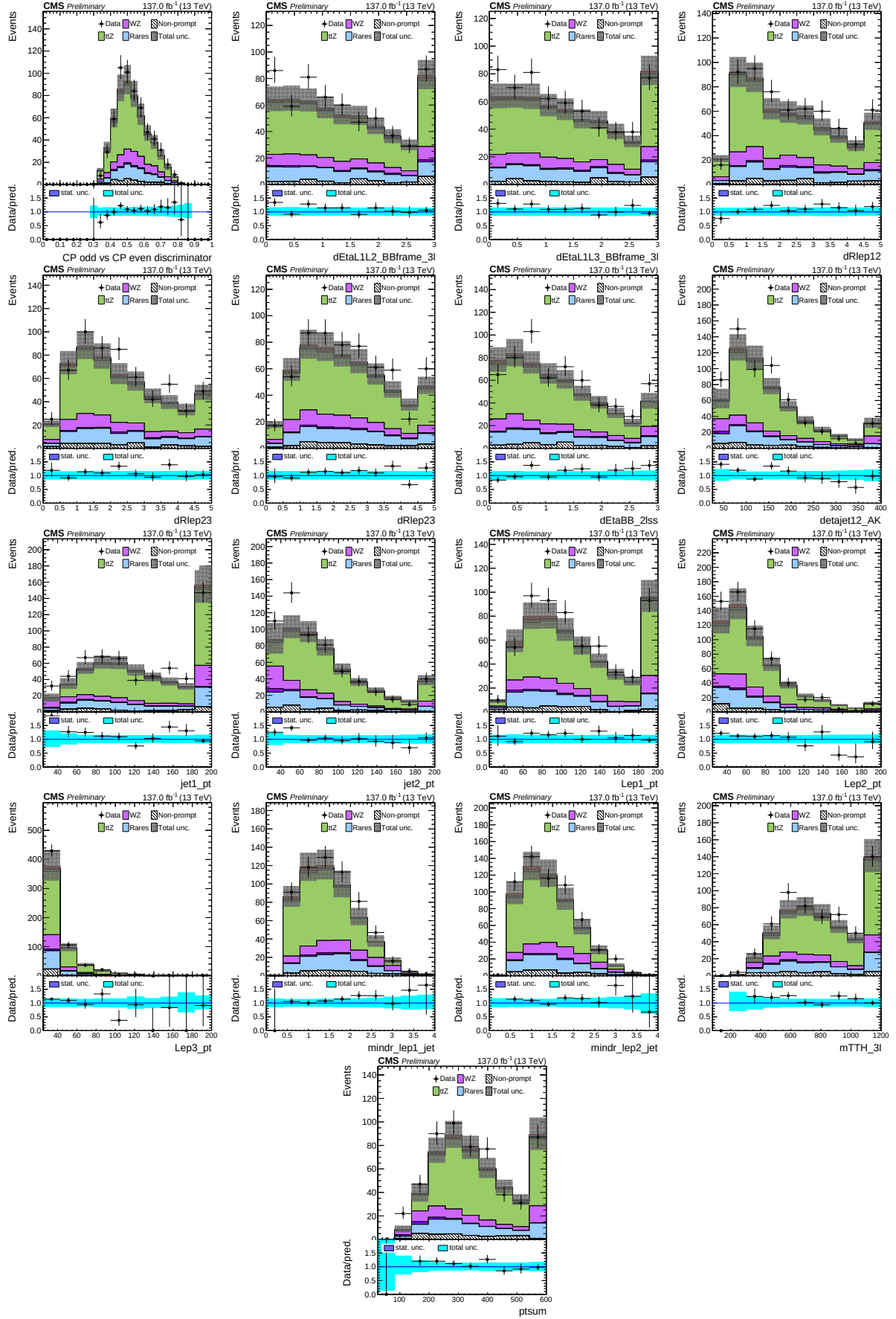


Figure 5.5: Plots for the ttZ VR

WZ Validation Region The WZ VR region is constructed starting from the $t\bar{t}Z$ control region and inverting the b tag jet multiplicity requirement in that region. Such a region is enriched in WZ events with additional jets and allows us to validate objects and modelling independent of Drell-Yan events. The corresponding plots can be seen in Fig. 5.6 and show a good agreement.

5.7 CP Discrimination

In order to separate CP-even and CP-odd scenarios, three separate Boosted Decision Tree (BDT) classifiers are trained, one for each of the channels: $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$, and $3\ell + 0\tau_h$.

For all three classifiers, we use 50% of our samples to train the BDTs, 40% for testing and 10% as validation dataset during training. Tab. 5.5 shows the various inputs used for the BDTs.

The hyperparameters of each classifier are optimized using a sequential grid search, resulting in a different optimal selection of input features for each BDT.

The transverse momentum, η , and ϕ of the final-state particles are used as input variables in all BDTs. The jet three-vectors are directly used only in the $3\ell + 0\tau_h$ category. Other variables, such as the momentum vectors of the four leading jets, have also been tested in the other final states. We found that they don't provide any increase in performance with respect to the current set, and their removal did not result in any performance loss. Other kinematic quantities such as the distance in the (η, ϕ) plane between the final-state objects are also used in all three categories.

The mass of the reconstructed $t\bar{t}H$ system ($m_{t\bar{t}H}$), which is composed by the leptons in the final state (including τ), the p_T^{miss} , and an appropriate number of jets (depending on the final state), proves to be a useful variable to discriminate between CP-even and CP-odd states.

In the $2\ell ss + 0\tau_h$ final state, the transverse masses of each lepton paired with p_T^{miss} are also considered in the training. The transverse mass is defined as:

$$m_T(l_i, p_T^{\text{miss}}) = \sqrt{(|\vec{p}_{T,l_i}| + |\vec{p}_T^{\text{miss}}|)^2 - |\vec{p}_{T,l_i} + \vec{p}_T^{\text{miss}}|^2}, \quad (5.2)$$

where $\vec{p}_{T,l_i}$ is the transverse momentum of the respective lepton.

Additional parameters like jet multiplicity, p_T^{miss} , the ϕ component of $\vec{p}_T^{\text{miss}}$, and the mean separation in the (η, ϕ) plane among jets further enhance performance in the $2\ell ss + 0\tau_h$ and $2\ell ss + 1\tau_h$ categories.

Moreover, jets resulting from a top quark's hadronic decay, where a dedicated BDT evaluates jet triplets to identify those originating from a top quark's hadronic decay [25], are useful for distinguishing between CP scenarios. In the $2\ell ss + 0\tau_h$ and $2\ell ss + 1\tau_h$ categories, the highest scoring triplet from all possible combinations in the event is used as an input. For the $2\ell ss + 1\tau_h$ category, an additional BDT classifier discerns jets from W boson decays in the $H \rightarrow WW$ decay chain, also in Ref. [25].

The number of input features for each BDT classifier ranges from 16 to 25. Tab. 5.5 lists all the input features for these BDTs. The modeling of these variables is checked in three validation regions enriched with misidentified lepton background, $t\bar{t}Z$, and WZ, respectively, which are discussed in Sec. 5.6.3.

The change of the most important import variables depending on the two CP scenarios [84, 168] is shown in Fig. 5.7 and 5.8 for the $2\ell ss + 0\tau_h$ and $3\ell + 0\tau_h$ channels.

Generally, the performance of our discriminator is bounded by the likelihood ratio between the CP odd and CP even components of the $t\bar{t}H$ signal. In our case, the likelihood ratio can

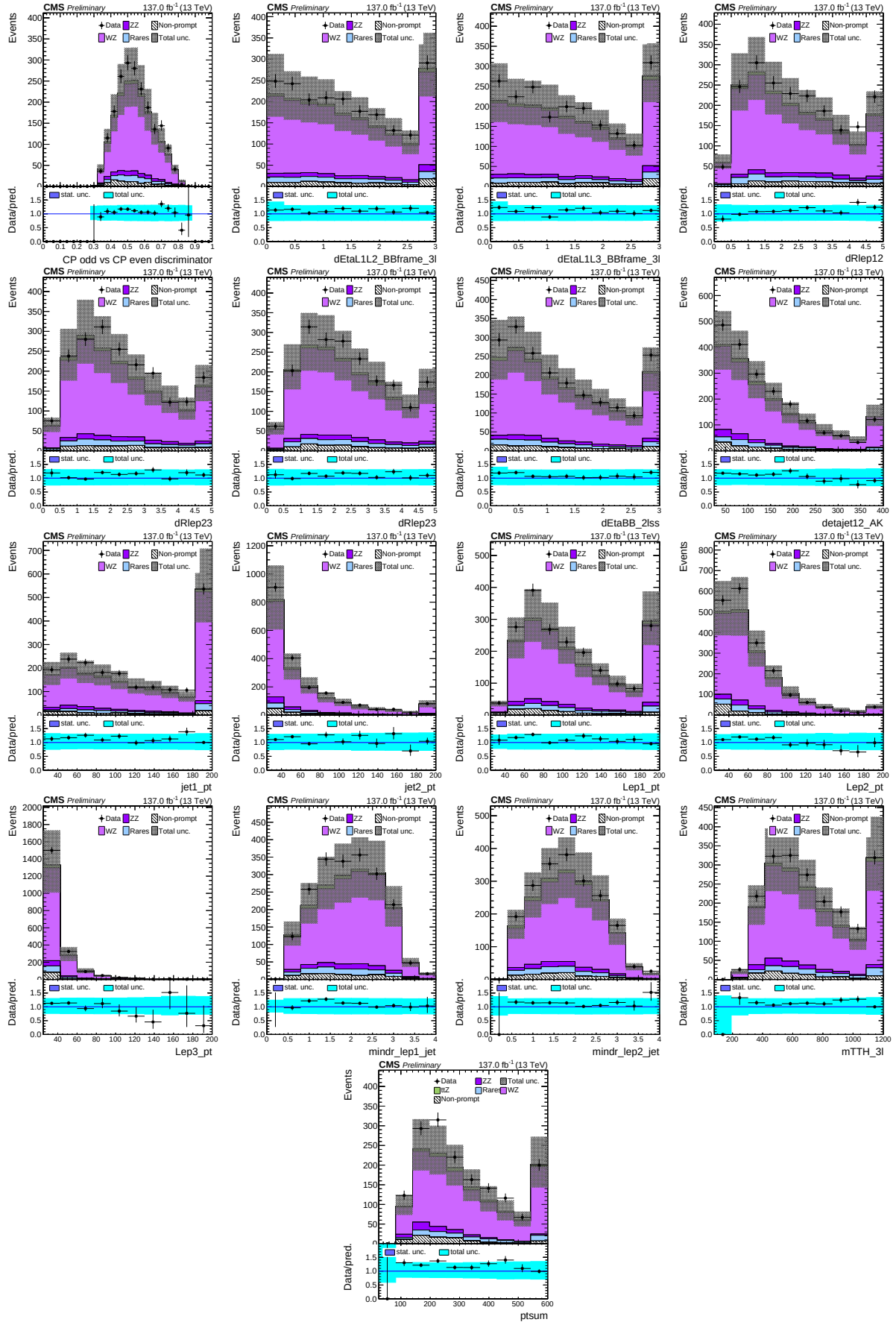


Figure 5.6: Plots WZ for the VR

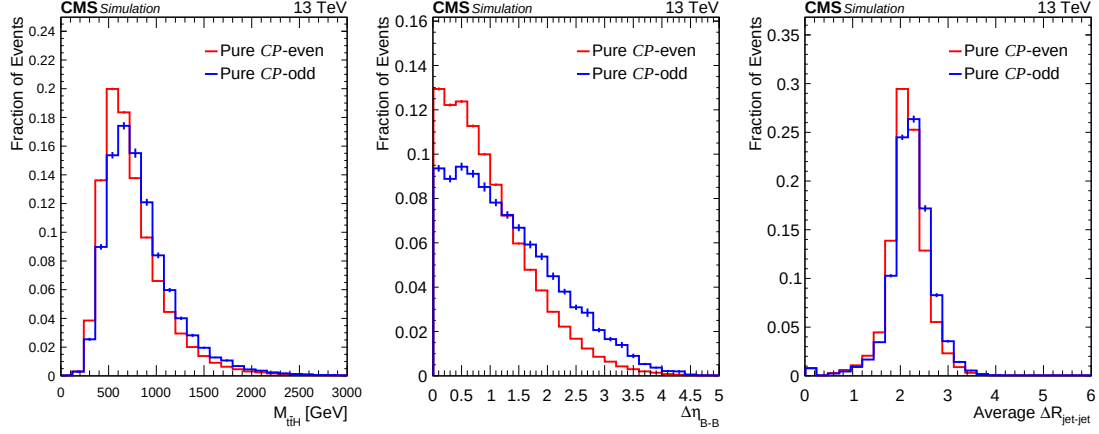


Figure 5.7: Most important input variables to the BDT used for CP discrimination in the $2\ell ss + 0\tau_h$ channel, defined in Tab. 5.5. The vertical bars represent the statistical uncertainty originating from the limited amount of simulated events. When not visible, the bars are smaller than the line width.

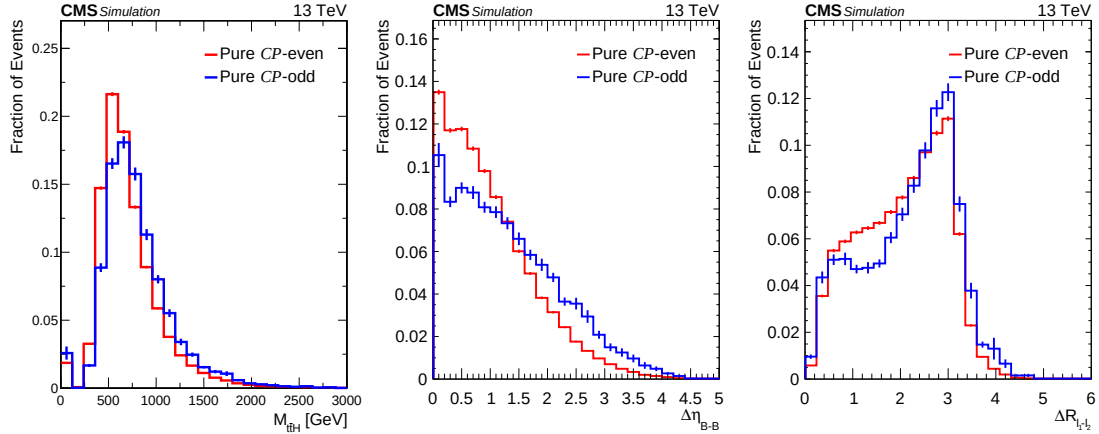


Figure 5.8: Most important input variables to the BDT used for CP discrimination in the $3\ell + 0\tau_h$ channel, defined in Tab. 5.5. The vertical bars represent the statistical uncertainty originating from the limited amount of simulated events. When not visible, the bars are smaller than the line width.

be determined in simulations, since it corresponds to the weights that are used to obtain the CP-odd distributions in samples generated under the CP-even scenario. This lets us calculate the maximum performance any classifier is able to achieve by directly using the likelihood ratios of both scenarios as a discriminator, which can be seen in Fig. 5.9. The weights are functions of the $t\bar{t}H$ kinematics of generator-level particles of the simulated samples. However, since the $t\bar{t}H$ kinematics cannot be reconstructed in data, it is impossible to actually reach this theoretical limit.

Table 5.5: Input features for the three BDTs. A check mark ($\checkmark$) indicates the variable is used in a given final state, whereas a long dash ($—$) indicates the variable is not used in that final state.

Variable description	$2\ell ss + 0\tau_h$	$2\ell ss + 1\tau_h$	$3\ell + 0\tau_h$
Jet variables*			
$j_1(p_T)$	—	—	$\checkmark$
$j_2(p_T)$	—	—	$\checkmark$
Number of jets	$\checkmark$	$\checkmark$	—
Lepton variables*			
$l_1(p_T)$	$\checkmark$	$\checkmark$	$\checkmark$
$l_1(\eta, \phi)$	$\checkmark$	$\checkmark$	—
$l_2(p_T)$	$\checkmark$	$\checkmark$	$\checkmark$
$l_2(\eta, \phi)$	$\checkmark$	$\checkmark$	—
$l_3(p_T)$	—	—	$\checkmark$
$\tau_h(p_T, \eta, \phi)$	—	$\checkmark$	—
Low level variables			
MET	$\checkmark$	$\checkmark$	—
Φ_{MET}	$\checkmark$	$\checkmark$	—
High level variables			
$t_{\text{had}}(\text{BDT score})^\dagger$	$\checkmark$	$\checkmark$	—
Higgs jet tagger †	—	$\checkmark$	—
Angle between two t in $t\bar{t}$ -frame	—	$\checkmark$	—
Angle of $t\bar{t}$ and H boson in $t\bar{t}H$ system	—	$\checkmark$	—
$m_{t\bar{t}H}$	$\checkmark$	$\checkmark$	$\checkmark$
m_T of l_1 and MET system	$\checkmark$	—	—
m_T of l_2 and MET system	$\checkmark$	—	—
dR of l_1 to the closest jet	$\checkmark$	$\checkmark$	$\checkmark$
dR of l_2 to the closest jet	$\checkmark$	$\checkmark$	$\checkmark$
dR between l_1 and l_3	—	—	$\checkmark$
dR between l_1 and l_2	—	—	$\checkmark$
dR between l_2 and l_3	—	—	$\checkmark$
Avg. dR distance among all jets	$\checkmark$	$\checkmark$	—
$d\eta$ of two jets with highest b score in the laboratory frame	$\checkmark$	$\checkmark$	$\checkmark$
$d\eta$ of the two leptons in frame of two most-likely b jets	$\checkmark$	$\checkmark$	—
$d\eta$ of two jets with highest b score in the dilepton system frame	$\checkmark$	$\checkmark$	—
$d\eta$ of two jets with highest b score in the ℓ_1 - ℓ_2 system frame	—	—	$\checkmark$
$d\eta$ of two jets with highest b score in the ℓ_1 - ℓ_3 system frame	—	—	$\checkmark$
$d\phi$ of the two leptons in frame of two most-likely b jets	—	$\checkmark$	—
$d\phi$ of two jets with highest b score in the dilepton system frame	—	$\checkmark$	—
$j_1(\eta) + j_2(\eta)$	—	—	$\checkmark$
$j_1(p_T) + j_2(p_T) + j_3(p_T) + \text{MET}$	—	—	$\checkmark$
Total number of variables	19	25	16

* Order determined by p_T

† Variables come from the Resolved Hadronic Top Tagger algorithm described in App. F in Ref. [150].

Table 5.6: Hyperparameters of the Classifiers DNNs

Variable	$2\ell_{ss} + 0\tau_h$	$2\ell_{ss} + 1\tau_h$	$3\ell + 0\tau_h$
Number of hidden layers	32, 10×16 , 5×8 , 5	2×50 , 30, 4×20 , 4	111, 2×16 , 8, 4
Activation on hidden layers	ReLu	PRelu	PRelu
Activation on output layer	Softmax	Softmax	Softmax
Optimiser	Adam (lr = 1e-3)	NAdam (lr = 1e-3)	NAdam (lr = 1e-3)
Batch size	500	500	500
Between hidden layers	batch normalization, 0.1 dropout	batch normalization, 0.1 dropout	batch normalization, 0.1 dropout

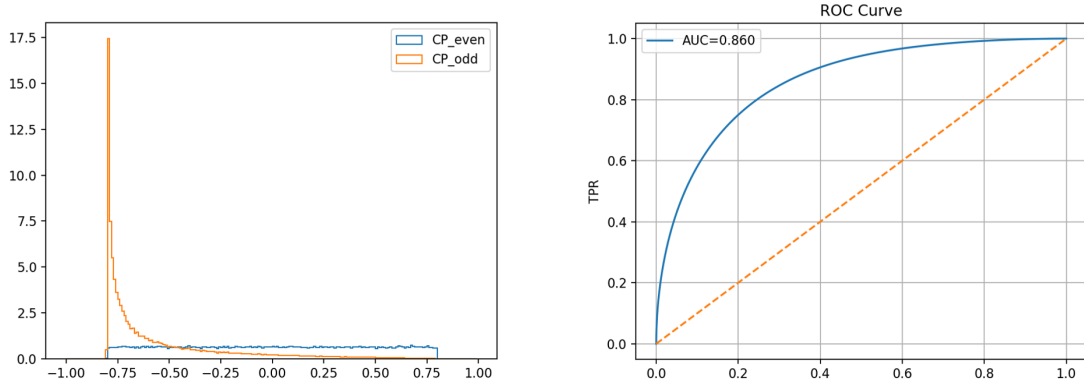


Figure 5.9: Maximum performance of the CP classifier in the $2\ell_{ss} + 0\tau_h$ category. The plot on the left shows the distributions of the Likelihood ratios determined from the simulated events and the plot on the right shows the ROC curve ($AUC = 0.863$) derived from the left plot.

5.8 Systematic Uncertainties

The various experimental systematic uncertainties have already been discussed in Sec. 3.2.8 and will not be discussed in detail here. Overall, this analysis considers the following systematic uncertainties: trigger efficiency, e and μ identification and isolation, τ_h identification efficiency, e , μ and τ_h energy scale, JES and JER, b jet tagging scale factors, MET resolution and response, integrated luminosity, pileup, L1 ECAL trigger efficiency corrections, misidentified lepton rate and charge misconstruction rate, renormalization (μ_R) and refactorization scales (μ_F) and theoretical cross section. Below, the theoretical systematic uncertainties are discussed.

Signal Rate: The measurement is affected by uncertainties in the $t\bar{t}H$ and tH cross sections, as the signal rates are measured in units of the SM $t\bar{t}H$ and tH production rates. The uncertainties associated to these processes are the following:

- The uncertainty in the SM $t\bar{t}H$ cross section, computed at NLO accuracy, amounts to $^{+6.8\%}_{-10.0\%}$, of which $^{+5.8\%}_{-9.3\%}$ are due to missing higher orders and 3.6% arises from uncertainties in the PDF and α_s [30].
- The uncertainty in the SM tH cross section, computed at NLO accuracy, amounts to $^{+4.2\%}_{-6.8\%}$, of which $^{+4.1\%}_{-6.7\%}$ are due to missing higher orders and 1.0% arises from uncertainties in the PDF and α_s [30].
- The uncertainty in the ITC tH cross section, computed at NLO accuracy, amounts to $^{+2.8\%}_{-4.0\%}$, of which $^{+2.7\%}_{-3.9\%}$ are due to missing higher orders and 0.9% arises from uncertainties in the PDF and α_s [30].
- The uncertainty in the branching fraction for the H boson to decay into WW ($\tau\tau$) amounts to 1.54% (1.65%).
- Uncertainties in the acceptance that are due to missing higher orders are treated as shape systematics, as they affect the shape of the distribution in the observable used for signal extraction. They are estimated by varying the renormalization (μ_R) and factorization (μ_F) scales between 0.5 and 2 times their default values, with the constraint that $0.5 \leq \mu_F/\mu_R < 2$.
- As $t\bar{t}H$ is simulated at LO in this analysis, the discrepancies between NLO and LO simulation need to be considered. The uncertainty is constructed as the symmetrized ratio of yields with LO and NLO samples.
- All the theoretical uncertainties associated to the signal rate are correlated across years.

Background Rates: The uncertainties associated to each of the relevant background contributions in this analysis are the listed below:

- The contribution of the WZ +jets background is known with an uncertainty of 30%, representing the uncertainty in the extrapolation to the SR from the WZ +jets-dominated CR (3l CR) described in Sec. 5.6.1. The uncertainty includes: the statistical uncertainty in the data yields in the CR; the uncertainty in the b tagging efficiency and mistag rate; and the uncertainty in the relative composition of light quark and gluon, c quark, and b quark jets in WZ +jets events contributing to the CR and to the SR.

- A 30% normalization uncertainty is applied to the WZ+jets and ZZ+jets background processes which contain 3 or more jets, to account for the mismodelling observed in the MC in these regions.
- The total normalization of WZ+jets and ZZ+jets backgrounds is floated in the fit and constrained by the dedicated CRs defined in Sec. 5.6.
- The uncertainty in the background arising from production of top quark pairs in association with real or virtual photons amounts to 30%.
- An uncertainty of 50% is assigned to other rare backgrounds which are modeled using MC simulation.
- No assumption is made on the rates of the irreducible $t\bar{t}W$, $t\bar{t}WW$ and $t\bar{t}Z$ backgrounds. The normalization of these backgrounds is determined simultaneously with the rate of the $t\bar{t}H$ and tH signals by the ML fit used for the signal extraction, described in Sec. 5.9.
- An additional uncertainty of 30% is assigned to the contribution of background events estimated using MC, which arise in the $2\ell ss + 1\tau_h$ category from events in which the reconstructed leptons are genuine prompt leptons and the reconstructed τ_h originates from the misidentification of a quark or gluon jet. This uncertainty is added because not all effects are well encapsulated by the current systematic uncertainties associated with the estimation of the misidentified leptons.
- The uncertainty on the yield of the charge flip background in the $2\ell ss + 0\tau_h$ and $2\ell ss + 1\tau_h$ categories amounts to 30%.

5.9 Signal Extraction

A Maximum Likelihood (ML) fit is performed on the distributions of chosen observables in the SR for the $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$, and $3\ell + 0\tau_h$ categories, as well as the CR for the 3ℓ and 4ℓ categories. These regions are further divided into subcategories targeting various processes, employing DNN classifiers as outlined in Sec. 5.4.4.

In the specific case of the $2\ell ss + 0\tau_h$ category, events are additionally separated based on the type of leptons involved (ee , $e\mu$ and $\mu\mu$), although this lepton flavour classification is not applied in the $t\bar{t}H$ node.

For the $3\ell + 0\tau_h$ category, the tH and $t\bar{t}H$ nodes are separated based on the number of b-tagged jets. Moreover, in the node that predominantly includes background events, a further classification is made considering the combinations of lepton flavours (eee , $ee\mu$, $e\mu\mu$, and $\mu\mu\mu$).

In the three SRs ($2\ell ss + 0\tau_h$, $3\ell + 0\tau_h$, and $2\ell ss + 1\tau_h$), the $t\bar{t}H$ -like categories described above are further split depending on the score of the CP classifiers described in Sec. 5.7.

The diagram depicted in Fig. 5.10 shows the classification described above.

This categorization allows us to exploit the different kinematic characteristics of the $t\bar{t}H$ process depending on the CP scenario. Additionally, the dedicated tH node in each category allows us to gain sensitivity to the sign of κ_t .

The discriminating observables, which are optimized for the $t\bar{t}H$ signal, used in the ML fit are shown in Fig. 5.11, showing the agreement between data and our statistical model evaluated at the best-fit point.

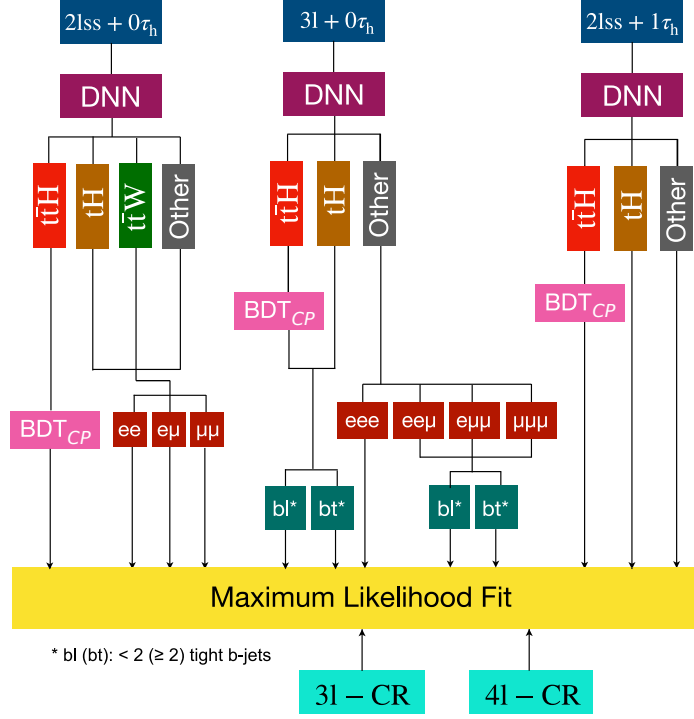


Figure 5.10: Diagram showing the categorization strategy used for the signal extraction. Besides the three SRs, also the two CRs enter the ML fit.

5.9.1 Beyond Standard Model Interpretation

To investigate BSM scenarios, particularly potential anomalous effects on the H boson couplings to fermions, we adopt the approach detailed in Sec. 5.2, which involves parameterizing the amplitude based on κ_t and $\tilde{\kappa}_t$. Corresponding to the amplitudes of the CP even and CP odd contributions of the top H coupling, they modify both the kinematics and normalization of the tH and t̄tH processes.

Additionally, as the tH process is sensitive to interference effects related to the top quark's coupling to the W boson, we set κ_V to its SM value. Similarly, the branching fractions of the H boson are also set to their SM predictions.

5.9.2 Results

Fig. 5.12 shows the expected and observed likelihood scans as a function of κ_t and $\tilde{\kappa}_t$, with the fit being compatible with the SM within 68% CL. The non-zero postfit value of $\tilde{\kappa}_t$ is driven by a small excess in the most CP-odd enriched regions of the $2lss + 0\tau_h$ and $3l + 0\tau_h$ categories.

By fixing $\tilde{\kappa}_t$ to its SM value, we are also able to determine one-dimensional limits at 68 and 95% CL for κ_t , which can be seen in Tab. 5.7.

We also parametrize the t̄tH process using two parameters: a signal strength multiplier, $\mu_{t\bar{t}H}$, applied to the SM t̄tH cross section, and $|f_{CP}^{Htt}|$, which is defined as $\frac{|\tilde{\kappa}_t^2|}{(|\tilde{\kappa}_t|^2 + |\kappa_t|^2)}$, where we set the H boson interactions with other particles to their corresponding SM predictions. The tH process is modified based on both $|f_{CP}^{Htt}|$ and $\mu_{t\bar{t}H}$.

This approach allows us to probe for possible fractional CP odd contributions and yields a best fit value of $|f_{CP}^{Htt}| = 0.59$ with an interval of (0.24, 0.81) at 68% CL. This result is compatible with the SM pure CP even scenario at 95% CL while the pure CP odd scenario is

Table 5.7: One-dimensional confidence intervals at 68 and 95% CL for κ_t ($\tilde{\kappa}_t$ fixed to SM expectation) and $\tilde{\kappa}_t$ (κ_t fixed to SM expectation). The upper part of the table shows the expected limits while the lower part shows the observed limits.

Parameter	68% CL	95% CL
Expected		
κ_t	(0.87, 1.14)	(0.74, 1.27)
$\tilde{\kappa}_t$	(-0.71, 0.71)	(-1.01, 1.01)
Observed		
κ_t	(0.89, 1.17)	(-1.09, -0.74) or (0.77, 1.3)
$\tilde{\kappa}_t$	(0.37, 1.16) or (-1.16, -0.37)	(-1.4, 1.4)

¹⁶¹⁸ excluded at more than 95% CL.

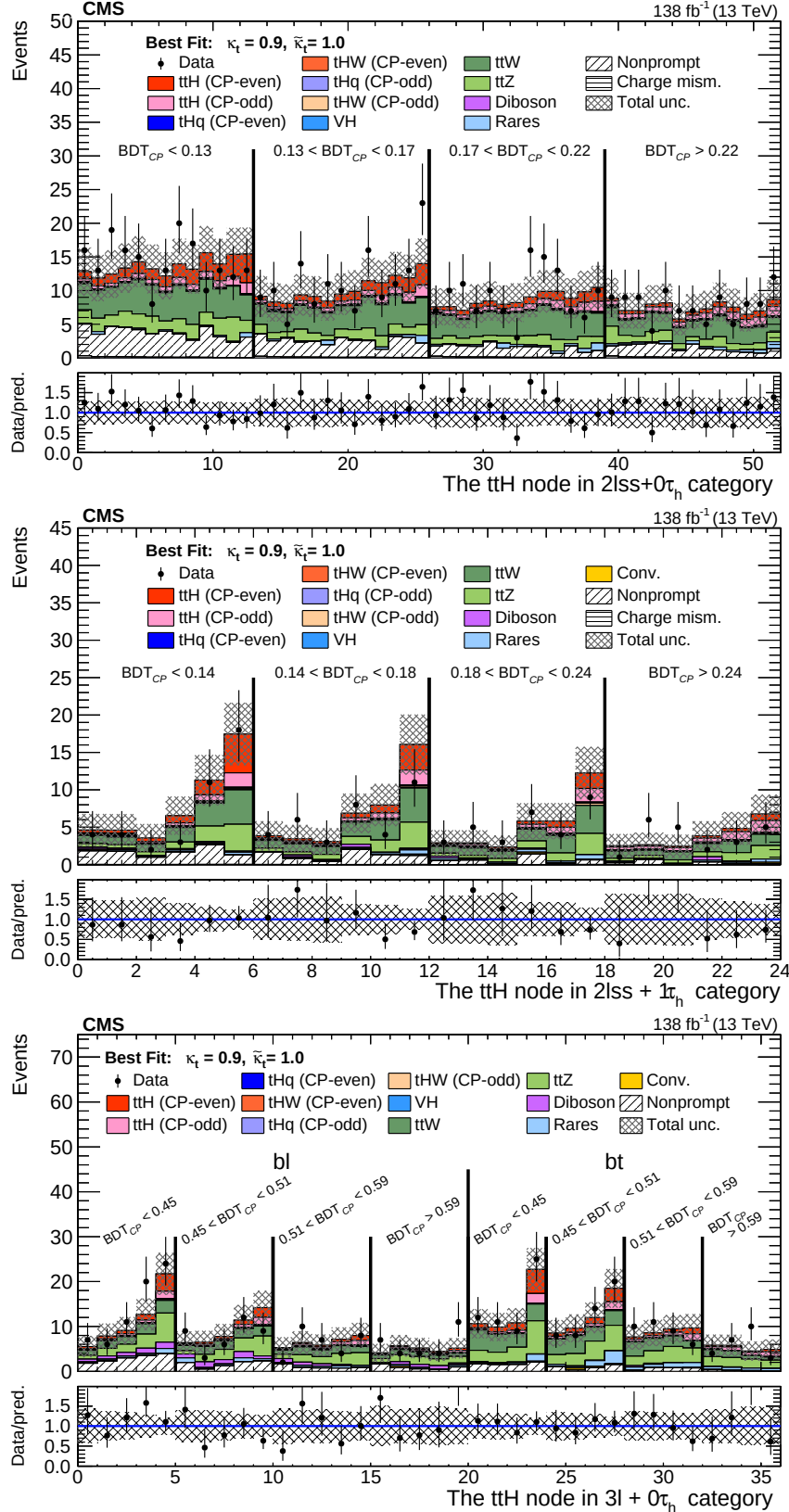


Figure 5.11: Postfit discriminating distributions used as input to the fit. Events in the $t\bar{t}H$ node are categorized as described in Sec. 5.9 for the three categories: $2\ell ss + 0\tau_h$ (top), $2\ell ss + 1\tau_h$ (center), and $3\ell + 0\tau_h$ (bottom). For the $2\ell ss + 1\tau_h$ bl (bt) denotes events with less than (at least) two b -tagged jets. The $t\bar{t}H$ CP-even (red) and CP-odd (pink) contributions are determined from the fit. The contribution labeled as “Nonprompt” refers to the backgrounds arising from misidentified leptons while the label “Charge mism.” alludes to the backgrounds arising from lepton charge mismeasurement.

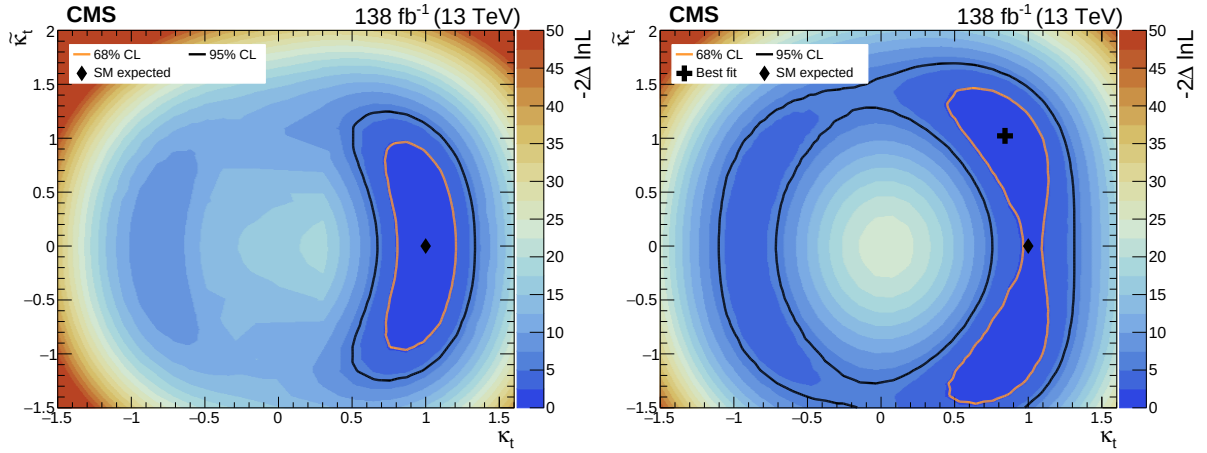


Figure 5.12: The expected (left) and observed (right) limits of κ_t and $\tilde{\kappa}_t$ are shown with both the 68 and 95% CL limits. The black cross shows the best value for κ_t and $\tilde{\kappa}_t$ given by the fit. The black diamond shows the expected SM values for κ_t and $\tilde{\kappa}_t$. κ_V and the H boson branching fractions are set to their SM values.

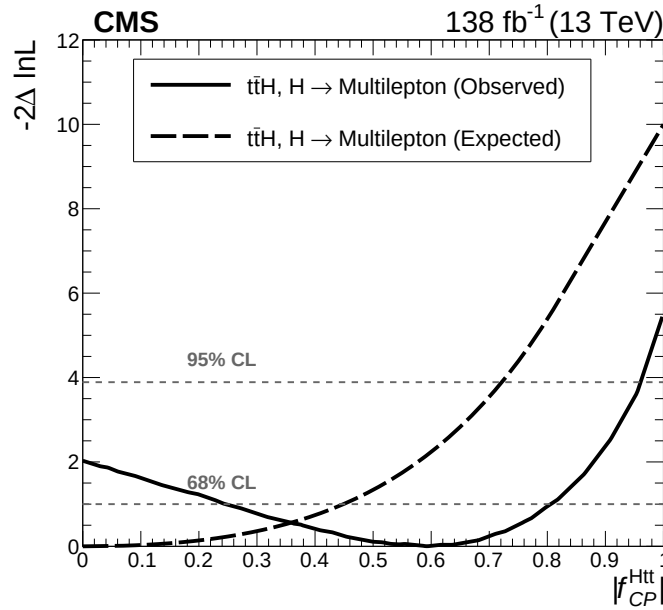


Figure 5.13: Likelihood scan as a function of $|f_{CP}^{Htt}|$ for multilepton final states. The solid (dashed) line shows the observed (expected) scan.

5.10 Combined Results for CP in $t\bar{t}H$ Events

The results presented in Sec. 5.9 are also combined with previously published CMS results on the CP parameter in other $t\bar{t}H$ decay channels. The combination includes the $H \rightarrow \gamma\gamma$ [77] and $H \rightarrow ZZ$ [79] results.

Uncertainties that are common between the various channels are taken as fully correlated. The detailed treatment of the systematic uncertainties can be seen in Ref. [169].

The combination provides a significant improvement in sensitivity, as shown in Fig. 5.14. Fig. 5.15 shows the extracted limits, as a function of κ_t and $\tilde{\kappa}_t$, for the combination of the multilepton, $H \rightarrow ZZ$, and $H \rightarrow \gamma\gamma$ decay modes.

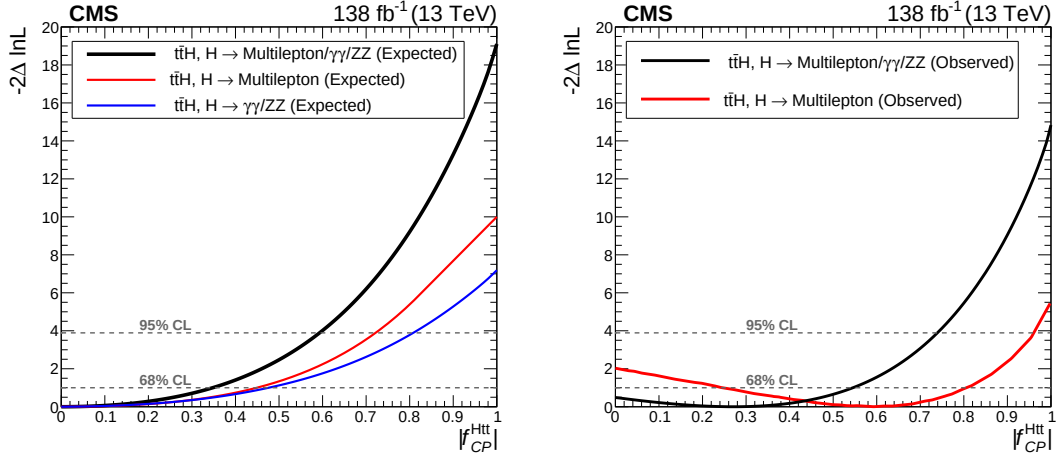


Figure 5.14: Likelihood scan as a function of $|f_{CP}^{Htt}|$. The left plot shows the expected limits for the multilepton final states, $H \rightarrow \gamma\gamma$, and $H \rightarrow ZZ$ final states, and the combination of multilepton, $H \rightarrow \gamma\gamma$, and $H \rightarrow ZZ$ final states. The right plot shows the observed likelihood scan for multilepton final states and the combination of multilepton, $H \rightarrow \gamma\gamma$, and $H \rightarrow ZZ$ final states.

One-dimensional confidence intervals at 68 and 95% CL are also obtained for κ_t ($\tilde{\kappa}_t$ fixed to SM expectation) and $\tilde{\kappa}_t$ (κ_t fixed to SM expectation), as listed in Tab. 5.8.

Table 5.8: One-dimensional confidence intervals at 68 and 95% CL for κ_t and $\tilde{\kappa}_t$.

Parameter	68% CL	95% CL
κ_t	(0.96, 1.16)	(0.86, 1.26)
$\tilde{\kappa}_t$	(-0.86, 0.85)	(-1.07, 1.07)

The observed limits of $|f_{CP}^{Htt}|$, while profiling $\mu_{t\bar{t}H}$, are shown for the combination of the multilepton, $H \rightarrow ZZ$, and $H \rightarrow \gamma\gamma$ decay modes in Fig. 5.14 and yields a best fit value of $|f_{CP}^{Htt}| = 0.28$ with an interval of $|f_{CP}^{Htt}| < 0.55$ at 68% CL. The result is compatible with the SM purely CP-even scenario within 68% CL. In addition, the scenario with $|f_{CP}^{Htt}| = 1$ is excluded with 3.7 standard deviations.

5.11 Summary

A measurement of the CP structure of the Yukawa coupling between the H boson and top quarks at tree level, when the H boson is produced in association with one (tH) or two ($t\bar{t}H$) top quarks, is presented. The measurement is based on data collected in proton-proton collisions

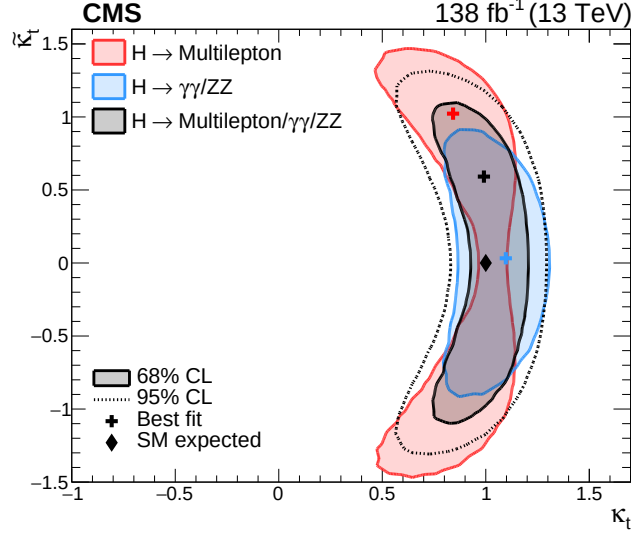


Figure 5.15: Likelihood scan as a function of κ_t and $\tilde{\kappa}_t$. Two-dimensional confidence intervals at 68% CL are depicted as shaded areas, for multilepton (red), the combination of $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ$ (blue), and the combination of the three channels (black). The 95% CL for the combination is shown as a dashed line. The best fit for each is shown as a cross of the corresponding colour. The plot is symmetric with respect to the line $\tilde{\kappa}_t=0$, hence there are two points corresponding to the best fit, here we only show one for simplicity. The black diamond shows the SM expected value. The nontrivial correlation between the measurements are the source of the change in the best fit value and shape of the confidence regions. The coupling κ_V and the H boson branching fractions are kept to their SM values.

at $\sqrt{s} = 13 \text{ TeV}$ by the CMS experiment at the CERN LHC, corresponding to an integrated luminosity of 137 fb^{-1} . The analysis targets events where the H boson decays to leptons and the top quark(s) decay either leptonically or hadronically. Separation of CP-even from CP-odd scenarios is achieved by using dedicated BDTs in each channel. Two-dimensional confidence regions are set on κ_t and $\tilde{\kappa}_t$ which are respectively the CP-even and CP-odd top-Higgs Yukawa coupling modifiers: one-dimensional confidence intervals are also set, constraining κ_t to be within $(-1.09, -0.74)$ or $(0.77, 1.30)$ and $\tilde{\kappa}_t$ to be within $(-1.4, 1.4)$ at 95% CL. No significant CP-odd contribution is observed, and the corresponding fraction parameter is determined to be $|f_{\text{CP}}^{\text{Htt}}| = 0.59$ with an interval of $(0.24, 0.81)$ at 68% CL. The results are combined with previously published analyses covering the $H \rightarrow ZZ$ and $H \rightarrow \gamma\gamma$ decay modes. Two- and one-dimensional confidence regions are set on κ_t and $\tilde{\kappa}_t$, constraining κ_t to be within $(0.86, 1.26)$ and $\tilde{\kappa}_t$ to be within $(-1.07, 1.07)$ at 95% CL. The possibility of a CP-odd contribution is also investigated in the combination, yielding a best fit of $|f_{\text{CP}}^{\text{Htt}}| = 0.28$ with an interval of $|f_{\text{CP}}^{\text{Htt}}| < 0.55$ at 68% CL. The results are compatible with predictions for the SM H boson.

6 Differential $t\bar{t}H$ Production in the Multilepton Final State

The work presented in this chapter corresponds to the paper "Differential $t\bar{t}H$ Production in the Multilepton Final State" and is currently in the internal approval process of the CMS experiment. This thesis is endorsed by the CMS experiment, which means that all plots and results shown in this chapter are to be understood as work in progress and as such might differ from the final published results and plots. As a result there will be significant overlaps with the paper mentioned above once it will be published. The analysis was performed in collaboration with the involvement of researchers from all the universities listed below:

- University of Zurich, Switzerland
- Universidad de Oviedo and ICTEA, Spain
- Universite Catholique de Louvain, Belgium
- Karlsruhe Institute of Technology, Germany
- Cornell University, USA
- Vilnius University, Lithuania

During this analysis I took a central role in many aspects of the analysis, often coordinating and delegating other team members as well as further developing the analysis framework. Below is a list of the most important contributions.

DNN Regression of Higgs Boson p_T : I trained and implemented DNNs to regress the Higgs boson p_T , improving over conventional approaches trying to reconstruct it directly via kinematic variables.

DNN Event Categorization: I introduced and executed the classification of events by process type via specialized DNN classifiers in each SR with the approach adapted from [25]. The implementation of said classifiers improved the sensitivity of the analysis significantly.

Validation: I was heavily involved in validating our data in the corresponding validation and control regions.

Optimization of the Binning: I derived the binning used in the signal regions for both the Higgs p_T and $m_{t\bar{t}H}$ based measurements to optimize our sensitivity.

6.1 Introduction

The Higgs (H) boson production in association with top quarks provides an interesting way to test the top-Higgs Yukawa coupling. The intricacies of tH and ttH production are described in more detail in Sec. 2.6.1.

This analysis builds on the approach developed in Ref. [25] which probed the Yukawa coupling to the H boson (y_t) divided by its SM expectation $\kappa_t := y_t/y_t^{SM}$ in multilepton final states.

Like in the approach of the CP measurement presented in Sec. 5, this analysis also uses the same three Signal Regions (SR), which correspond to the most sensitive channels of the measurement presented in Ref. [25]. These channels contain enough ttH events to be sensitive to signal kinematic properties, which makes them ideal to investigate the differential behavior of the top-Higgs system.

The measurement is based on data recorded by the CMS experiment in pp collisions at $\sqrt{s} = 13$ TeV during the LHC Run 2, corresponding to an integrated luminosity of 137 fb^{-1} , with an in-depth description of the CMS detector to be found in Sec. 3. It targets final states with electrons, muons, and hadronically decaying tau (τ_h) leptons and includes the signatures $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$, and $3\ell + 0\tau_h$. These signatures account for the H decay modes $H \rightarrow WW$ and $H \rightarrow \tau\tau$ targeting events in which at least one top quark decays leptonically. The symbol ℓ denotes light leptons (e, μ), and “ss” means same-sign.

As in the previous analysis [25], the separation of the ttH signal from backgrounds is improved with machine learning techniques like Deep Neural Networks (DNN).

We perform a so-called “SM analysis”, where we unfold to particle level the H boson p_T or alternatively the mass of the ttH-system ($m_{t\bar{t}H}$). The differential analysis observables are reconstructed using either combinations of final state objects (for the $m_{t\bar{t}H}$ based measurement) or via DNN-based regression (for the H p_T based measurement). The unfolding is performed via χ^2 minimization. For the H p_T , we use the latest Les Houches agreement on the Simplified Template Cross Section (STXS) binning of that observable, but we will also present results with a binning optimized based purely on the experimental sensitivity. For the $m_{t\bar{t}H}$ measurement, the binning scheme is not related to STXS agreements, and is optimized based purely on the experimental sensitivity.

Using the same inputs as for the differential cross section measurement, we measure the trilinear Higgs coupling κ_3 , exploiting the fact that it contributes to ttH production at loop level. The measurement of the trilinear Higgs coupling will be referred to as the “BSM measurement”.

As this analysis and the CP measurement presented in Chap. 5 are closely related, only the parts exclusive to this analysis are discussed in this chapter while the shared parts are discussed in Chap. 5.

6.2 Data Samples

The analyzed data was collected in pp collisions at $\sqrt{s} = 13$ TeV center-of-mass energy and with a 25ns bunch crossing period. The events were recorded using a combination of single, double, and triple lepton triggers. Only data-taking periods where all detector systems were fully operational are included in the analysis. The integrated luminosity of the analyzed dataset amounts to 36.3 fb^{-1} in 2016, 41.4 fb^{-1} in 2017 and 59.7 fb^{-1} in 2018, totalling 137 fb^{-1} in the full LHC Run 2. Approximately 30 inelastic pp interactions (PU) occurred per bunch crossing on average. The SM cross sections for the ttH and tH signals and for the most relevant background

processes estimated from simulation are reported in Tab. 5.2 in Chap. 5.

A combination of single, double, and triple lepton triggers is used to collect the data included in this analysis.

Samples of the $t\bar{t}H$ signal and of background events ($t\bar{t}Z$, $t\bar{t}W$ and other backgrounds), produced by Monte Carlo simulation, are used for the purpose of estimating signal and background yields in the analysis and to train machine learning algorithms. The following processes are simulated: Z +jets, W +jets, single top, top quark pairs, diboson (WW , WZ , ZZ , $W\gamma$, and $Z\gamma$), triboson (WWW , WWZ , WZZ , ZZZ , and $WZ\gamma$) production, the production of a single H boson by gluon-gluon fusion (ggF) and by vector-boson fusion (VBF), the associated production of a H boson with vector bosons (WH and ZH), double-Higgs production (HH), as well a few selected “rare” processes. The exotic processes, such as $t\bar{t}t\bar{t}$ and the production of same-sign WW boson pairs, typically have very small cross sections, but may nevertheless yield non-negligible background contributions in some event categories. All the simulated samples are produced setting the H boson mass to $m_H = 125$ GeV.

The cross sections of the $t\bar{t}H$ signal as well as single top quark [170–172], $t\bar{t}Z$, tHq , and tHW production [32], are computed at NLO accuracy. The Z +jets, W +jets, and $t\bar{t}$ +jets processes are normalized to cross sections computed at next-to-next-to-leading-order (NNLO) accuracy [173–176]. Special care is taken when scaling the $t\bar{t}Z$ background to the NLO cross-section of Ref. [32]: there are subtle differences between the process generated in the CMS simulated samples and the process for which the NLO calculation was performed. Details are given in Ref. [150], boiling down to the fact that the NLO computations are done without including Z/γ^* contribution, whereas the CMS simulated samples properly include that contribution.

In the case of the $t\bar{t}W$ background, besides the NLO samples, we use additional privately produced samples to improve the modeling of this background in the three years. In these samples, the $t\bar{t}W$ process is modeled including the higher order NLO3+NLO4 electroweak corrections, as recently derived in [162].

6.3 Event Selection

This analysis builds on the approach developed of the $t\bar{t}H$ inclusive measurement in the multilepton channel [25]. More specifically, three different channels covered in this analysis are $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$ and $3\ell + 0\tau_h$, where ℓ refers to an electron or muon and the τ_h refers to a hadronic τ , while the “ss” (“os”) refers to same-sign (opposite-sign) electrons or muons are targeted. These three channels correspond to the three most sensitive channels of the measurement in Ref. [25] and contain enough $t\bar{t}H$ events to be sensitive to signal kinematic properties.

An in depth description of the channels can be found in Sec. 5.4.

Generally, the event selection is designed to detect the rare $t\bar{t}H$ and tH (tHq and tHW) signals in multilepton final states despite the presence of other SM processes with larger cross sections also yielding to leptons in the final state. More specifically, the H boson decays where H decays into a pair of W bosons or τ leptons are targeted. The W subsequently decay either hadronically or into electrons or muons, while the τ can decay to electrons, muons or τ_h .

Within each channel, processes are further separated by means of a specialized DNN classifier. This adapts the strategy developed in Ref. [25] and improves upon it. A discussion of the channel specific event classification and a comparison to the classifier DNN in place for Ref. [25] is presented in the following section.

6.3.1 Event Classification

To increase the separation between signal and background we trained channel specific DNN classifiers.

In the approach developed in the inclusive measurement [25], events get classified into three classes each based on a different process or a group of processes. Namely they are $t\bar{t}H$ -like, tH -like and other events, where the other class (also called “bkg-like” in this analysis) is a class used to collect all events not fitting into any of the other classes. Additionally in the $2\ell ss + 0\tau_h$, the $t\bar{t}W$ -like class gets introduced to account for the relevant $t\bar{t}W$ background in this channel.

Even though this approach works reasonably well for $t\bar{t}H$ -like events, one observes that $t\bar{t}H$ events with high $H p_T$ are classified correctly with roughly the same accuracy as low $H p_T$ events which is reflected in similar AUC-scores for both low and high $H p_T$ events. Kinematically however, high $H p_T$ events should be easier to discriminate from other events, which hints at the DNN not discriminating high $H p_T$ events optimally.

To motivate the classifier to pay more attention at high Higgs p_T events, the $t\bar{t}H$ -like class is split into two classes. The first class contains $t\bar{t}H$ -like events with a Higgs p_T below 300 GeV while the second one contained $t\bar{t}H$ -like events with a Higgs p_T above 300 GeV.

The samples used for training and testing can be seen in Tab. 6.1. To each of the samples we applied the same cuts as of the corresponding SR.

To each event we applied the fake-rate weights and the GenWeight. Next, oversampling was applied to each events class if the sum of events in that class amounted to less than 10% of the overall sum of events. In that case, oversampling was applied until the sum of events in that class made up at least 10% of the overall events, which helped to create a more even distribution of events withing batches. Finally, additional weights on a per class level were applied so that the overall sum of all weighted events in each class was the same. 45% of the events were used for training, 5% for validation during the training and the remaining 50% for the testing of the classifiers.

A combination of low and high level variables was used to train the classifiers. Tab. 6.2 shows all the variables used in each channel together with a short explanation of the variable.

The choice of hyperparameters of the classifier DNNs is shown in Tab. 6.3.

Lastly, the performance of the classifier DNN is shown for $2\ell ss + 0\tau_h$ in Fig. 6.1, $2\ell ss + 1\tau_h$ in Fig. 6.2 and $3\ell + 0\tau_h$ in Fig. 6.3.

All classes in all three channels show a similar or improved ROC-AUC score compared to the DNN classifier presented in Ref. [25]. To compare the new classifier with the DNN in Ref. [25], we simply compare the output of the $t\bar{t}H$ -like node with either the $t\bar{t}H$ low or high $H p_T$ node of the new classifier. The $t\bar{t}H$ high $H p_T$ class shows a significant improvement, which confirms that the DNN of the inclusive analsis was not performing optimally for high $H p_T$ events. This improvement helps significantly to better constrain the kinematics of $t\bar{t}H$ in events with high $H p_T$ as we can extract them with a much higher purity. Finally, the ROC-AUC score in the $t\bar{t}H$ low $H p_T$ region stays comparable to the inclusive DNN.

Table 6.1: List of samples used to train the classifier DNNs in the $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$ and $3\ell + 0\tau_h$ categories. For the $2\ell ss + 1\tau_h$ and $3\ell + 0\tau_h$ categories the $t\bar{t}W$ -like class was included in the bkg-like class.

class	samples
$t\bar{t}H$ -like	TTHnobb_pow
tH -like	THQ_ctcvcp
$t\bar{t}W$ -like	TTWJetsToLNu_EWK_5f_NLO TTWToLNu_fxfr
bkg-like	TTLep_pow TTSemi_pow TTZToLLNuNu_amc TTZToLLNuNu_m1to10 THW_ctcvcp TTWW WZTo3LNu_fxfr VHToNonbb TTTT TTWH TZQToLL tWll_thad_wlep tWll_tlep_whad tWll_tlep_wlep WWTo2L2Nu WWZ WZG WZZ ZZZ

Table 6.2: Input variables for the classifier DNNs. A check mark ($\checkmark$) indicates the variable is used in a given channel, whereas a long dash ($—$) indicates the variable is not used in that channel.

Variable description	$2\ell ss + 0\tau_h$	$2\ell ss + 1\tau_h$	$3\ell + 0\tau_h$
Jet variables*			
$j_1(p_T, \eta, \phi)$	$\checkmark$	$\checkmark$	$\checkmark$
$j_2(p_T, \eta, \phi)$	$\checkmark$	$\checkmark$	$\checkmark$
$j_3(p_T, \eta, \phi)$	$\checkmark$	$\checkmark$	$\checkmark$
$j_4(p_T, \eta, \phi)$	$\checkmark$	$—$	$—$
Number of jets	$\checkmark$	$\checkmark$	$\checkmark$
Number of forward jets	$\checkmark$	$\checkmark$	$\checkmark$
Leading forward jet (η, p_T)	$\checkmark$	$\checkmark$	$\checkmark$
Number of med. b-tagged jets	$\checkmark$	$\checkmark$	$\checkmark$
Number of loose b-tagged jets	$\checkmark$	$\checkmark$	$\checkmark$
Lepton variables*			
$l_1(p_T, \eta, \phi, \text{charge})$	$\checkmark$	$\checkmark$	$\checkmark$
$l_1(m_T)$	$\checkmark$	$\checkmark$	$—$
$l_2(p_T, \eta, \phi)$	$\checkmark$	$\checkmark$	$\checkmark$
$l_2(m_T)$	$\checkmark$	$\checkmark$	$—$
$l_3(p_T, \eta, \phi)$	$—$	$—$	$\checkmark$
$\tau_h(p_T, \eta, \phi)$	$—$	$\checkmark$	$—$
Sum of lepton charges	$—$	$\checkmark$	$\checkmark$
Number of electrons	$—$	$\checkmark$	$\checkmark$
Sum of lepton IDs	$\checkmark$	$—$	$—$
Has same flavor os leptons	$—$	$—$	$\checkmark$
Low level variables			
MET	$\checkmark$	$\checkmark$	$\checkmark$
Maximum eta of an object	$\checkmark$	$—$	$—$
High level variables			
$t_{\text{had}}(\text{BDT score})^\dagger$	$\checkmark$	$\checkmark$	$—$
$t_{\text{had}}(p_T)^\dagger$	$—$	$—$	$\checkmark$
Higgs jet tagger †	$\checkmark$	$\checkmark$	$\checkmark$
$m_{t\bar{t}H}$	$—$	$\checkmark$	$—$
Mass of $l_{1,2}$ and τ_h ($\sum l_{1,2}(m) + \tau_h(m)$)	$—$	$\checkmark$	$—$
Mass of $b\bar{b}$ system**	$—$	$\checkmark$	$\checkmark$
Avg. dR distance among all jets	$\checkmark$	$\checkmark$	$\checkmark$
Min. dR between $l_{1,2}$ and j_1	$\checkmark$	$\checkmark$	$\checkmark$
Min. dR between l_3 and j_1	$—$	$—$	$\checkmark$
Min. dR between leptons	$—$	$\checkmark$	$\checkmark$
Min. dR between τ_h and j_1	$—$	$\checkmark$	$—$
Min. dR between leading forward jet and j_1	$—$	$\checkmark$	$\checkmark$
Total number of variables	36	41	37

* Order determined by p_T

** On loose b tagged jet working point.

† Variables come from the Resolved Hadronic Top Tagger algorithm described in App. F in Ref. [150]

Table 6.3: Hyperparameters of the Classifiers DNNs

Variable	$2\ell_{ss} + 0\tau_h$	$2\ell_{ss} + 1\tau_h$	$3\ell + 0\tau_h$
Number of hidden layers	32, 10×16 , 5×8 , 5	2×50 , 30, 4×20 , 4	111, 2×16 , 8, 4
Activation on hidden layers	ReLU	PReLU	PReLU
Activation on output layer	Softmax	Softmax	Softmax
Optimiser	Adam (lr = $1e-3$)	NAdam (lr = $1e-3$)	NAdam (lr = $1e-3$)
Batch size	500	500	500
Between hidden layers	batch normalization, 0.1 dropout	batch normalization, 0.1 dropout	batch normalization, 0.1 dropout

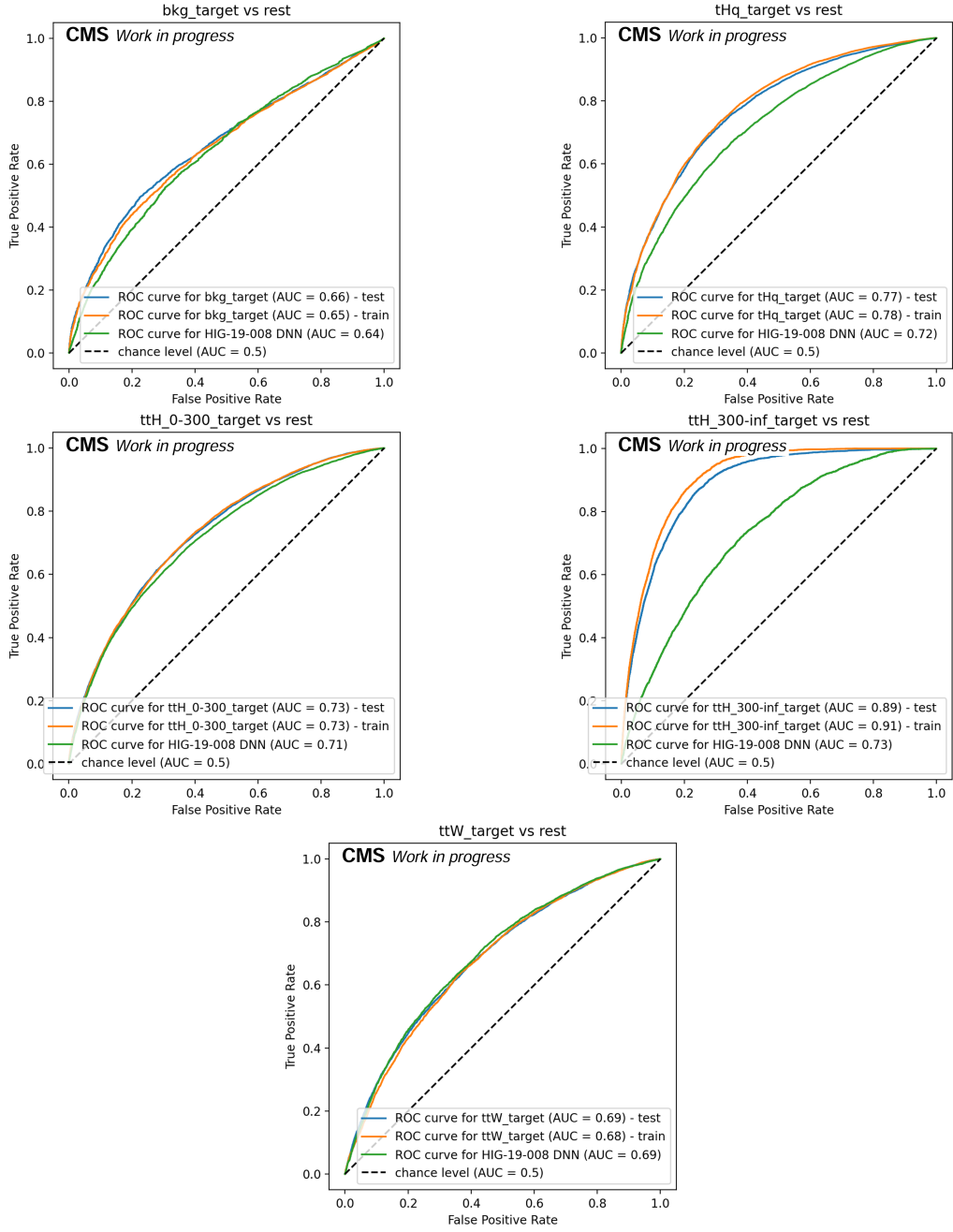


Figure 6.1: ROC curves for each of the classes in the SR $2\ell_{ss} + 0\tau_h$ with a comparison to the DNN used in [25].

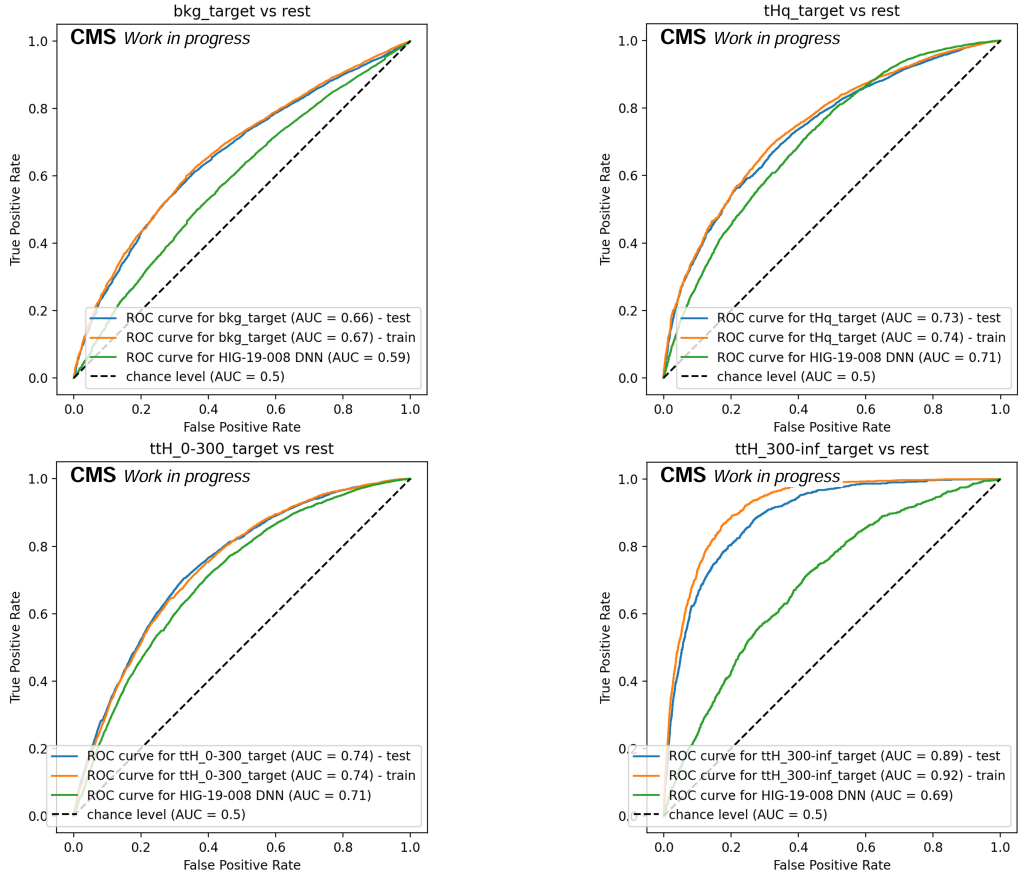


Figure 6.2: ROC curves for each of the classes in the $SR\ 2\ell ss + 1\tau_h$ with a comparison to the DNN used in [25].

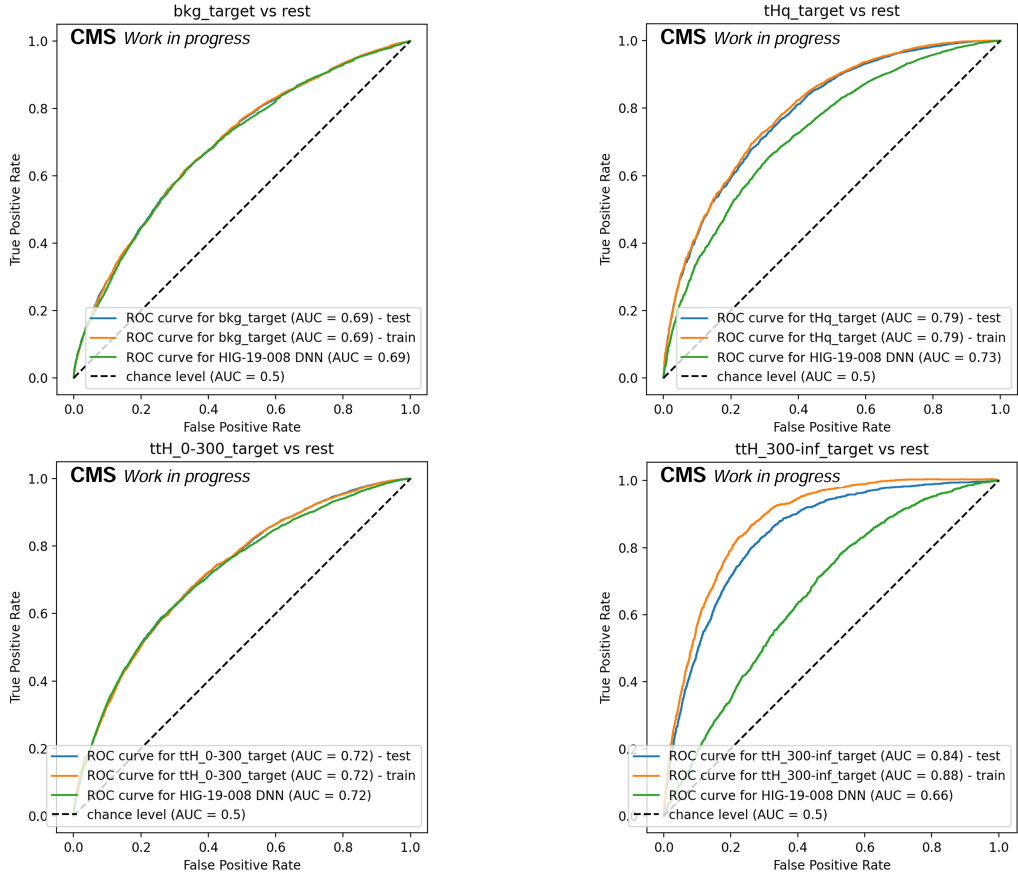


Figure 6.3: ROC curves for each of the classes in the SR $3\ell + 0\tau_h$ with a comparison to the DNN used in [25].

6.4 Background Control Regions

Similar as in Ref. [25] or the CP measurement in Chap. 5, this analysis uses a three and four lepton CR to constrain the WZ and ZZ backgrounds, which are floating during the final fit.

The selection of cuts applied to construct these two CR match the ones used in Sec. 5.6 to construct the corresponding CR. Consequently, a discussion of the construction of these CR will be omitted and only the plots corresponding to them are shown in Fig. 6.4. Even though the same set of cuts is used to construct them, they are still slightly different to the ones of the CP measurement as this analysis uses an updated set of data samples.

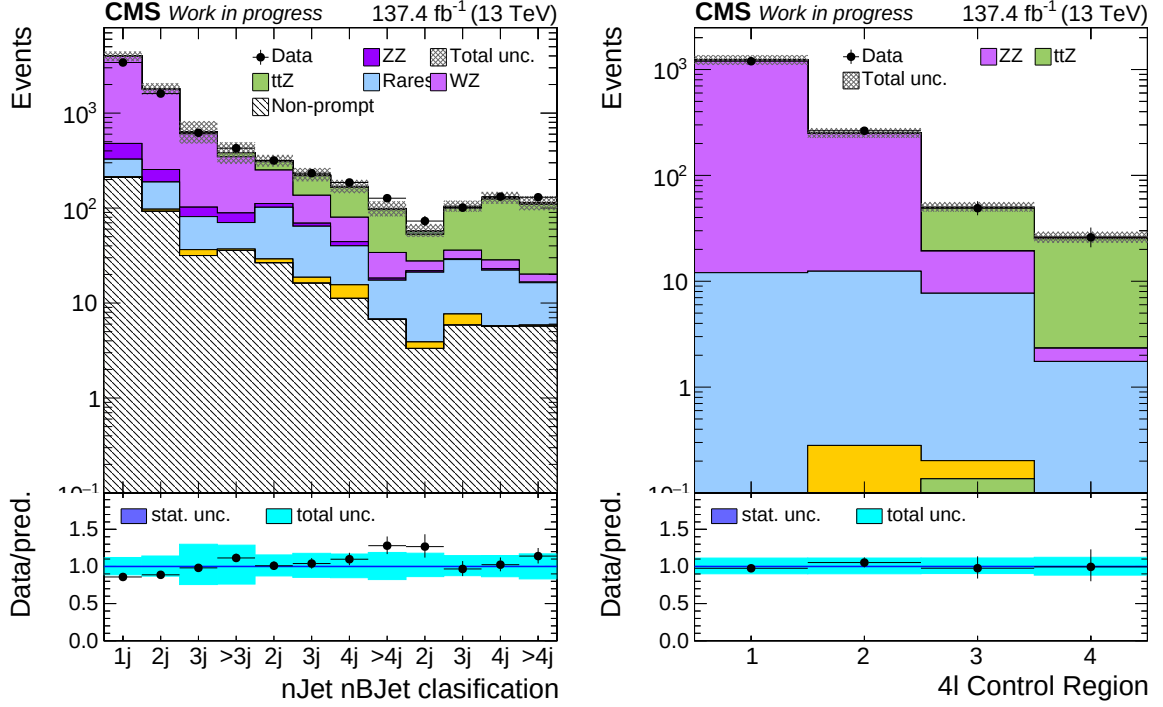


Figure 6.4: 3 lepton (left) and 4 lepton (right) CR distributions for all years combined.

The sensitivity to $t\bar{t}Z$ and ZZ background processes is driven by the 3ℓ CR, however, the 4ℓ CR provides a reasonably sensitive alternative measurement and is enriched in ZZ events.

Finally, in order to check the validity of the objects and background samples as well as our data driven background estimation, the same three Validation Regions (VR) as in the CP measurement are used, which are defined in Sec. 5.6.3. Fig. 6.5, 6.6 and 6.7 show the corresponding plots to check our objects and variables, focusing on the input parameters used for the DNN classifiers (Sec. 6.3.1) and the H p_T regression (Sec. 6.6.1).

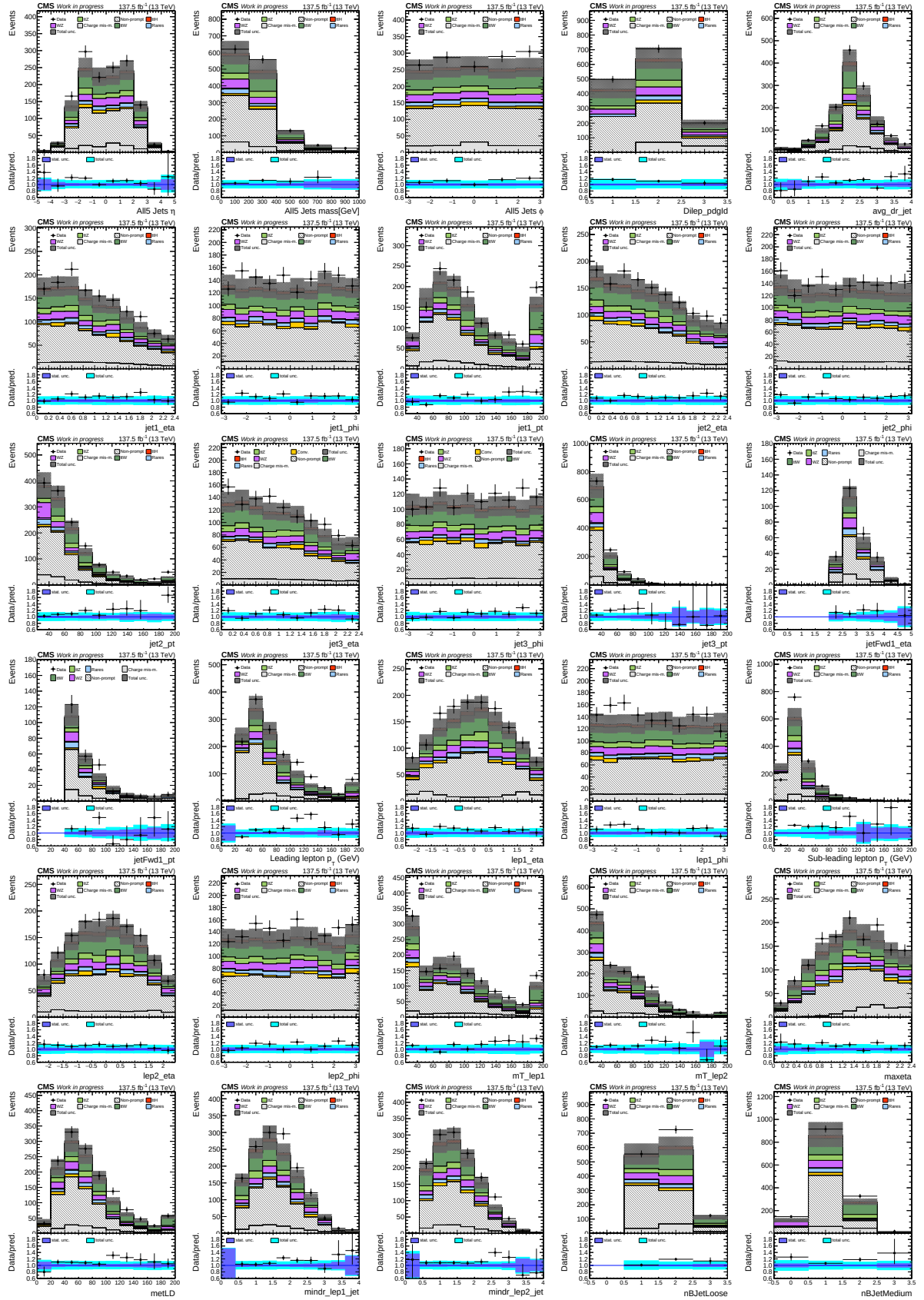


Figure 6.5: Validation region plots for the 3j validation region for all years combined.

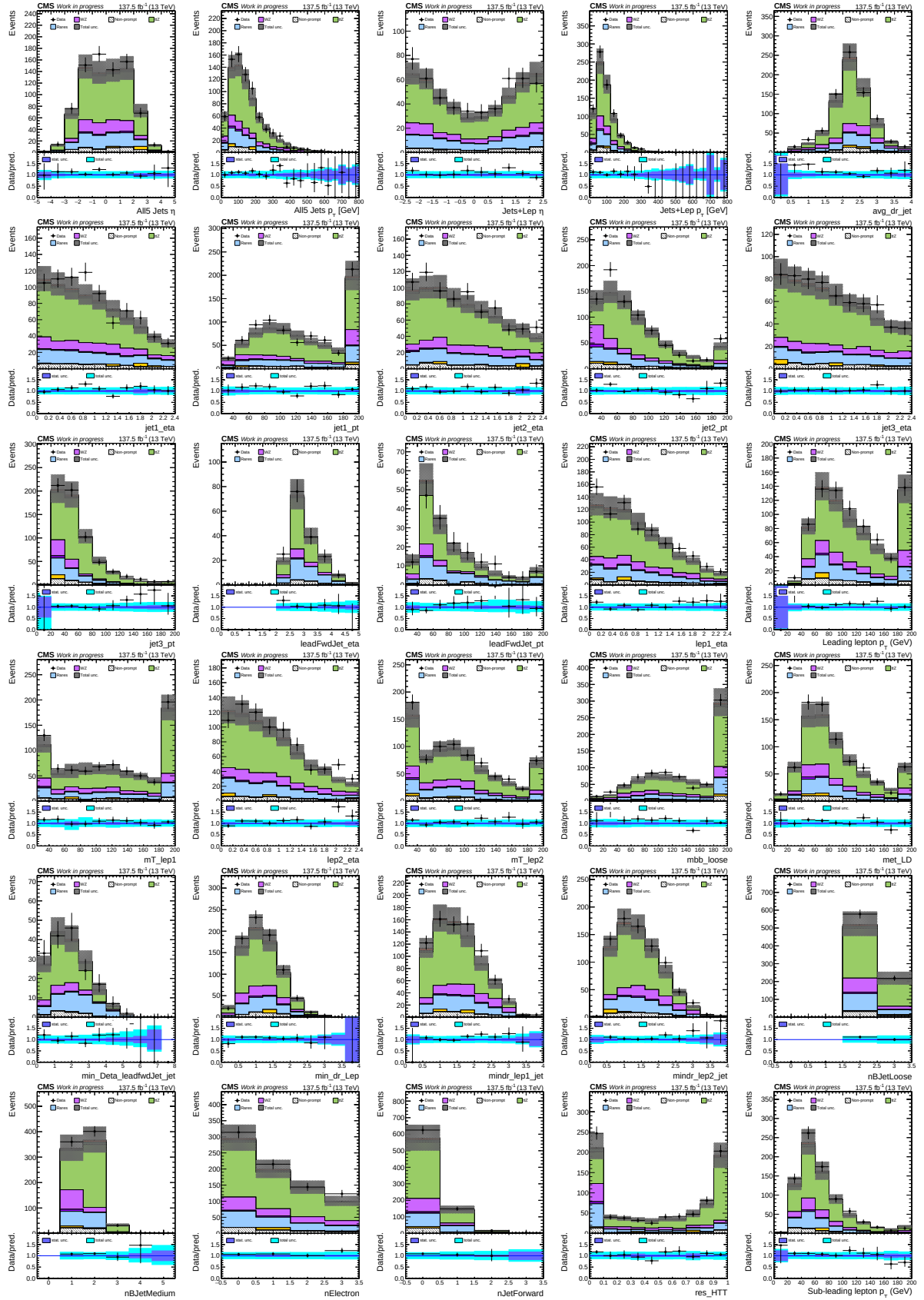


Figure 6.6: Validation region plots for the ttZ VR for all years combined.

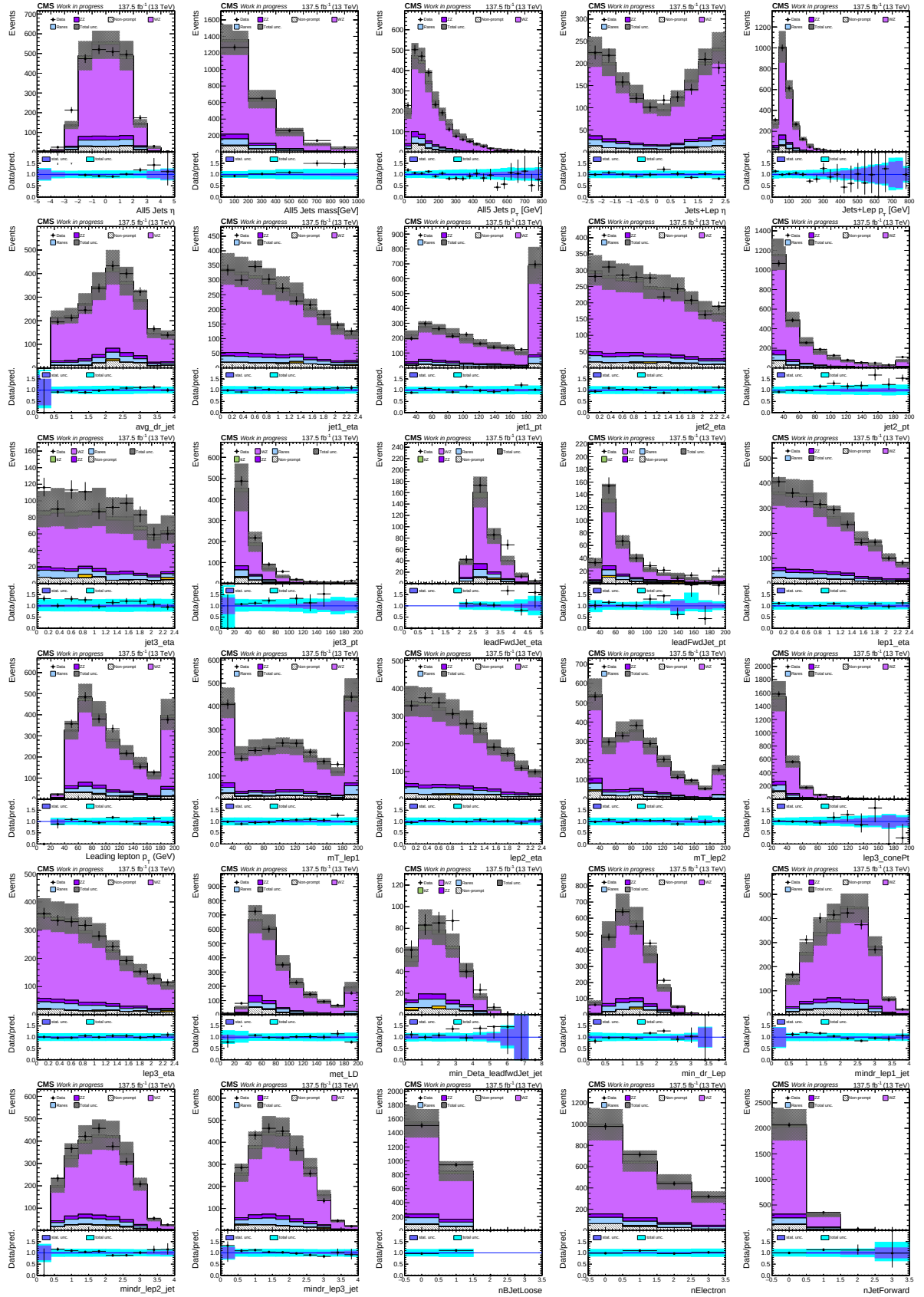


Figure 6.7: Validation region plots WZ for the VR for all years combined.

6.5 Systematic Uncertainties

The various experimental systematic uncertainties have already been discussed in Sec. 3.2.8 and will not be discussed in detail here. Overall, this analysis considers the following systematic uncertainties: trigger efficiency, e and μ identification and isolation, τ_h identification efficiency, e , μ and τ_h energy scale, JES and JER, b jet tagging scale factors, MET resolution and response, integrated luminosity, pileup, L1 ECAL trigger efficiency corrections, misidentified lepton rate and charge misconstruction rate, renormalization (μ_R) and refactorization scales (μ_F) and theoretical cross section. Below, the theoretical systematic uncertainties are discussed.

Signal Rate: The signal rates are measured in units of the SM $t\bar{t}H$ and tH production rates: the measurement is therefore affected by uncertainties in the $t\bar{t}H$ and tH cross sections. The uncertainties associated to these processes are the following:

- The uncertainty in the SM $t\bar{t}H$ cross section, computed at NLO accuracy, amounts to $^{+6.8\%}_{-10.0\%}$, of which $^{+5.8\%}_{-9.3\%}$ are due to missing higher orders and 3.6% arises from uncertainties in the PDF and α_s [30].
- The uncertainty in the SM tH cross section, computed at NLO accuracy, amounts to $^{+4.2\%}_{-6.8\%}$, of which $^{+4.1\%}_{-6.7\%}$ are due to missing higher orders and 1.0% arises from uncertainties in the PDF and α_s [30].
- The uncertainty in the branching fraction for the H boson to decay into WW ($\tau\tau$) amounts to 1.54% (1.65%).
- Uncertainties in the acceptance that are due to missing higher orders are treated as shape systematics, as they affect the shape of the distribution in the observable used for signal extraction. They are estimated by varying the renormalization (μ_R) and factorization (μ_F) scales between 0.5 and 2 times their default values, with the constraint that $0.5 \leq \mu_F/\mu_R < 2$.
- All the theoretical uncertainties associated to the signal rate are correlated across years.

Background Rates: The uncertainties associated to each of the relevant background contributions in this analysis are the listed below:

- The contribution of the WZ +jets background is known with an uncertainty of 30%, representing the uncertainty in the extrapolation to the SR from the WZ +jets-dominated CR. This CR is defined on the $3\ell + 0\tau_h$ category and is described in Sec. 5.6.1. The uncertainty includes: the statistical uncertainty in the data yields in the CR; the uncertainty in the b tagging efficiency and mistag rate; and the uncertainty in the relative composition of light quark and gluon, c quark, and b quark jets in WZ +jets events contributing to the CR and to the SR.
- A 30% normalization uncertainty is applied to the WZ +jets and ZZ +jets background processes which contain 3 or more jets to account for the mismodelling observed in the MC in these regions.
- The total normalization of WZ +jets and ZZ +jets backgrounds is floated in the fit and constrained by the dedicated CR defined in Sec. 5.6.

- The uncertainty in the background arising from production of top quark pairs in association with real or virtual photons amounts to 30%.
- An uncertainty of 50% is assigned to other rare backgrounds which are modeled using MC simulation.
- An additional uncertainty of 30% is assigned to the contribution of background events estimated using MC, which arise in the $2\ell ss + 1\tau_h$ category from events in which the reconstructed leptons are genuine prompt leptons and the reconstructed τ_h originates from the misidentification of a quark or gluon jet. This uncertainty is added because not all effects are well encapsulated by the current systematic uncertainties associated with the fake rate method.
- The uncertainty on the yield of the charge flip background in the $2\ell ss + 0\tau_h$ and $2\ell ss + 1\tau_h$ categories amounts to 30%.

6.6 Standard Model Analysis

We perform a Maximum Likelihood (ML) fit of the distributions of the selected observables in the SR defined for the $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$, and $3\ell + 0\tau_h$ categories as well as the CR on the 3ℓ and 4ℓ categories. Each SR channel is further separated into subcategories based on the different classes provided by the DNN classifier described in Sec. 6.3.1. For all three channels, within the $t\bar{t}H$ -like nodes, events are binned based on either their regressed $H p_T$ value or their reconstructed value of $m_{t\bar{t}H}$, which will be described in Sec. 6.6.1 and 6.6.2. In the $2\ell ss + 0\tau_h$ category, events are further classified depending on the flavour of the leptons ($ee/e\mu/\mu\mu$), except in the $t\bar{t}H$ node, where no flavour categorization is applied. In the $3\ell + 0\tau_h$ category, the tH and $t\bar{t}H$ nodes are separated according to the number of b-tagged jets. A detailed description of the binnings used for the $m_{t\bar{t}H}$ and $H p_T$ based measurements is presented in Sec. 6.6.3.

The $H p_T$ measurement will be interpreted in terms the Simplified Template Cross Section (STXS) framework which provides a global binning of $H p_T$, which permits the integration of top-Higgs coupling results into global fits for the properties of the H boson. Additionally, the $H p_T$ measurement will also be performed in terms of a custom binning, which is optimized for sensitivity. The $m_{t\bar{t}H}$ measurement will only be performed with a custom binning, also optimized for sensitivity, as there exists not STXS framework binning selection for $m_{t\bar{t}H}$.

6.6.1 DNN for Higgs p_T Regression

Each channel of the SR uses a separately trained DNN to regress the $H p_T$. For each of the trainings, 70% of the data was used for training (including validation) and the remaining 30% were used for testing.

Similar to the classifiers described in Sec. 6.3.1, the DNNs to regress the $H p_T$ use a combination of low and high level variables which are described in detail in Tab. 6.4.

As the performance of the DNNs was only weakly dependant of the choice of hyperparameters, the same architecture was chosen for all three channels and listed in Tab. 6.5.

Each DNN was trained for 100 epochs and used the custom loss function, which was developed to help the DNN to correctly model the $H p_T$ distribution and is shown in Eq. (6.1).

Table 6.4: Input variables for the H p_T regression DNN. A check mark ($\checkmark$) indicates the variable is used in a given channel, whereas a long dash ($—$) indicates the variable is not used in that channel.

Variable description	$2\ell ss + 0\tau_h$	$2\ell ss + 1\tau_h$	$3\ell + 0\tau_h$
Jet variables*			
$j_1(p_T, \eta, \phi)$	—	$\checkmark$	—
$j_2(p_T, \eta, \phi)$	—	$\checkmark$	—
Score of DeepJet Discriminator ($j_{1,2}$)	—	$\checkmark$	—
Number of jets in event ($j_{1,2}$)	—	$\checkmark$	—
Lepton variables*			
$l_1(p_T, \eta, \phi)$	$\checkmark$	$\checkmark$	$\checkmark$
$l_1(m_T)$	—	$\checkmark$	—
$l_2(p_T, \eta, \phi)$	$\checkmark$	$\checkmark$	$\checkmark$
$l_2(m_T)$	—	$\checkmark$	—
$l_3(p_T, \eta, \phi)$	—	—	$\checkmark$
$\tau_h(p_T, \eta, \phi)$	—	$\checkmark$	—
Low level variables			
MET	$\checkmark$	$\checkmark$	$\checkmark$
Φ_{MET}	$\checkmark$	—	$\checkmark$
High level variables			
$t_{\text{had}}(p_T, \eta, \phi)^\dagger$	$\checkmark$	—	$\checkmark$
$t_{\text{had}}(\text{BDT score})^\dagger$	$\checkmark$	—	$\checkmark$
Higgs jet tagger †	—	$\checkmark$	—
Jet is from from hadronic top flag † ($j_{1,2}$)	—	$\checkmark$	—
Variables of visible H (p_T, η)	—	$\checkmark$	—
Sum of variables of first five jets ($\sum_{n=1}^5 j_1(p_T, \eta, \phi)$)	$\checkmark$	—	$\checkmark$
Sum of variables of remaining jets ($\sum_{n>5} j_1(p_T, \eta, \phi)$)	$\checkmark$	—	$\checkmark$
Sum of all jet and fakeable lepton variables ($\sum_n j_n + \sum_n l_n(p_T, \eta, \phi)$)	$\checkmark$	—	$\checkmark$
Avg. dR distance among all jets	—	$\checkmark$	—
$m_{t\bar{t}H}$	—	$\checkmark$	—
Total number of variables	21	29	21

* Order determined by p_T

† Variables come from the Resolved Hadronic Top Tagger algorithm described in App. F in Ref. [150]

Table 6.5: Hyperparameters of the H p_T regression DNNs

Variable	$2\ell ss + 0\tau_h, 2\ell ss + 1\tau_h, 3\ell + 0\tau_h$
Nodes per layer	(512,256,128,64)
Activation on hidden layers	SELU
Before output layer	10% Dropout
Activation on output layer	Abs
Optimiser	Adam (lr = 1e-4)
Batch size	128

$$L = \frac{1}{N_{\text{batch}}} \sum [p_T^{\text{true}} - p_T^{\text{pred}}]^2 \times |\sigma_{\text{true}}^2 - \sigma_{\text{pred}}^2| \quad (6.1)$$

The loss function is based on the mean square loss but has an additional term to punish large differences of the variance between the true and the regressed value, which was needed as all

three DNNs tended to regress a wider H p_T distribution than the truth data. An exemplary comparison in the $3\ell + 0\tau_h$ channel of the H p_T regression trained with the mean squared error and the custom loss function is shown in Fig. 6.8.

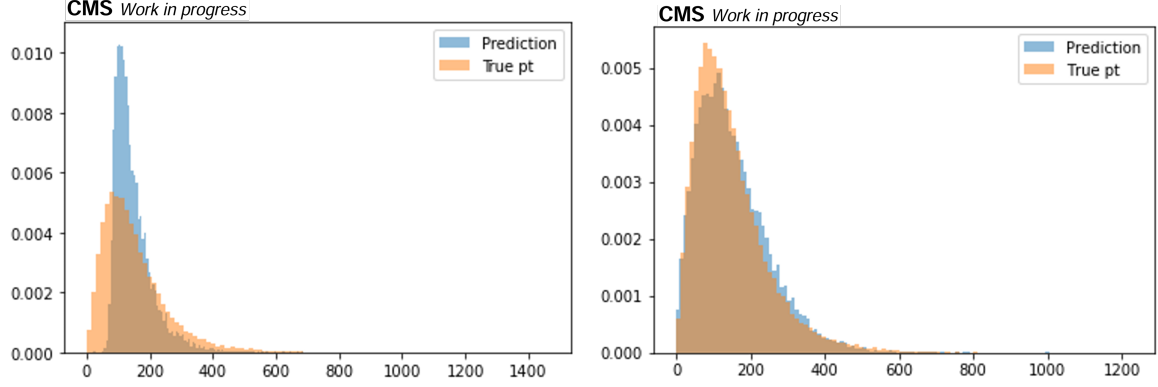


Figure 6.8: The H p_T distribution predicted by the DNN when using the mean squared error loss function, overlayed on the True H p_T distribution (left) and when using the custom loss function (right) in the $3\ell + 0\tau_h$ channel.

Fig. 6.9 shows the response matrix of the H p_T regression DNNs in all three SR channels.

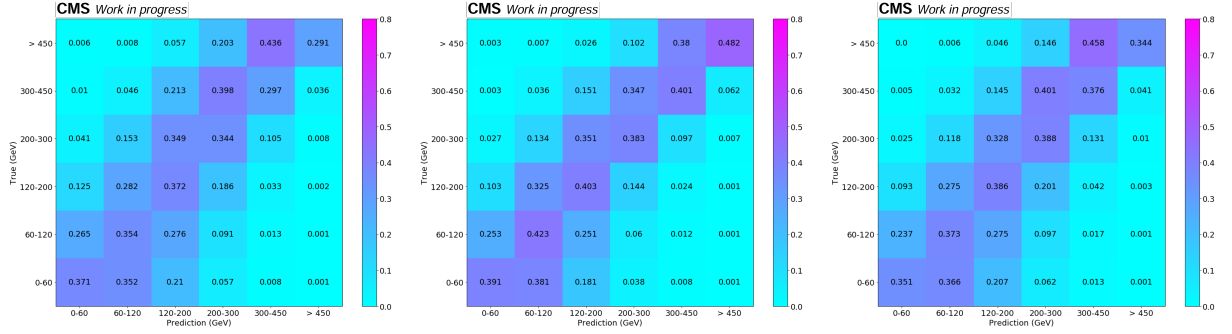


Figure 6.9: The response matrix H p_T DNN for the $2lss + 0\tau_h$ (left), $2lss + 1\tau_h$ (middle) and $3\ell + 0\tau_h$ (right) channels. The H p_T bins correspond to the STXS binning. Each row is normalized to unity, so that each cell (i, j) corresponds to the conditional probability that an event which originates in truth bin i will also be reconstructed in the reconstructed bin j .

6.6.2 $m_{t\bar{t}H}$ Reconstruction

A simple reconstruction algorithm was used to reconstruct $m_{t\bar{t}H}$. A DNN regression, similar to the $H p_T$ DNN regression was studied but as the performance was similar, the simple reconstruction algorithm was chosen.

The reconstruction builds the four-momenta of the $t\bar{t}H$ system by kinematically summing together the first two leptons when sorted from highest to lowest p_T , the first six jets when sorted from highest to lowest p_T and the MET.

6.6.3 Signal Region Binning Strategy

Events in each SR channel are separated based on the output of the different classes provided by the DNN classifier described in Sec. 6.3.1, where events get assigned their corresponding class based on the highest classifier score.

In the $2\ell ss + 0\tau_h$ channel, background events get further split by their lepton flavor combination (ee, em, mm). In the $3\ell + 0\tau_h$ channel, background events get split according to their number of medium tagged b-jets. Finally, in the $2\ell ss + 1\tau_h$ channel, no additional separation based lepton flavor or number of medium tagged b-jets is made due to low number of events.

Within each group of the background classes formed this way, n-tiles to spread the amount of non-class like events based on the classifier score are defined. As a result, the purity of class like events increases in subsequent bins of the same group.

Depending on if the measurement is performed in terms of the $H p_T$ or $m_{t\bar{t}H}$, the $t\bar{t}H$ -like classes are binned differently. In the $H p_T$ measurement, $t\bar{t}H$ -like events are binned in terms of the regressed $H p_T$ and are split based on the low $H p_T$ and high $H p_T$ classes. Events in the low $H p_T$ class use the binning $[0, 60, 120, 200, \infty]$, where the lowest three bins correspond to the first three bins of the STXS convention with the last three STXS bins merged to form the last bin. As the low $H p_T$ class mainly features low $H p_T$ events, the higher $H p_T$ bins are sparsely populated leading to the decision to merge these bins into one. The opposite goes for the high $H p_T$ class, there the low $H p_T$ bins are sparsely populated. Consequently, we use the binning $[0, 200, 300, 450, \infty]$, which is again based on the STXS convention, but this time the three lowest $H p_T$ bins are merged into one. In case of the $m_{t\bar{t}H}$ measurement, all $t\bar{t}H$ -like events are grouped together and binned in terms of the custom binning $[0, 750, 1000, \infty]$. Also similar to the background classes, for each group withing the $t\bar{t}H$ -like classes, n-tiles based on the amount of background events are formed for each iteration of the corresponding binning. As such, the amount of background per iteration of the binning within each group stays constant, while the amount of signal events increases for each iteration.

A comprehensive list of the number of bins for each channel is shown in Tab. 6.6 for the $H p_T$ measurement and in Tab. 6.7 for the $m_{t\bar{t}H}$ measurement. The corresponding plots can be seen in Fig. 6.10 and 6.11.

Table 6.6: Binning for the H p_T measurement for each channel.

class	$2\ell ss + 0\tau_h$	$2\ell ss + 1\tau_h$	$3\ell + 0\tau_h$
t $\bar{t}$ H _low	6×4	2×4	(< 2 bjet med., ≥ 2 bjet med.) 2×4
t $\bar{t}$ H _high	2×4	1×4	1×4
tH	(ee) 4 (em) 11 (mm) 7	4	(< 2 bjet med., ≥ 2 bjet med.) 2
bkg	(ee) 8 (em) 14 (mm) 11	5	(eee) 1 (eem: < 2 bjet med., ≥ 2 bjet med.) 2 (emm: < 2 bjet med., ≥ 2 bjet med.) 2 (mmm: < 2 bjet med., ≥ 2 bjet med.) 2
t $\bar{t}$ W	(ee) 6 (em) 19 (mm) 15	—	—
Total	127	21	21

Table 6.7: Binning for the $m_{t\bar{t}H}$ measurement for each channel.

class	$2\ell ss + 0\tau_h$	$2\ell ss + 1\tau_h$	$3\ell + 0\tau_h$
t $\bar{t}$ H	11×3	4×3	(< 2 bjet med.) 2×3 , (≥ 2 bjet med.) 2×3
tH	(ee) 4 (em) 11 (mm) 7	4	(< 2 bjet med., ≥ 2 bjet med.) 2
bkg	(ee) 8 (em) 14 (mm) 11	5	(eee) 1 (eem: < 2 bjet med., ≥ 2 bjet med.) 2 (emm: < 2 bjet med., ≥ 2 bjet med.) 2 (mmm: < 2 bjet med., ≥ 2 bjet med.) 2
t $\bar{t}$ W	(ee) 6 (em) 19 (mm) 15	—	—
Total	128	21	21

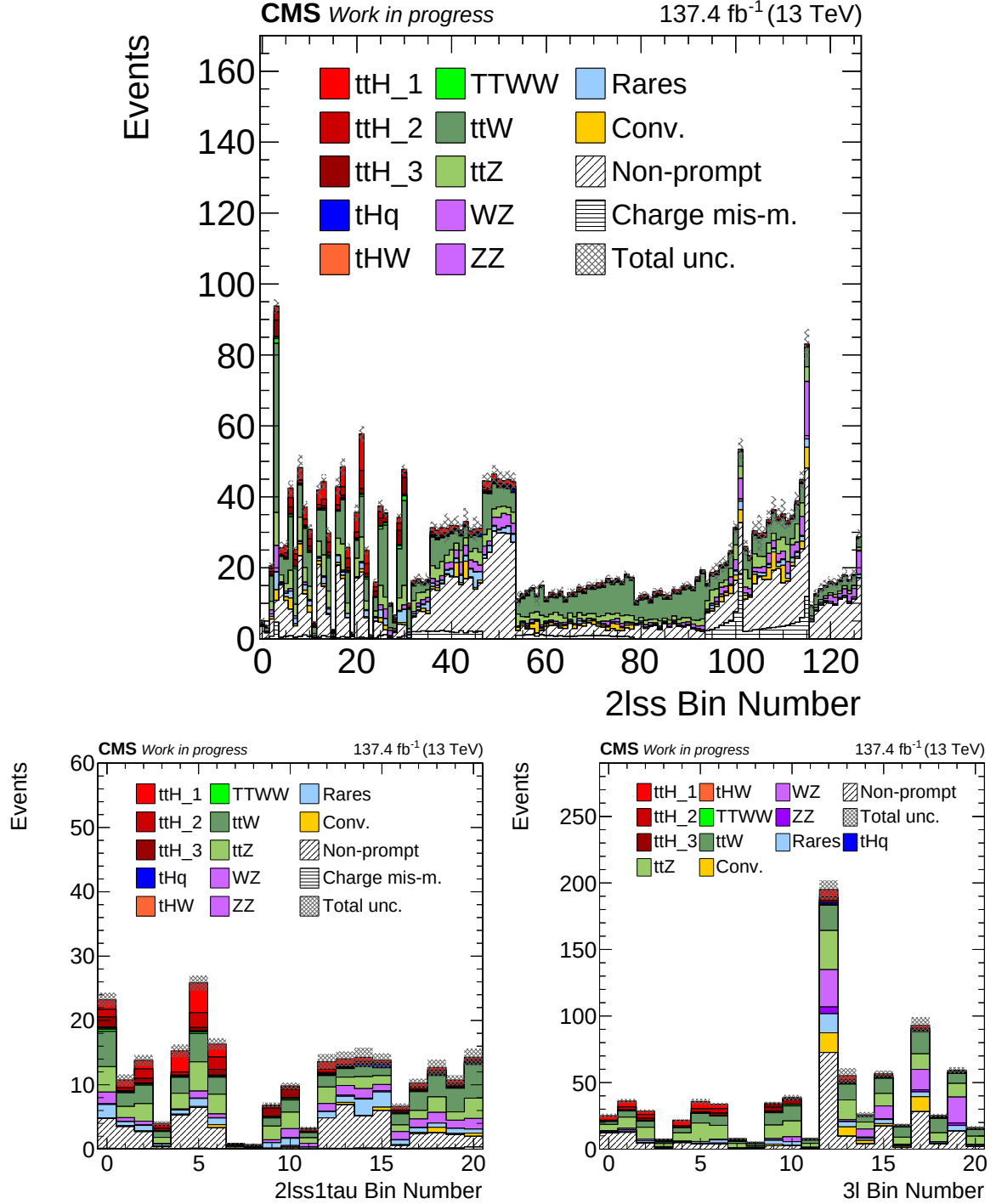


Figure 6.10: Binning used for each SR. ttH_1 to ttH_3 correspond to the bins of the Higgs p_T custom binning [0, 120, 200, ∞].

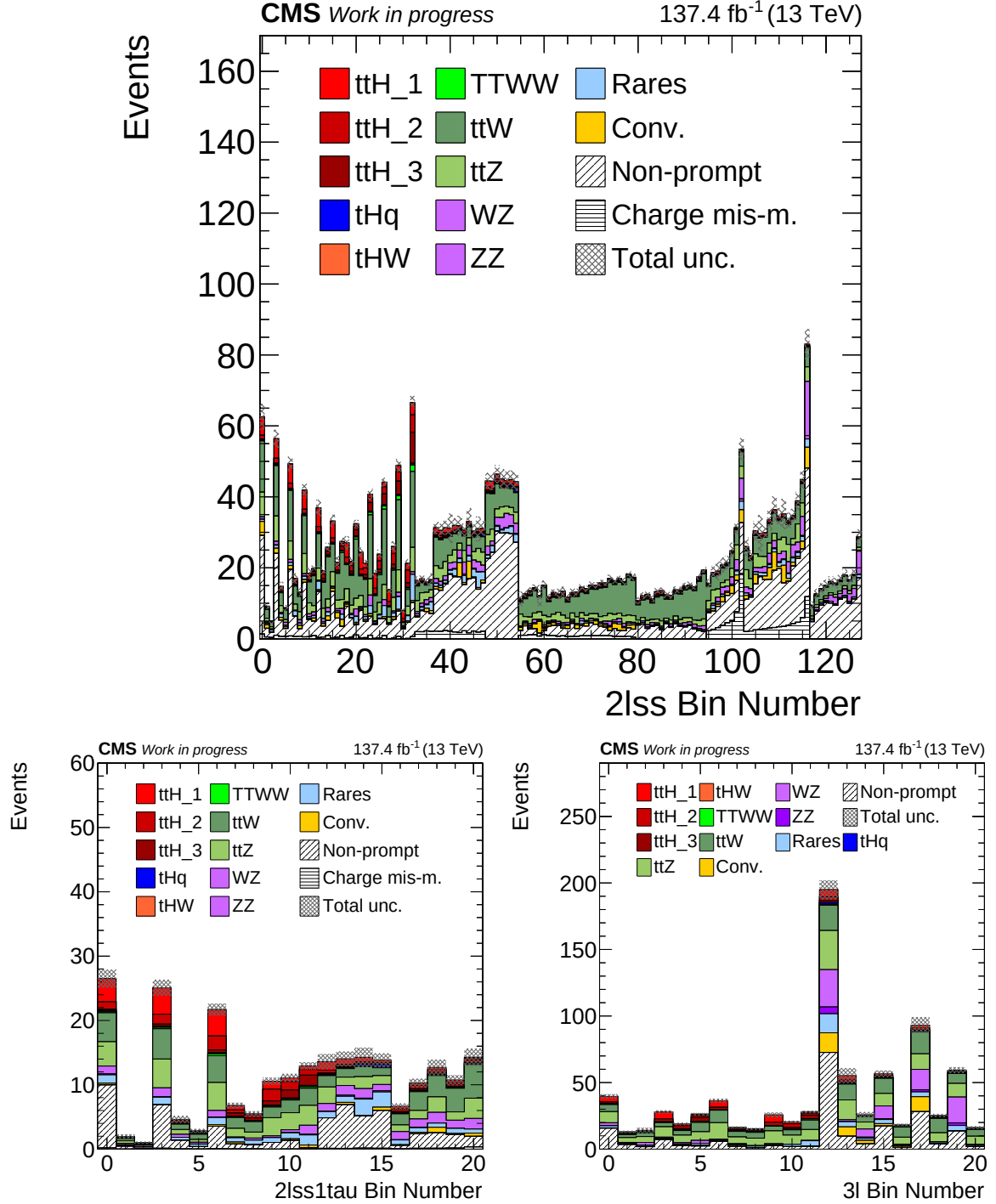


Figure 6.11: Binning used for each SR. ttH_1 to ttH_3 correspond to the bins of the mttH binning in mttH [0, 750, 1000, ∞].

6.6.4 Signal Extraction

A ML fit to the distributions of either the H p_T or the $m_{t\bar{t}H}$ based distributions is performed using the SR defined in $2\ell ss + 0\tau_h$, $2\ell ss + 1\tau_h$, $3\ell + 0\tau_h$ as well as the 3l and 4l CR.

For the H p_T based measurement, the STXS binning convention $[0, 60, 120, 200, 300, 450, \infty]$ and a custom binning $[0, 120, 200, \infty]$ derived by merging several of the STXS bins are used. The $m_{t\bar{t}H}$ based measurement is performed in terms of a custom binning $[0, 750, 1000, \infty]$ which was chosen for optimal sensitivity.

The expected sensitivity of the H p_T based measurement in terms of the STXS binning are listed in Tab. 6.8.

Table 6.8: SM measurement expected sensitivity in terms of the H p_T STXS binning computed on the Asimov dataset.

H p_T bin	Signal strength relative to SM	Uncertainty (68%)
$[0, 60)$	1.000	$-2.189 / + 2.202$
$[60, 120)$	1.000	$-1.620 / + 1.623$
$[120, 200)$	1.000	$-1.334 / + 1.348$
$[200, 300)$	1.000	$-1.852 / + 1.898$
$[300, 450)$	1.000	$-2.811 / + 2.829$
$[450, \infty)$	1.000	$-3.554 / + 3.980$

The expected sensitivity of the H p_T based measurement in terms of the custom binning are listed in Tab. 6.9.

Table 6.9: SM measurement expected sensitivity in terms of the H p_T custom binning computed on the Asimov dataset.

H p_T bin	Signal strength relative to SM	Uncertainty (68%)
$[0, 120)$	1.000	$-0.599 / + 0.606$
$[120, 200)$	1.000	$-1.095 / + 1.107$
$[200, \infty)$	1.000	$-0.782 / + 0.805$

The expected sensitivity of the $m_{t\bar{t}H}$ based measurement are listed in Tab. 6.10.

Table 6.10: SM measurement expected sensitivity in terms of the $m_{t\bar{t}H}$ binning computed on the Asimov dataset.

$m_{t\bar{t}H}$ bin	Signal strength relative to SM	Uncertainty (68%)
$[0, 750)$	1.000	$-0.473 / + 0.475$
$[750, 1000)$	1.000	$-0.912 / + 0.939$
$[1000, \infty)$	1.000	$-0.845 / + 0.861$

6.7 Constraints on Trilinear Higgs Coupling κ_3

To look for deviations of the κ_3 parameter in $t\bar{t}H$ production, the SM assumption is dropped. This study follows the phenomenological studies proposed in Ref. [177], that proposes ways to

probe this coupling by measuring single Higgs production. They compute the contributions from loop diagrams involving this coupling and derive a way to compute any observable (cross section, yields) as

$$\sigma(\kappa_3) = Z_H \Sigma_{LO} (1 + \kappa_3 C_1 + \delta Z_H + \delta_{EWK}), \quad (6.2)$$

where Σ_{LO} is the prediction including corrections that factorize with the EWK contributions. In our case, this would correspond to NLO in QCD. Z_H is a term corresponding to a renormalization of the external H leg, which is universal for all single H production processes and is independent of the kinematics. Its value can be computed as a function of κ_3 as

$$Z_H = \frac{1}{1 - (\kappa_3^2 - 1)\delta Z_H}. \quad (6.3)$$

δZ_H is computed by the authors of Ref. [177] to be equal to -1.536×10^{-3} . Finally, C_1 is a term that depends on the process considered and on the event kinematics. Out of the processes considered in Ref. [177], it is the highest for $t\bar{t}H$ production.

The Madgraph NLO signal samples described in Sec. 6.2 are reweighted, using the Madgraph model provided by the authors of Ref. [177], as a function of the $t\bar{t}H$ kinematics. Since the code to reweight the samples is developed for LO samples, we perform the reweighting as a function of the kinematics of the top quarks and H boson produced in the rest frame of the $t\bar{t}H$ system, in order to avoid the effect from outgoing partons other than the $t\bar{t}H$ system.

In order to extract limits in κ_3 , we use the same classification of events as described in Sec. 6.6.3. The analysis sensitivity has been computed for both the $m_{t\bar{t}H}$ and H p_T based binning. As the H p_T based binning outperforms the $m_{t\bar{t}H}$ based binning, only the H p_T based results are shown.

Limits are obtained by implementing Eq. (6.2) in a ML fit, accounting for both the quadratic dependence of the signal normalization, given by Z_H , and the effect on the signal kinematics, given by C_1 .

The SM expectation is computed for each of the fitted distributions using the nominal simulation. The correction term C_1 is computed per bin by weighting each event with the relevant weight obtained via Madgraph. In this fit, we leave the rest of the H boson couplings fixed to their SM expectation.

The distribution of the $t\bar{t}H$ SM production in the bins considered in this analysis is shown in Fig. 6.12, along with the c_1 contribution. The bottom panel shows the ratio between the two, showing a large expected impact of the c_1 contribution on the process kinematics.

The expected sensitivity to κ_3 is shown in Fig. 6.13, which depicts the likelihood as a function of this parameter. We get better sensitivity to negative values of κ_3 due to the fact that the changes induced in the total yield by c_1 and Z_H go in the same direction for negative κ_3 values, while they tend to cancel out for positive κ_3 .

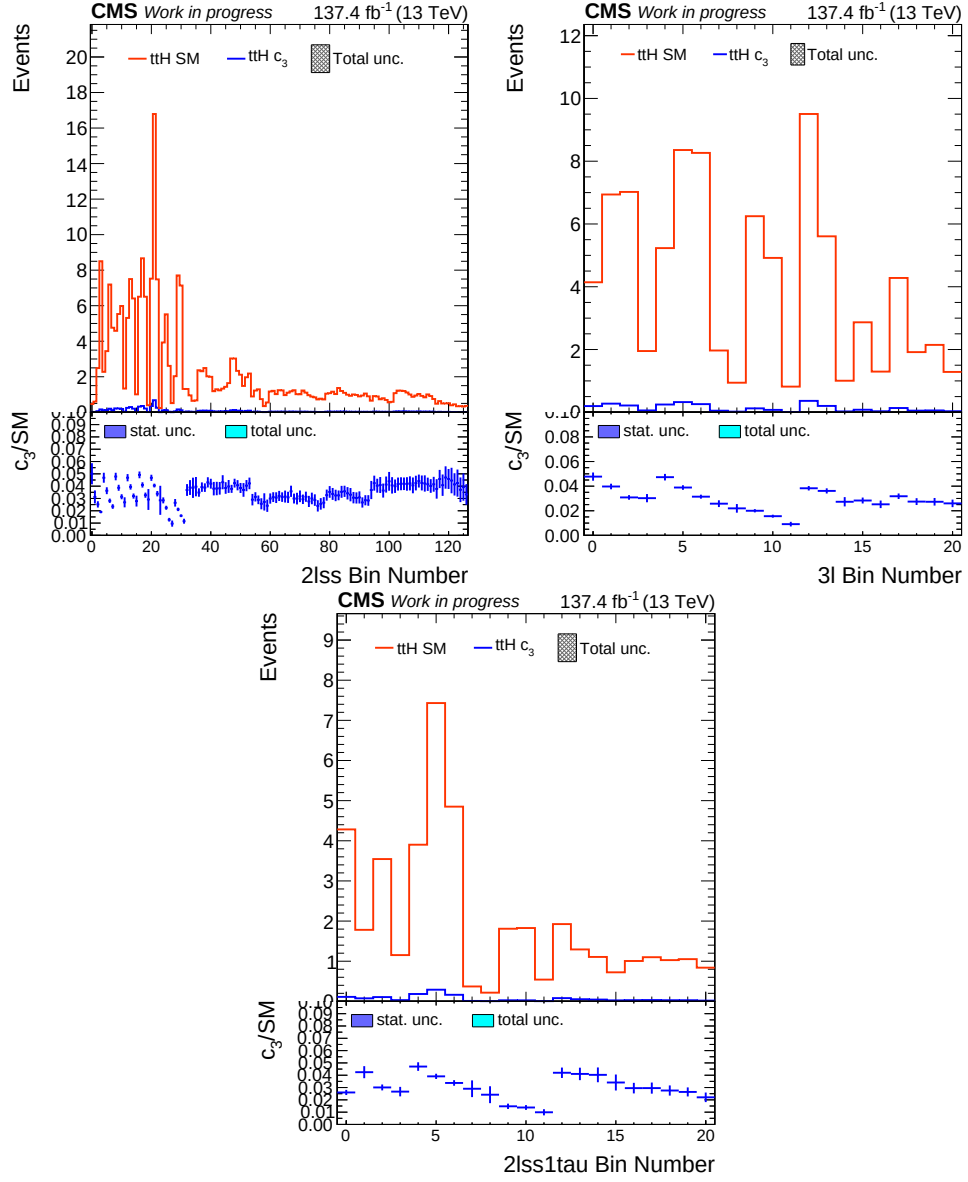


Figure 6.12: Distribution of the $t\bar{t}H$ signal in SM events in the variables used for the signal extraction, along with the c_3 contribution.

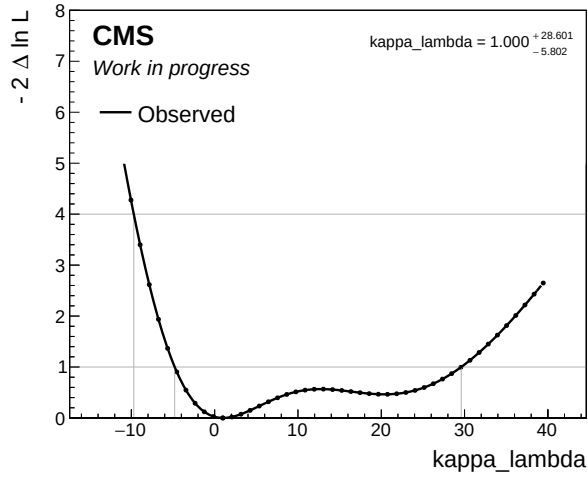


Figure 6.13: Likelihood as a function of κ_3 for the analysis computed on the Asimov dataset.

6.8 Summary

The first differential measurement of the production of H bosons in association with either one (tH) or two (ttH) top quarks is measured in final states with electrons, muons and taus, using proton-proton collision data recorded at $\sqrt{s} = 13$ TeV center-of-mass energy during the period 2016 to 2018, corresponding to an integrated luminosity of 137 fb^{-1} . The sensitivity of the analysis is improved by using machine learning methods to separate the signal from backgrounds. The H boson transverse momentum and the mass of the ttH system are reconstructed, and differential cross sections for ttH production are calculated at particle level, assuming a lack of new physics effects. We are able to measure the cross section in three independent categories with an expected uncertainty between $[-1.10, 1.11]$ of the SM expectation at 68% CL on the Asimov dataset. Also, a measurement of the H trilinear coupling (κ_3) is performed. The H trilinear coupling is expected to be constrained within $[-5.90, 28.60]$ at 68% CL from the Asimov dataset.

The analysis is in the internal review process of the CMS experiment. As a result, everything presented in this chapter is to be understood as work in progress and all the results only show the expected sensitivity based on the Asimov dataset as the analysis is still blind at the moment.

7 CMS Inner Tracker Endcap Pixel Upgrade

The work presented in this section includes the material published in Ref. [178] and the studies that followed from that publication. All the work presented in this section was done in collaboration with the teams involved in the upgrade of the CMS Inner Tracker Endcap Pixel (TEPX) detector at UZH and PSI.

My contribution to this project can be summarized in the following three main points:

Thermal Design Validation: I validated the TEPX thermal design by employing Finite Element Analysis (FEA) methodologies. This involved rigorous testing and evaluation of both the final design and its interim stages, ensuring robust thermal performance under operational stresses.

Design Optimization: The insight provided by my FEA studies helped optimizing the overall design and material choices to ensure optimal thermal efficiency and structural integrity of the TEPX detector.

Prototype Testing: I configured the prototype testing apparatus and conducted extensive tests to validate the detector's design and function prior to full-scale production.

Additionally, I had the chance to present these studies at the ICHEP conference in Bologna, Italy in 2022 and publish them in the subsequent proceedings [178].

7.1 Introduction

During the Long Shutdown 3 (LS3), the LHC will be significantly upgraded and is expected to collide protons at an increased centre-of-mass energy of 14 TeV (before 13.6 TeV) and reach the unprecedented peak instantaneous luminosity of $7.5 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$. Due to the increased instantaneous luminosity, more simultaneous pp collisions are happening during a single bunch crossing, which results in an average number of Pile-Up (PU) vertices of up to 200. This upgrade is widely known as the High-Luminosity LHC (HL-LHC) and will allow the ATLAS and CMS experiments to collect a data sample with an integrated luminosity of the order of 300 fb^{-1} per year (assuming a run-time of 10 years, this results in up to 3000 fb^{-1} in total).

To adapt to these harsh conditions, which are discussed in more detail in Sec. 7.2, the CMS detector will be substantially upgraded before the start of the HL-LHC, a plan known as the CMS Phase-2 upgrade [179–182]. The entire CMS Inner Tracker (IT) will be replaced and the new detector will feature increased radiation hardness, higher granularity and capability to handle higher data rate and longer trigger latency.

7.2 High Luminosity Upgrade

The HL-LHC upgrade significantly improves our ability to measure rare and statistically limited Standard Model (SM) and Beyond SM (BSM) processes [179, 183–185].

A good example to showcase the motivation for the HL-LHC upgrade is the study of the SM H boson Yukawa couplings. The HL-LHC enables us to test the properties of the H boson, like the CP structure of its Yukawa coupling to fermions with significantly improved sensitivity [179, 183, 184]. As a result, we expect to be able to set significantly more stringent limits on H boson measurement like the one presented in Chap. 5, where we measure the H top Yukawa CP structure. However, it also allows us to measure the H Yukawa couplings to many particles that were not explorable before [183]. Measurements that probe the H boson self-coupling, like the trilinear H boson coupling measurement in Sec. 6.7, are also expected to be significantly more constrained. Additionally, proposed measurements like $HH \rightarrow b\bar{b}b\bar{b}$ [183] allow for improved measurements.

Simultaneously, new channels open up allowing for completely new measurements. An example is the proposed measurement of J/Ψ reconstruction in top quark events [185]. It targets final states containing $J/\Psi \rightarrow \mu\bar{\mu}$ from b quark fragmentation. This allows for a much more precise measurement of the top quark mass, as it only relies on charged particles which can be measured with much higher precision than jets, which current measurements of the top quark mass rely on.

Indirect searches of new physics, like the analysis presented in Chap. 4, also profit immensely from the increased integrated luminosity. However, also direct BSM searches profit, as they gain access to new channels and are able to reach higher masses of potential new particles.

7.2.1 Requirements of the CMS detector

The HL-LHC poses a harsh environment for any detector due to its high radiation levels and the large amounts of data to be recorded and evaluated. The CMS experiment is expected to collect up to 300 fb^{-1} each year, providing a significant increase in recorded collisions, especially when compared to the full Run 2 where the CMS experiment recorded around 150 fb^{-1} of data. To be

able to function properly in the harsh conditions the HL-LHC provides, the CMS detector needs to fulfil several requirements with some highlights listed below. Although the HL-LHC promises significant improvements, there are still many problems to overcome to achieve the conditions needed to make the measurements.

Radiation Hardness: The higher luminosity significantly increases the radiation levels in the CMS detector which in turn results in more radiation damage on the detector components. Radiation damage occurs primarily through ionization, where the radiation damages the crystal structure of the sensor components, which degrades the sensors efficiency and accuracy. Over time, this leads to increased noise, reduced sensitivity, and changes in electrical properties. The radiation level is mainly dependent on the radius r from the beampipe and only weakly dependant on z . As a result, the whole IT needs to be especially radiation hard to ensure it stays functional up to a target integrated luminosity of 3000 fb^{-1} while needing as little maintenance as possible.

Level-1 Trigger: Selecting interesting physics events at the stage of the level-1 trigger becomes extremely challenging at the HL-LHC. Besides the increased rate of collisions, selection algorithms become increasingly inefficient at high PU. As a result, the CMS trigger will operate with increased latency and output rates and will use tracking information in the L1 event selection, which was exclusive to the high-level trigger before.

Increased Granularity: To ensure an effective tracking despite the high level of PU, the occupancy of the channels in the IT (and OT) needs to stay below the per mille level (below 1%). Consequently, a high number of channels is needed where PU levels of 140 and 200 serve as target values to benchmark the performance of the tracking.

Improved Two-Track Separation: The current tracker struggles to find the track of highly energetic jets due to hit merging issues within the pixel detector. To be able to optimally utilize the large amounts of data taken during the HL-LHC, the two track separation needs to be improved.

Reduced Material in Tracking Volume: As the tracking performance is affected by the amount of material in the detector, the new tracker will need to be lighter. This helps to greatly enhance the tracking capabilities of the new tracker and improves the performance of the calorimeters. This will result in an overall improved event reconstruction.

Robust Pattern Recognition: With increasing levels of PU, track finding becomes significantly more difficult and time consuming. This means that at the level of the HLT, the upgraded tracker needs to provide fast and efficient track finding.

Extended Tracking Acceptance: The new CMS detector will feature extended acceptance of the tracker and calorimeters in the forward region [183] providing efficient tracking up to $|\eta| = 4$. The improved acceptance improves the overall CMS physics capabilities.

7.2.2 Planned Inner Tracker

Like in the current design of the CMS detector, the tracker is divided into an Inner Tracker (IT) and Outer Tracker (OT). Fig. 7.1 shows the dimensions of the tracker and its individual components.

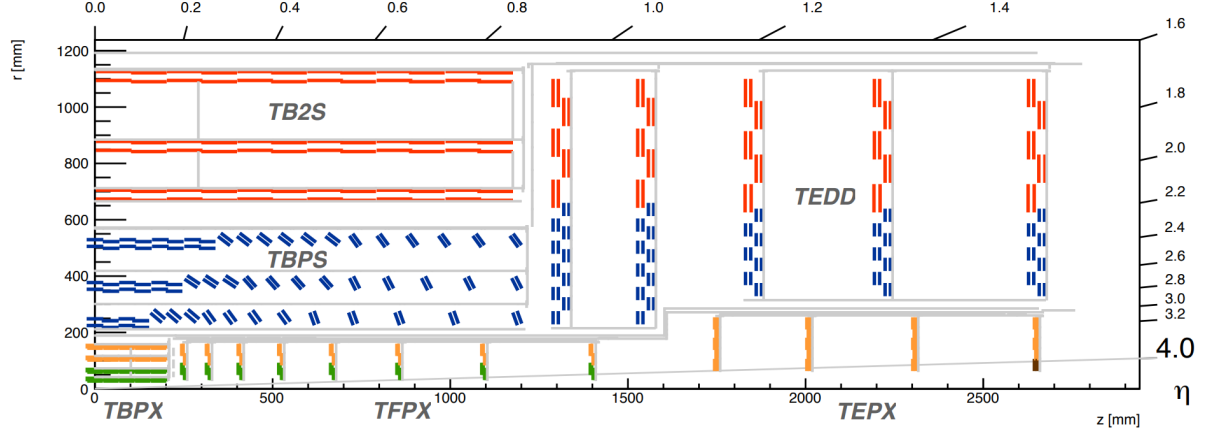


Figure 7.1: Tracker layout and dimensions (taken from [186]).

The inner Tracker Barrel Pixel detector (TBPX) is the part of the pixel detector closest to the interaction point and is arranged in concentric cylindrical layers. Next to it is the inner Tracker Forward Pixel detector (TFPX). At the endcap section of the inner tracker is the TEPX detector, which extends the coverage of the IT up to $\eta \leq 4$ (compared $\eta \leq 2.5$ at the current CMS detector). Both the TFPX and the TEPX consist of several semicircular disks, called dees, on which the modules are arranged in concentric rings. The contribution of the UZH and PSI groups to the IT upgrade for the HL-LHC involves the upgrade and design of the TEPX section of the IT. As a result, in this chapter, the TEPX detector will be discussed in depth, with a special focus on the thermal design.

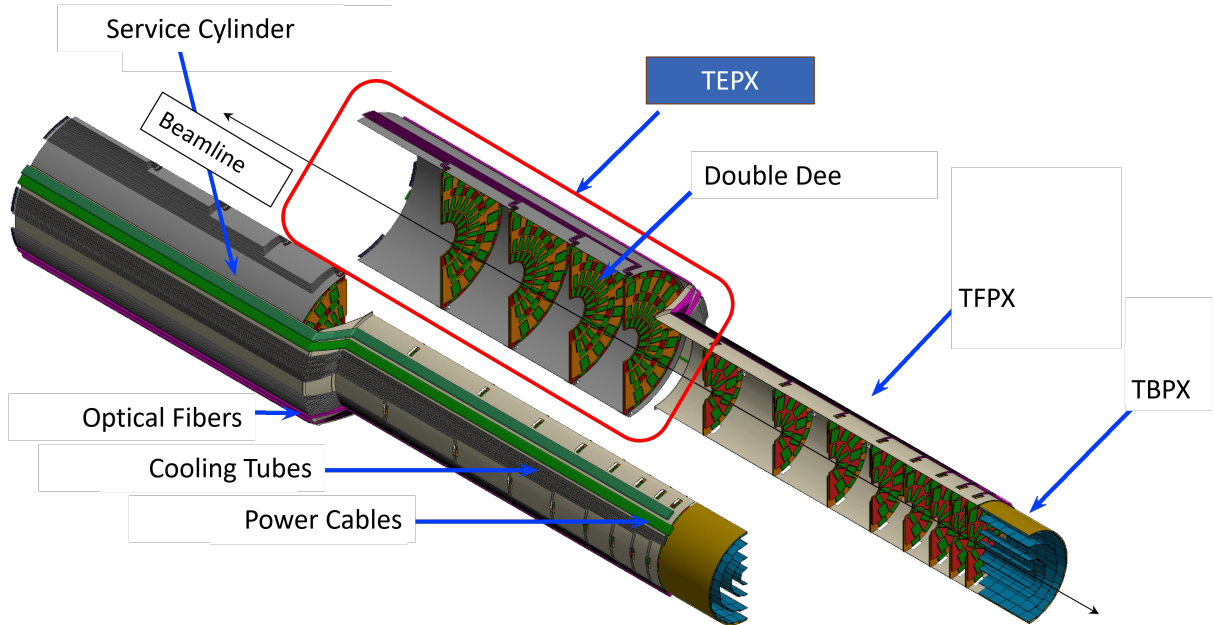


Figure 7.2: IT layout of the CMS experiment for the HL-LHC.

7.3 Tracker Endcap Pixel Detector

7.3.1 Supply Tubes

The TEPX detector consists of four separate structures at each end of the detector (see Fig. 7.3), each containing two double dees, for a total of 16 double dees in the whole detector. The

structures on which the dees are mounted on will be referred to as “supply tubes” from now on. Besides providing structural support and stability for the TEPX detector, the supply tubes also house the readout electronics (divided into 12 portcards which handle power and data transmission), the CO₂ cooling input and output lines, and the electrical cables carrying data and power. Fig. 7.3 shows a prototype of a supply tube. The portcards are cooled by the CO₂ cooling lines in the supply tube, which features a base out of 3D printed carbon shells.

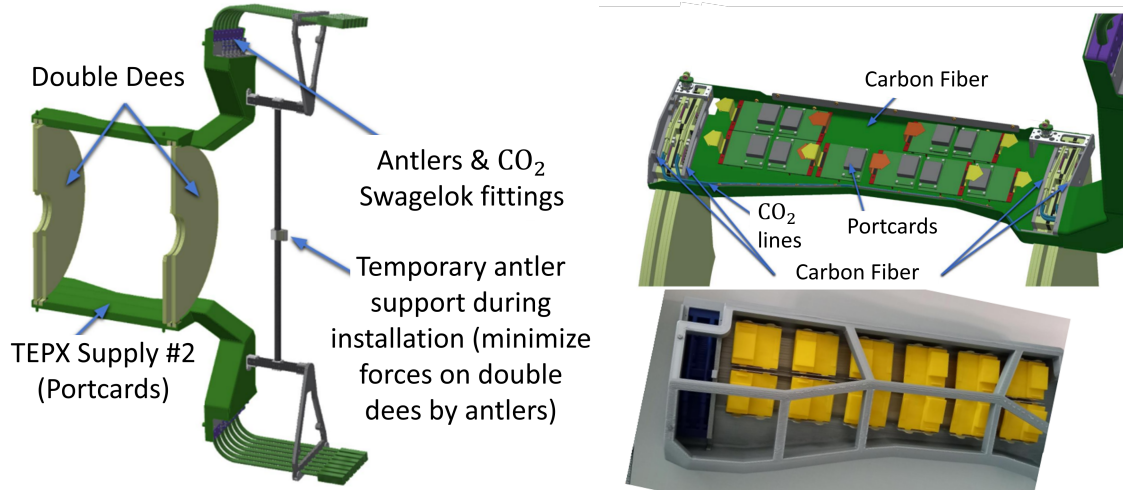


Figure 7.3: The left diagram shows the TEPX supply tubes on which the TEPX double dees are mounted on. The right one shows a comparison between a drawing of the service channel on the top and a dummy prototype to check the spacing of the components on the bottom.

7.3.2 Dee Design

The geometry and the design of the dees is chosen such that the dee consists of as little material as possible to help reduce the material in the IT and keep the radiation length large while also providing sufficient cooling.

Each dee is populated with 44 modules, arranged in five concentric rings with the arrangement shown in Fig. 7.4. When in use, each module generates approximately 11.4 W of heat resulting in a total thermal load of approximately 500 W.

Fig. 7.5 shows the transversal plane of the dee, where we can see the different parts of the dee and their characteristics, such as their thermal conductivity λ , their thickness d and the surface convection coefficient H between the cooling tubes and the mixed phase CO₂, which is circulated at -35°C .

Thin cooling tubes run through the middle of the dee, one for each half of the dee. These tubes, shown both in both Fig. 7.4 and 7.5, are made of stainless steel (SS) and feature a flower-like shape to cover the dee surface and ensure proper cooling of the modules populating the dee. We also tested, how using Titanium (Ti) instead of SS tubes affects the cooling properties of the dee. Compared to SS tubes Ti tubes have twice the radiation length and half the thermal conductivity. Ti featuring double the radiation length of SS makes it an attractive candidate as one of the main requirements of the new IT is to reduce the material budget.

Even though Ti has only half of the thermal conductivity of SS, we don’t expect the reduced thermal conductivity of Ti to significantly impact the cooling capabilities of the dee. The cooling performance is expected to be limited by other factors like the thermal conductivity of the glue or through plane conductivity of the carbon fiber. Mechanically however, Ti is a more difficult

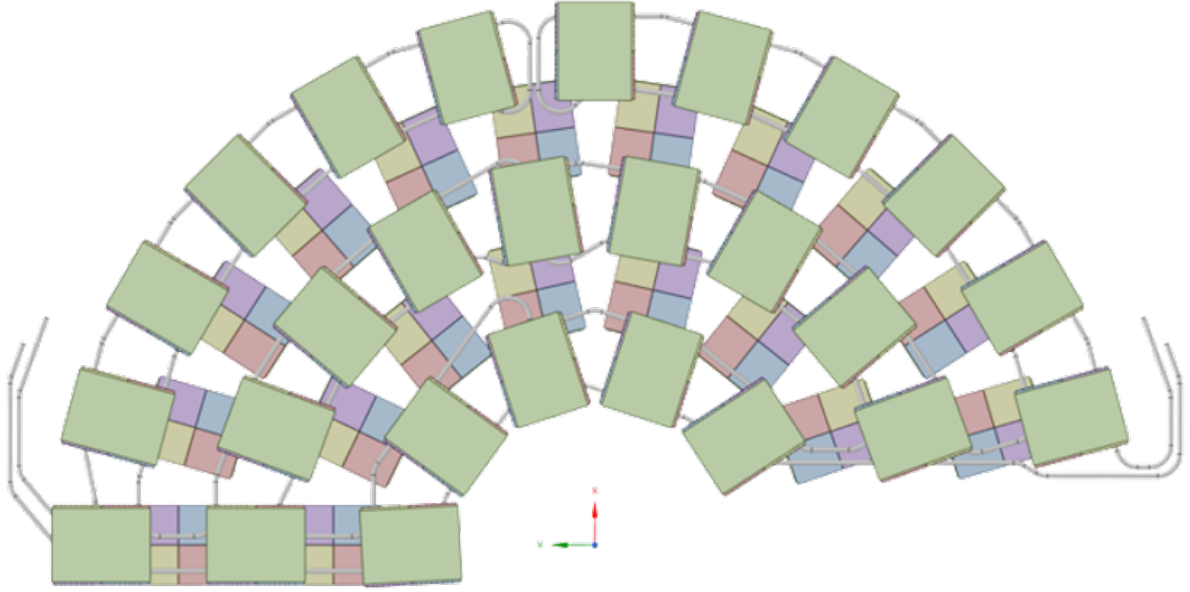


Figure 7.4: The arrangement of the modules on each dee of the TEPX tracker and in relation to the cooling pipes running through the dee showing the five concentric rings.

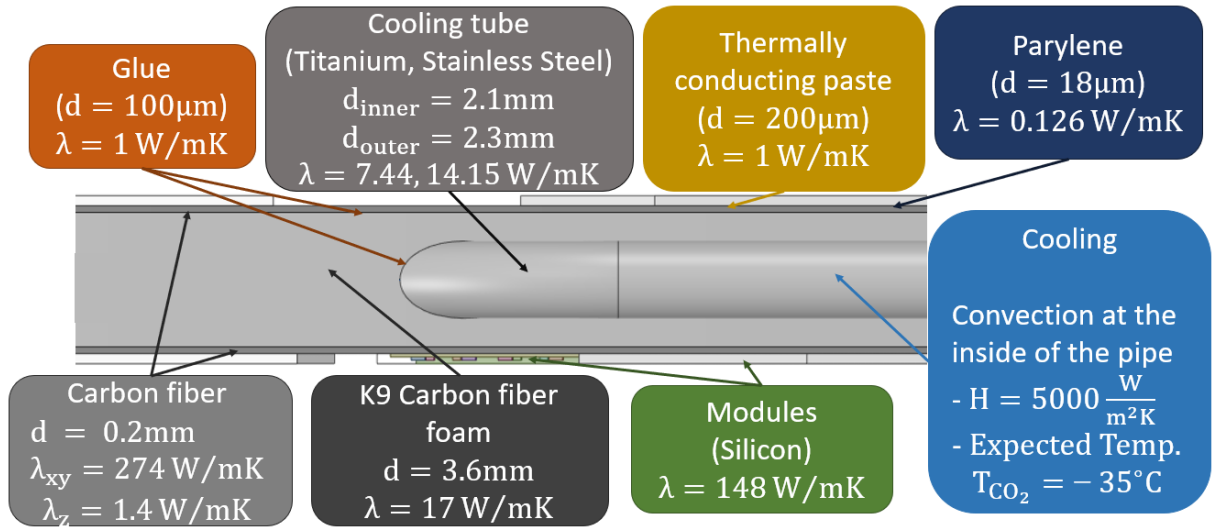


Figure 7.5: A diagram showing a transversal cut through the dee, with the respective thicknesses of the material layers and their corresponding thermal conductivities.

material in terms of bending the pipes into the correct shape and ensuring good connections to the CO_2 tubes outside of the TEPX detector which are made out of SS as connecting different material increases the complexity of the connections.

The cooling tubes are connected to highly thermally conductive carbon foam using thermal glue. To enclose the cooling tubes in the carbon foam, a small trench is milled out of the carbon foam at the width of the cooling pipes to place the tubes in the center of the carbon foam, as can be seen in Fig. 7.6. To ensure good thermal contact between the cooling tubes and the rest of the disk, the cooling tubes are covered in thermal glue and the milled out trench is filled with thermal glue as well.

Compressed Carbon Fiber (CFK) sheets are bonded to both sides of the carbon foam via thermal glue. They feature a high thermal conductivity in the direction of the plane λ_{xy} , thus helping to distribute the heat more evenly but a rather low thermal conductivity transversal to the plane λ_z .

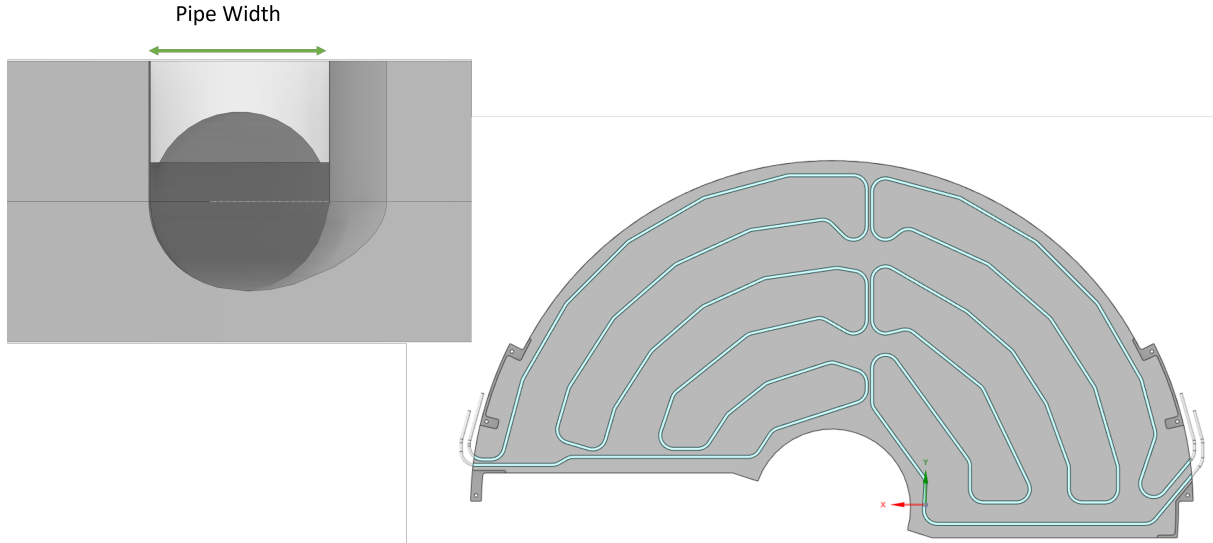


Figure 7.6: Schematic view of the trench milled out of the carbon foam and its glue filling.

The pixel modules, often referred to as CROC modules, are connected to the CFK via thermal paste. They consist of four RD53A readout chips [187], which is a new chip specifically developed for the HL-LHC CMS and ATLAS detectors. They feature a sufficiently high radiation hardness to survive the harsh conditions of the HL-LHC and allow for serial powering, which reduces the amount of material in the detector and losses due to long cables. The four RDA53A chips are connected to the sensor and the High-Density Interconnect (HDI), which is then connected to the PCB placed on top of the CFK, which carries power and data to and from the modules (not shown in Fig. 7.5). The modules are placed on the dee with the chips facing the CFK and the side with the HDI is facing away from the CFK.

The total thermal load of all module components while active is estimated to be approximately 10 W. However, as a safety measure, we conduct our studies with an additional load of 15%, which equates to 11.4 W.

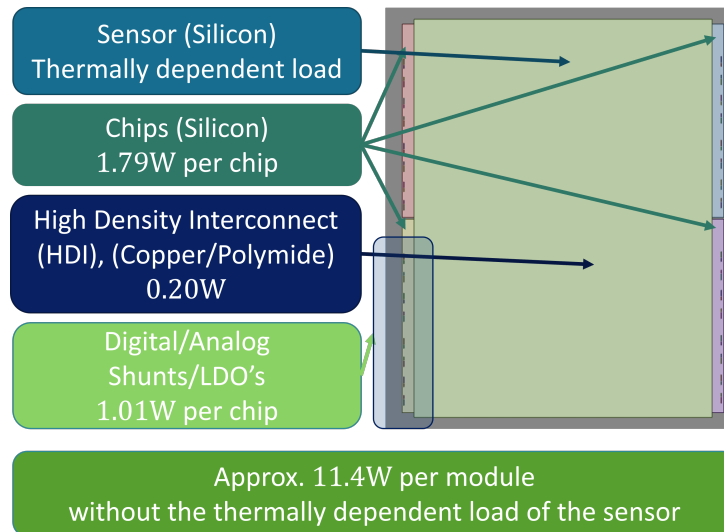


Figure 7.7: Schematic view of a model with its individual components and their corresponding thermal load and conductivity

Each component of the module other than the sensor is expected to have a constant thermal load when active. In the sensor however, we expect to observe a temperature dependent leakage

current, resulting in a temperature dependent thermal load that can be described as follows:

$$p(T) = U_{\text{bias}} \cdot \Phi(r) \cdot \alpha_0 \cdot V \cdot \frac{T^2}{T_0^2} \cdot \exp\left(C \frac{T - T_0}{T T_0}\right) \quad (7.1)$$

where $U_{\text{bias}} = 600 \text{ V}$ and corresponds to the bias voltage applied to the module. $\Phi(r)$ corresponds to the fluence and can be approximated via $\Phi(r) = \frac{b}{1000 \cdot r^2} + \frac{c}{1000 \cdot r^{0.55}}$ with $b = 1.566e^{+19}$ and $c = 1.3093e^{+16}$ in $\left[\frac{\text{MeV} \cdot n_{\text{eq}}}{\text{cm}^2}\right]$. The values for b and c have been calculated with the FLUKA model layout OT801_IT701 with an integrated luminosity of 3000 fb^{-1} and correspond to the TEPX dee, which experiences the highest fluence. The corresponding fit of the fluence function with the extracted fluence values from FLUKA can be seen in Fig. 7.8. V is the volume of the sensor and $T_0 = 20^\circ\text{C}$ is a reference temperature at which the constant $C = 6624.58 \text{ K}$ was measured.

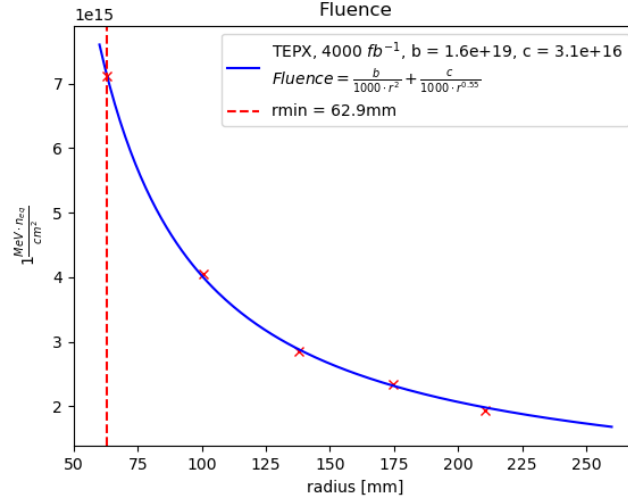


Figure 7.8: Fit of the fluence curve (blue) to the points extracted from the FLUKA model (red crosses).

As a result, the thermal load that the sensor experiences is exponentially dependent on its own temperature. This means that the leakage current in the sensor increases with temperature, which results in higher power dissipation. In the extreme case, where the increased thermal load cannot be completely absorbed by the cooling, the result is a loss of thermal stability. This uncontrollable rise in temperature is known as thermal runaway, which occurs when a critical temperature is reached. The cooling design must therefore ensure that the module temperature remains safely below the critical temperature during operation of the modules.

In addition, the modules are coated with a thin layer of parylene to isolate the readout chips from the sensor and the chip backside from the CFK of the dee. The effect of such a parylene layer on the cooling performance is also presented in the following sections.

7.3.3 Cooling of the Modules

The modules are cooled by thin pipes within which mixed phase CO_2 is circulated at -35°C . The mixture wets the surface of the pipe with liquid CO_2 . The cooling effect occurs when the CO_2 evaporates due to the heat of the dee. Using this CO_2 admixture allows us to achieve a large cooling effect with a small amount of material, while providing us with a small temperature

gradient along the cooling tube.

The CO₂ is supplied from a central plant and is then distributed to the individual components through a system of pipes. The ambient temperature in the CMS cavern is expected to be -20°C and is not expected to have a significant effect on the cooling of the dees.

As can be seen in Fig. 7.4, the cooling pipes are arranged in a flower-like shape. The flower shape ensures optimal coverage of the dee, which also results in optimal cooling, and has been optimised via finite element analysis during the course of these studies.

Fig. 7.9 shows the materials through which the heat flows before reaching the coolant.

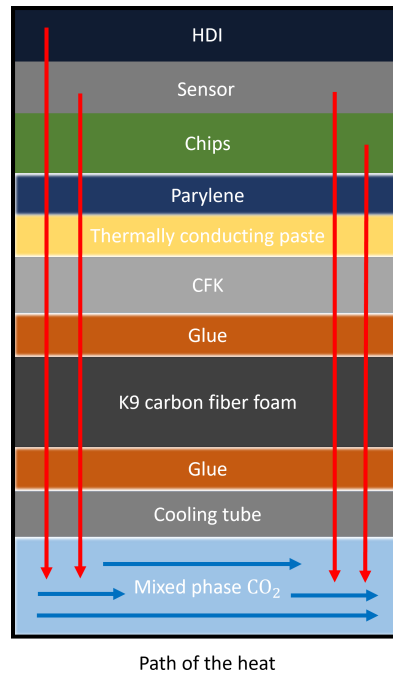


Figure 7.9: Diagram showing the different materials through which the heat flows until it reaches the cooling pipes

7.3.4 Thermal Design Studies Using Finite Element Analysis

Finite Element Analysis (FEA) is a powerful computational technique for simulating the behaviour of complex systems and structures. Developed to provide insight into complex engineering problems, it has also found its way into scientific fields where it is used, for example, in detector design. As the name suggests, the process involves breaking down the usually complex geometry of an object into smaller, manageable finite elements that are connected at nodes. By solving equations describing the behaviour of these finite elements and the interactions between them, FEA provides a way of simulating the behaviour of the whole system.

The intense conditions present during the HL-LHC raise the need for a powerful and optimized cooling solution. To simulate the behaviour of the cooling solution and test different design options, FEA analyses to compare the different design choices have been performed, which allows us to find the optimal configuration.

The results of these FEA studies are presented in the following sections and later compared to prototype tests, which are discussed in Sec. 7.3.5.

7.3.4.1 Parylene Coating of the Modules

In order to reduce noise and improve the durability of the modules to external conditions, the modules will be coated with a thin layer of parylene of approximately $18\text{ }\mu\text{m}$ thickness. The parylene is applied by vapor deposition and forms a protective layer around the module. It insulates the readout chips from the sensor and the chip backside from the CFK of the dee.

Although parylene has a low thermal conductivity of about 0.126 W/mK , we do not expect it to have a significant effect on the cooling of the modules as the layer is relatively thin.

Adding a parylene coating to the modules results in an average $+2^\circ\text{C}$ to the module temperature in the FEA simulations. This is in very good agreement with internal studies carried out by the TEPX group at PSI. Their tests with parylene coated prototype modules showed an increase in module temperature of about $+2.5^\circ\text{C}$.

7.3.4.2 Material Tests of the Cooling Pipes

To improve the material budget of the TEPX detector, we investigate the possibility of using Ti instead of SS for the cooling pipes. Tab. 7.1 shows the relevant parameters between the two materials. Ti has almost half the density of SS, which helps to reduce the material budget of the IT, while also featuring approximately twice the radiation length of SS. However, Ti is also mechanically more difficult to handle and features only approximately half the thermal conductivity. Bending the Ti cooling pipes into the flower pattern is a much more complex process using Ti pipes instead of SS pipes. The cooling pipes running between the central CO_2 plant and the TEPX pipes are made out of SS, which adds the additional mechanical complexity of ensuring a good connection between the two materials. Finally, the thermal conductivity of Ti is only about half that of SS. However, we do not expect this to have a significant effect on the cooling capabilities of the dee, as we expect the heat flow from the modules to the cooling pipes to be limited by other factors such as the through plane thermal conductivity of the CFK or the thermal conductivity of the glue, which both feature significantly lower thermal conductivities than Ti.

Table 7.1: Comparison of SS and Ti for values relevant values (from [188]).

	SS	Ti
Density [kg/m^3]	7870	4540
Rad. Length [cm]	1.757	3.560
Therm. Cond. [W/mK]	14.15	7.44

Running the FEA confirms our assumptions that changing the pipe material from SS to Ti only has a minimal effect on cooling. When running the same simulation and changing only the pipe material from SS to Ti, we find the change in the temperatures of the modules and dee to be smaller than 0.5°C , which is considered insignificant.

7.3.4.3 Cooling Pipe Insertion Techniques

In the early stages of designing the TEPX dee, two strategies to insert the cooling loop into the carbon foam were considered.

The first is to mill a trench out of the carbon foam and then place the pipe inside of the trench. The trench is then filled with a highly thermally conductive adhesive, which helps to smooth out small irregularities and ensure a good connection.

The other idea was to cut the carbon foam into two even pieces down the middle and then “sandwich” the pipe between the two halves. Instead of a milled trench filled with thermal adhesive, the two sides of the carbon foam are glued together over the entire surface.

FEA simulations showed slightly better cooling results for the first strategy, where a trench is milled out of the carbon foam, as we observe slightly lower module temperatures ($< 1.0^{\circ}\text{C}$).

However, as both approaches were comparable in terms of cooling performance, the TEPX team opted for the first approach as it was not only slightly better performing, but also mechanically easier to implement as there was more room to compensate for inaccuracies.

7.3.4.4 Carbon Foam Material Tests

At the start of the TEPX development, three candidates for the carbon foam were considered, which are listed in the Tab. 7.2.

Due to its non-uniformity and much larger pore size (also shown in Fig. 7.10), the CFoam35 HTC carbon foam was discarded as a candidate because the large pore size led to holes in the carbon foam sheet and severely reduced the structural integrity of the foam sheet.

Mechanically, milling out the trench to place the cooling tubes is easier to implement with the K9 foam compared to the POCO foam. Also, due to the smaller pore size, the parts where the trench for the cooling pipes was milled out are much more structurally stable compared to the POCO foam parts. Therefore, although POCO foam has better thermal conductivity, K9 foam is used in the final design of the TEPX disk due to the smaller pore size resulting in a mechanically superior design.

For completeness, FEA studies were also carried out comparing an identical disk with either K9 carbon foam or POCO foam. The resulting temperature difference was an increase of $dT \approx 3.0^{\circ}\text{C}$ when using K9 foam instead of POCO foam due to the difference in thermal conductivity.

Table 7.2: Comparison of pore size and thermal conductivity of the carbon foam candidates.

	K9 Foam	POCO Foam	CFoam35 HTC
Avg. pore size [mm]	0,15	0.4	< 4
Therm. Cond. [W/mK]	17	$\lambda_{xy} = 135, \lambda_z = 45$	140-180

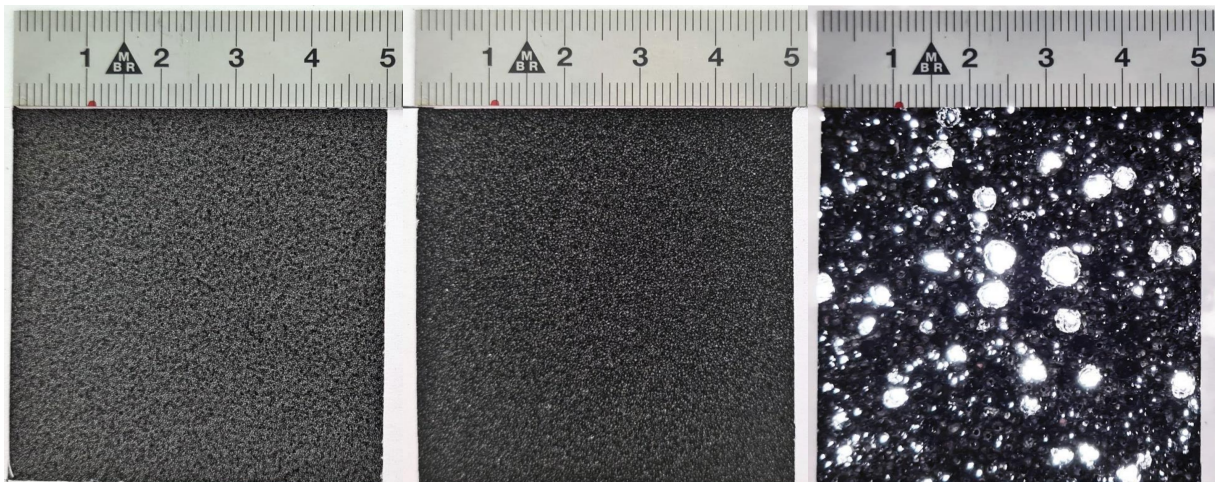


Figure 7.10: Comparison of the pore size of a milled 4 mm thick piece. Left K9 foam, middle POCO foam, right CFoam35 HTC.

7.3.4.5 Studies to Reduce the Material Budget

With the aim of reducing the material budget even further, we carried out studies where the amount of carbon foam is significantly reduced. Looking at Fig. 7.11, we can see that most of the heat is exchanged through the carbon foam close to the cooling pipe. To study if the cooling would still be sufficient with a reduced foam design, we removed all the carbon foam not located in the immediate vicinity of the cooling pipes (“reduced foam design”).

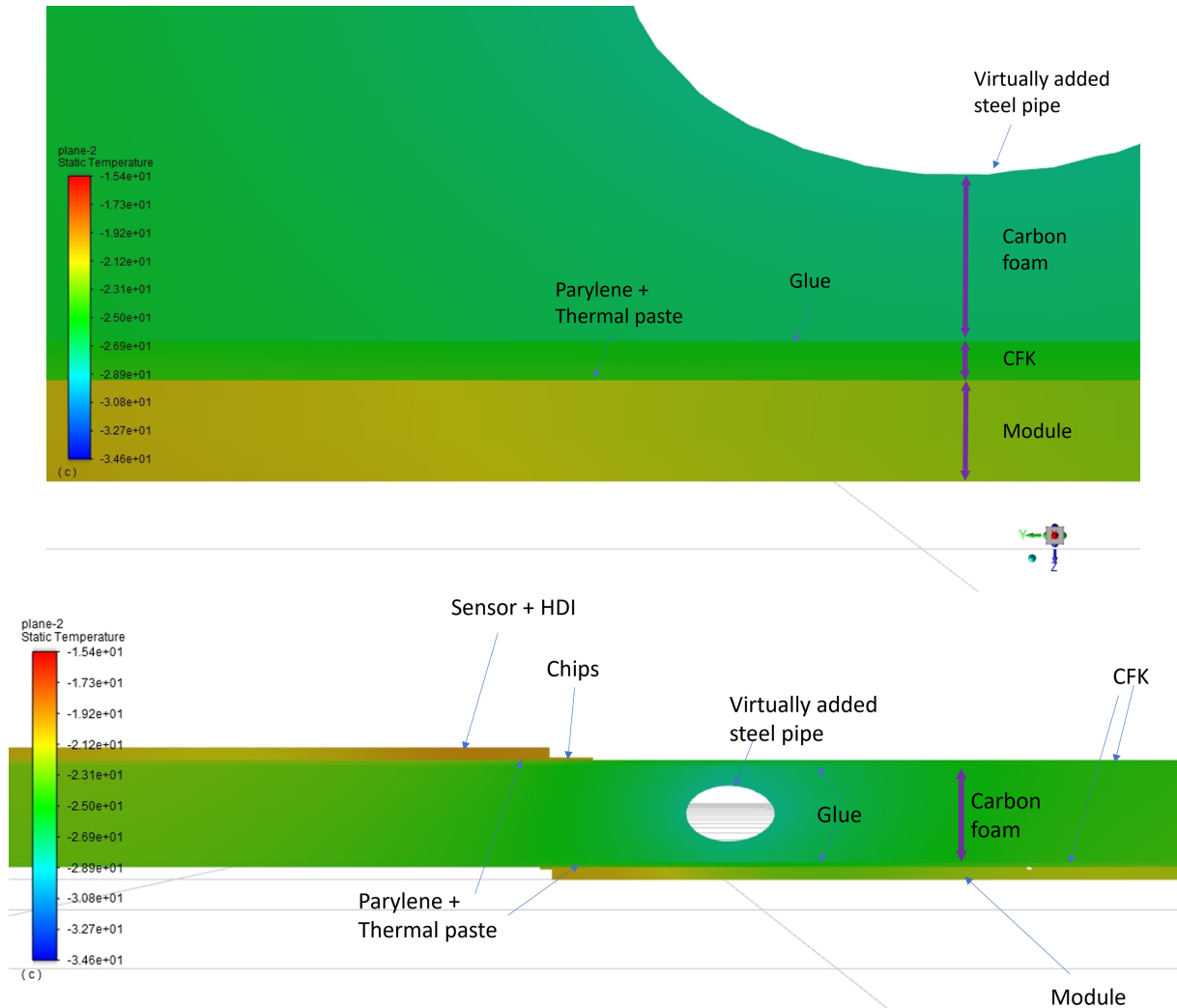


Figure 7.11: Cut through a transversal plane of a FEA featuring a full foam disc. It shows the the temperature of each component. The image on top is a zoomed in version of the bottom image.

By reducing the foam as shown in Fig. 7.12, the amount of foam is reduced by 84%. The FEA studies carried out, show an increase in module temperature of $dT \approx 5.0^\circ\text{C}$, when using a reduced foam setup. Although, this increase would still be acceptable, we decided to keep the design featuring the full foam disk as it provided a greater safety margin to the critical thermal runaway temperature.

7.3.4.6 Optimization of the Arrangement of the Cooling Tubes

During the FEA studies, we discovered a weakness in our cooling tube design when determining the critical temperature at which thermal runaway occurs. In general, thermal runaway, which

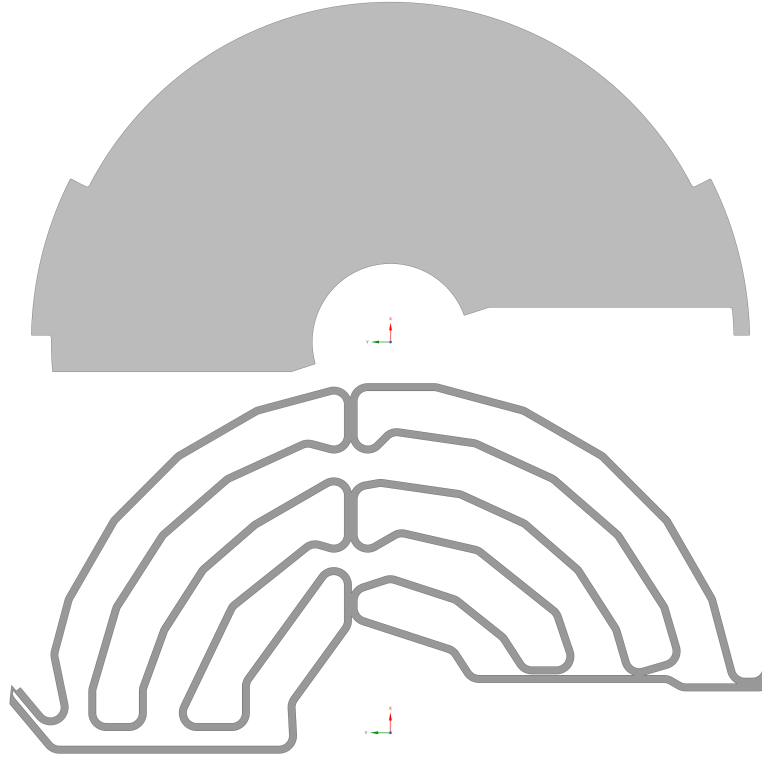


Figure 7.12: Comparison of the reduced foam design (bottom) with the conventional design (top).

2291 refers to the uncontrolled rise in temperature described by Eq. (7.1), tends to start in the
 2292 innermost ring of the dee, as these modules experience the highest fluence due to their proximity
 2293 to the interaction point. However, instead of all the modules in the first ring entering thermal
 2294 runaway at a similar temperature, the central module entered thermal runaway significantly
 2295 earlier than the other modules, which in turn raised the critical temperature of the entire dee.
 2296 We found that the reason for this was that the cooling of the module was reduced because some
 2297 areas of the module were not optimally covered by the cooling tubes. In particular, the bottom
 2298 edge showed increased temperatures compared to its neighbouring modules, as can be seen in
 2299 Fig. 7.13.

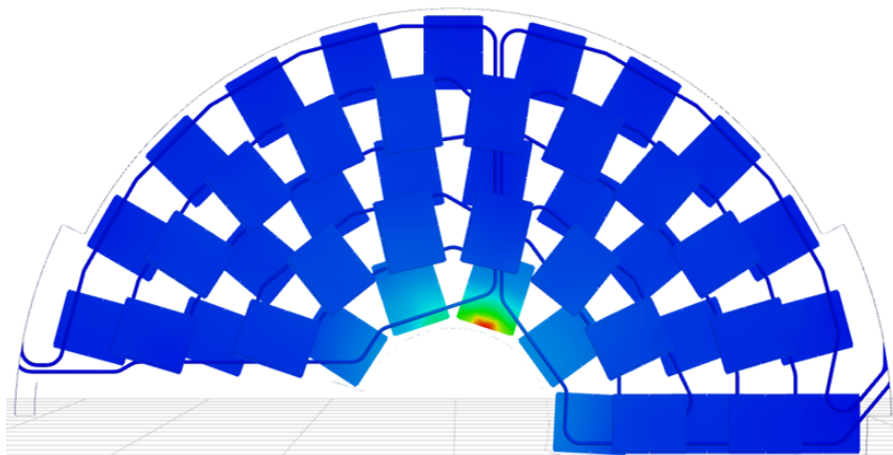


Figure 7.13: This graphic shows the start of thermal runaway at a coolant temperature of -25.0°C featuring the old pipe design. Note that the expected coolant temperature during operation is -35.0°C . So there is still a safety margin of 10.0°C , even with the old tube design.

To address this issue, I proposed an improved design with minimal changes to the existing design that provides better coverage of the module (Fig. 7.14). The new pipe design improves the module temperature by $dT \approx 4.0^\circ\text{C}$ and consequently improves the critical temperature by the same amount. Thus, the safety margin of the critical temperature could be improved by 3.0°C with this design change and is included in the current TEPX design plan.

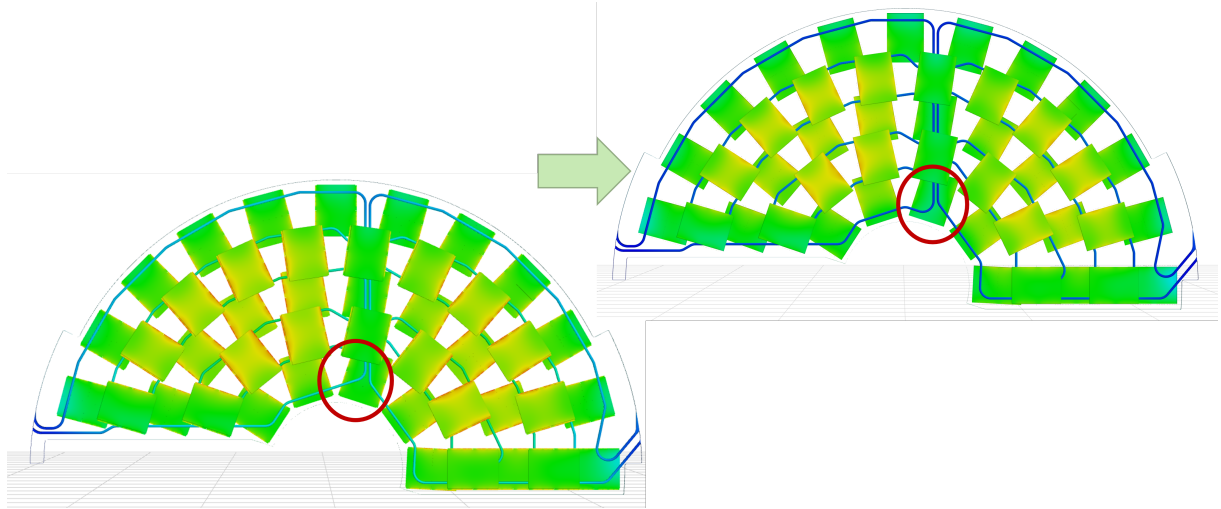


Figure 7.14: The diagram on the left shows the old pipe design with the changed part of the cooling pipe highlighted. The diagram on the right shows the new pipe design with better coverage of the critical module.

7.3.4.7 Thermal Runaway Studies

Some of the most essential FEA simulations involves studies to determine the critical temperature at which thermal runaway occurs. To ensure safe operation, the dee must be sufficiently cooled not only at the expected coolant temperature of -35.0°C , but also at higher coolant temperatures. This safety margin ensures that the system is able to compensate for mechanical inaccuracies and unexpected behaviour. Thermal runaway is usually described by a curve plotting the difference between the temperature of the hottest module and the coolant temperature against the coolant temperature. Due to the increasing thermally dependent load in the sensor, this temperature difference increases continuously up to the critical temperature where thermal stability is lost and the temperature rises uncontrollably.

Four different scenarios have been studied, which are described below with their results shown in Fig. 7.15.

The first scenario is called the “baseline scenario”, as it corresponds to the TEPX dee design that was in place before the improvements, that followed from the studies presented in this chapter, were implemented. It features a full K9 carbon foam plate with a thickness of $d = 3.6\text{ mm}$ and the cooling tube layout that includes the hot spot discussed in Sec. 7.3.4.6.

We also investigated the effect of reducing the material budget in two different ways. The first includes a reduced carbon foam scenario as presented in Sec. 7.3.4.5, where we remove the foam that is not in close proximity to a cooling tube. Due to the very high in-plane thermal conductivity of the CFK, this approach might still work reasonably well, as the heat can easily spread over the entire surface of the CFK.

Another idea to reduce the material budget was to reduce the overall thickness of the foam layer, which is limited by the thickness of the pipes embedded inside of the foam. For this

thin foam scenario, the thickness of the foam layer was reduced to $d = 2.6$ mm. Although, the extreme case of $d = 2.6$ mm is not mechanically rigid enough to actually be implemented, it still serves as a good indicator of the sensitivity of the cooling to the thickness of the carbon foam layer.

Finally, we have the scenario that corresponds to the current design of the TEPX detector. Compared to the baseline scenario, the only difference is that it includes the updated cooling pipe design, which provides better coverage of the center module in ring one of the dee.

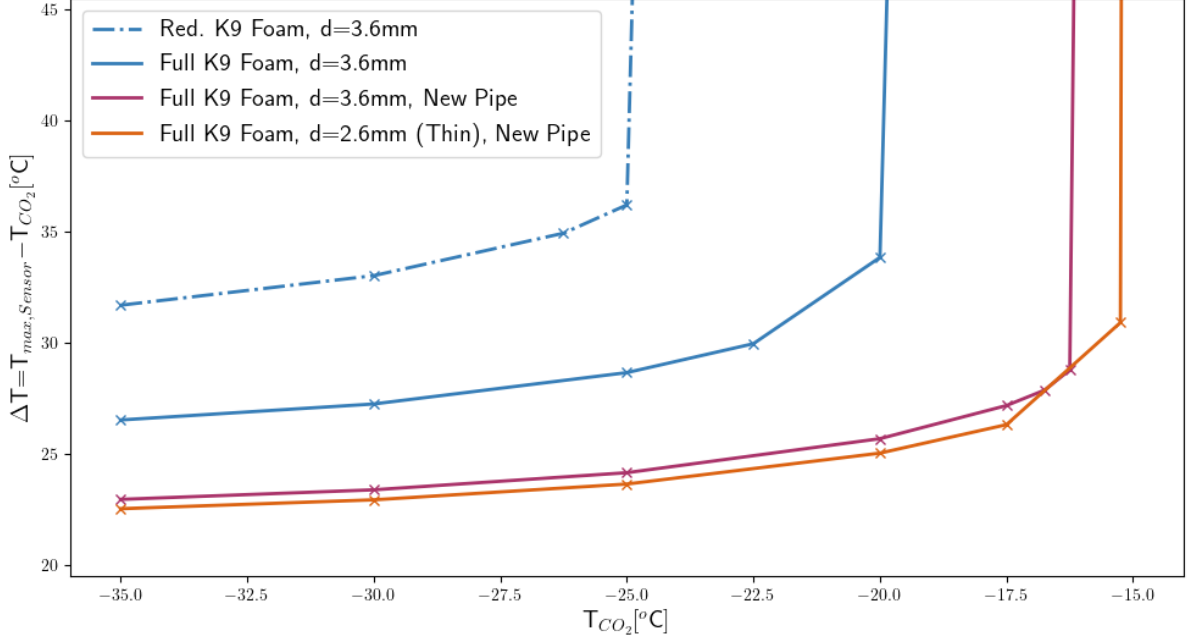


Figure 7.15: Plot showing different scenarios and their corresponding thermal runaway curves. The blue graph corresponds to the baseline while the blue striped graph corresponds to the same scenario with the old pipe design but also includes the reduced carbon foam. The red graph corresponds to the current design plan for TEPX with the cooling pipe improvements. The orange graph corresponds to the current TEPX design with the foam plate thickness reduced to $d = 2.6$ mm.

As it can be seen in Fig. 7.15, all four scenarios allow for at least a 10.0°C safety margin from the expected operating temperature. The baseline scenario has a safety margin of 15.0°C and therefore is safe to operate. The reduced K9 foam scenario significantly reduces the safety margin and as such will not be investigated further.

As discussed in Sec. 7.3.4.6, the sub-optimal coverage of the center module in ring 1 drives the critical temperature. As a result, we see a significant improvement in the safety margin from 15.0°C to approximately 19.0°C , even though only minimal changes have been made to the cooling tube design. As such, this design is preferable to the old design and will be used in future iterations and tests.

Lastly, we see that although reducing the carbon foam thickness has some limited effect, the cooling performance is limited by other factors such as the thermal conductivity of the CFK through the plane or the glue. This tells us, that a thicker foam plate of $d = 3.6$ mm thickness for improved mechanical stability can safely be used without sacrificing much cooling performance.

7.3.5 Prototyping and Testing

7.3.5.1 MARTA Cooling System

To simulate the conditions in which the TEPX dees will operate, a small local CO₂ cooling plant was required. For this we used a MARTA 2.0 machine, which provides the same CO₂ mixture for cooling as it will be used in the final design. Although, the machine is specified to be able to provide a coolant temperature of -30.0°C , due to mechanical issues of the machine, it is only able to cool down to -22.0°C . Therefore, the following tests and comparisons have been performed at this minimum temperature of -22.0°C .

One machine is capable of providing 300 W of cooling, which is not enough for an entire disk (approximately 500 W load per dee). Therefore, for studies where both sides of the dee are populated with modules and all five rings are active, two MARTA units are required to cool the dee. In this case, each MARTA unit cools one half of the disk via its respective cooling pipe circuit.

7.3.5.2 Dee Prototype

In order to investigate the compatibility of the FEA results with actual test data, a dee prototype was constructed. The prototype closely resembles the baseline scenario presented in Sec. 7.3.4.7. However, there are a few differences between the baseline scenario and the prototype. Fig. 7.16 shows the thermal conductivities of the prototype, while Fig. 7.17 shows the front and back of the prototype.

Firstly, as it can be seen in Fig. 7.17, only the side featuring rings 1, 3 and 5 (26 modules) is fully built with the other side being empty and not featuring anything beyond the CFK plate. Secondly, the glue used to construct the prototype dee, as in Fig. 7.5, has a thermal conductivity of $\lambda = 0.25 \text{ W/mK}$, while the one in the baseline scenario has a thermal conductivity of $\lambda = 1.0 \text{ W/mK}$. The module slots were populated with dummy modules, that are used to simulate a constant load. They feature several resistors on top of a thin HDI, which are able to generate the desired thermal load by adjusting the applied current and voltage. Finally, as the dummy modules are very thin compared to the CROC modules, a copper plate about the size of a module is placed in between the dummy module and the CFK, acting as a spacer to bridge the gap between them.

Like in the final TEPX design, the dummy modules are pressed onto the dee via spider clamps, which can be seen in the prototype setup shown in Fig. 7.18. There is no thermal bonding material such as thermal paste between the copper plate and the CFK, unlike the TEPX design, where we have thermal paste between the CFK and the modules. To account for the layer of air in between the CFK and the copper plate, we assume a small air gap of $d = 35 \mu\text{m}$. Between the copper plate and the dummy module, we place a highly thermally conductive graphite sheet to provide good thermal contact.

7.3.5.3 Experimental Setup

Our experimental setup consisted of the MARTA unit providing the CO₂ admixture for cooling, which was attached to a local box and can be seen in Fig. 7.18. The local box, which is an attachment of the MARTA unit, acts as an interface, where we connect CO₂ cooling tubes that run into the cooling box and from there into dee prototype. The cooling box itself is made out of foam boards with a very low thermal conductivity of approximately $\lambda = 0.024 \text{ W/mK}$. As such,

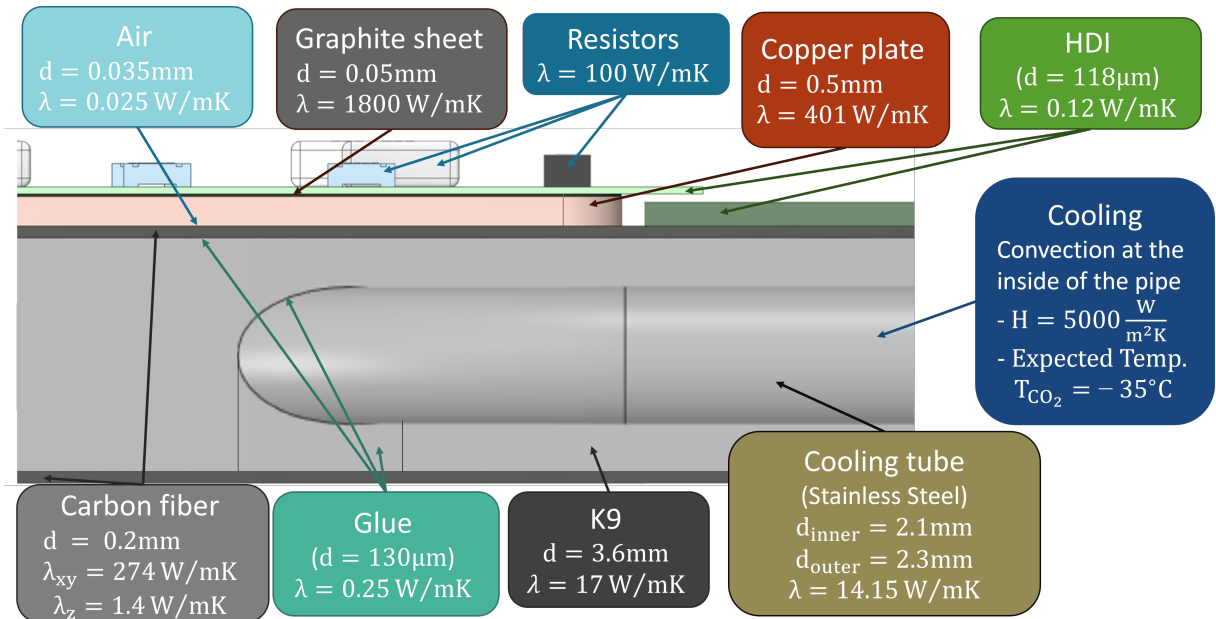


Figure 7.16: A diagram showing a transversal cut through the prototype dee, with the respective thicknesses of the material layers and their corresponding thermal conductivities.

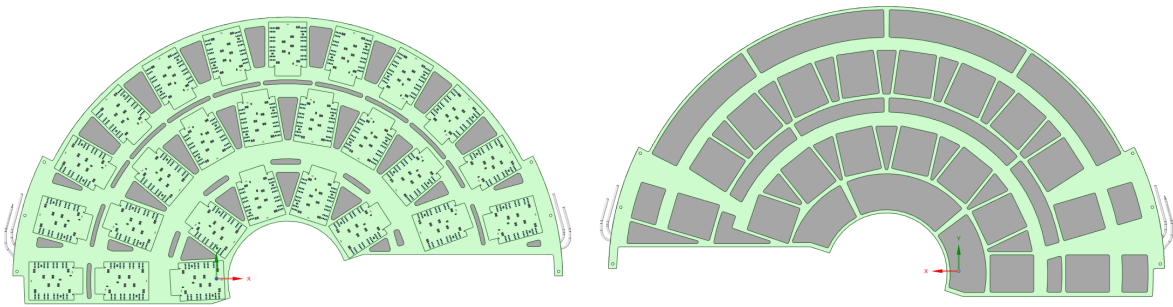


Figure 7.17: Front view (left) of the prototype dee featuring rings 1, 3 and 5 and back view of the dee (right), which is empty.

it is ideal to isolate the prototype during testing and create a dry, which prevents condensation on the dee during cooling, and thermally insulated environment. The dry environment is created by a constant flow of dry air into the cooling box. Located inside of the cooling box is a dew-point meter to monitor the humidity inside of the box during operation and prevent possible condensation on the disk.

In addition, several Pt100 temperature sensors were placed on the CFK and on selected modules. Fig. 7.19 shows the placement of the temperature sensors. The sensors were placed so that we could measure the temperature of one module in each ring, as well as on the CFK board next to the module being measured. Their signals were then read out via LabView and stored locally.

Finally, we were able to control the power for each ring individually and ramp it up to the expected thermal load. Due to limitations of the power supply of the modules, the maximum applied load per module was 9.6 W.

Tab. 7.3 shows the measured temperatures with a load of 9.6 W per module. One can see that the output coolant temperature is lower than the input temperature. This is an effect caused by the evaporation of CO_2 inside the cooling pipe and indicates that the cooling works as expected and has the correct mixture of liquid and gaseous CO_2 .

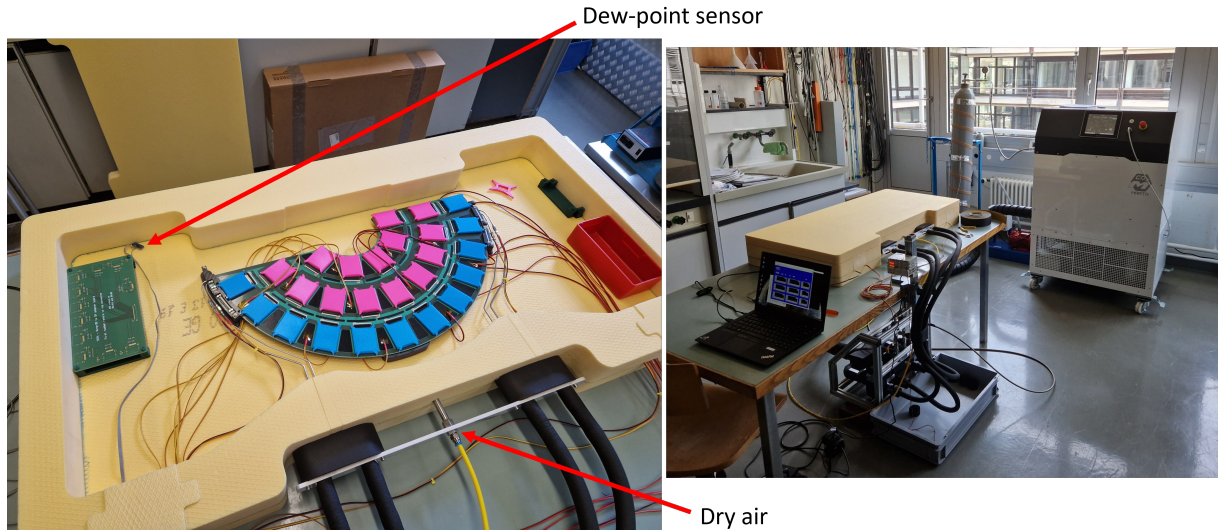


Figure 7.18: The picture on the left shows the cooling box with the dee prototype. The picture on the right shows the complete experimental setup including the MARTA unit used to cool the system.

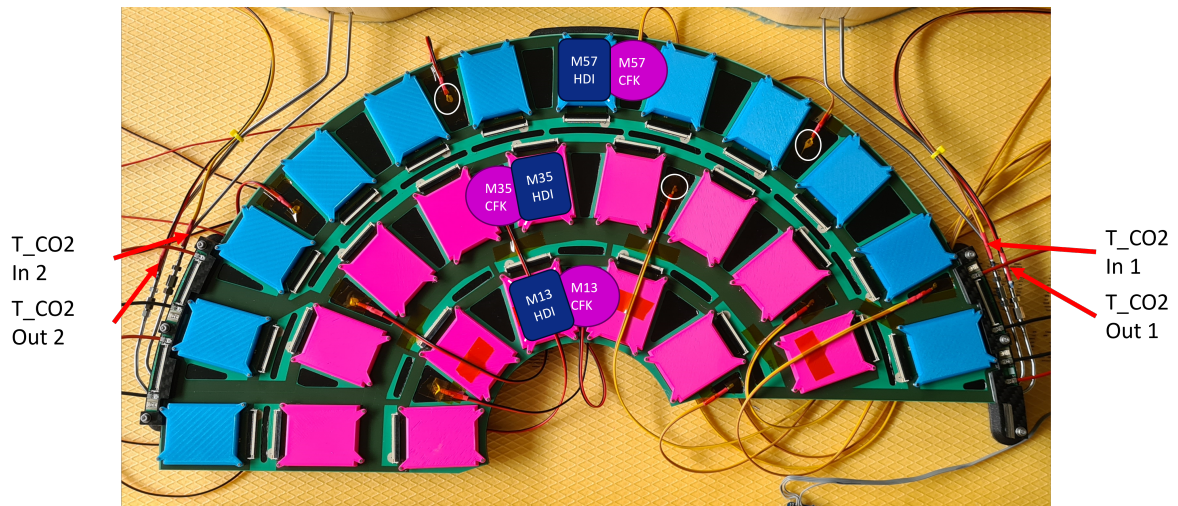


Figure 7.19: This figure shows the placement of the temperature sensors. Sensors M13 HDI, M35 HDI and M57 HDI are placed on the HDI of the prototype modules (also simply called M13, M35 and M57 in the rest of the document). The neighbouring sensors M13 CFK, M35 CFK and M57 CFK are placed on the CFK next to the corresponding modules. The naming scheme follows the logic “M - Ring Number - Module Number in the ring”.

Table 7.3: This table shows the results of a measurement with a thermal load of 9.6 W per module in °C. The first four columns show the input and output temperatures of the cooling pipes. The next six columns show the temperatures of the modules and the temperature of the CFK next to the module.

T_{In1}	T_{Out1}	T_{In2}	T_{Out2}	T_{M13}	$T_{M13,CFK}$	T_{M35}	$T_{M35,CFK}$	T_{M57}	$T_{M57,CFK}$
-17.7	-19.2	-18.5	-19.2	11.5	2.4	11.0	-1.1	11.3	-0.8

7.3.5.4 FEA of the Dee Prototype

Using the geometry of the prototype (see Fig. 7.17) a FEA analysis was performed using the parameters shown in Fig. 7.16. A total thermal load of 9.6 W was applied to each module. The results are shown in Fig. 7.20 and 7.21.

Fig. 7.20 shows that there are no obvious hotspots on the dee, indicating that the cooling

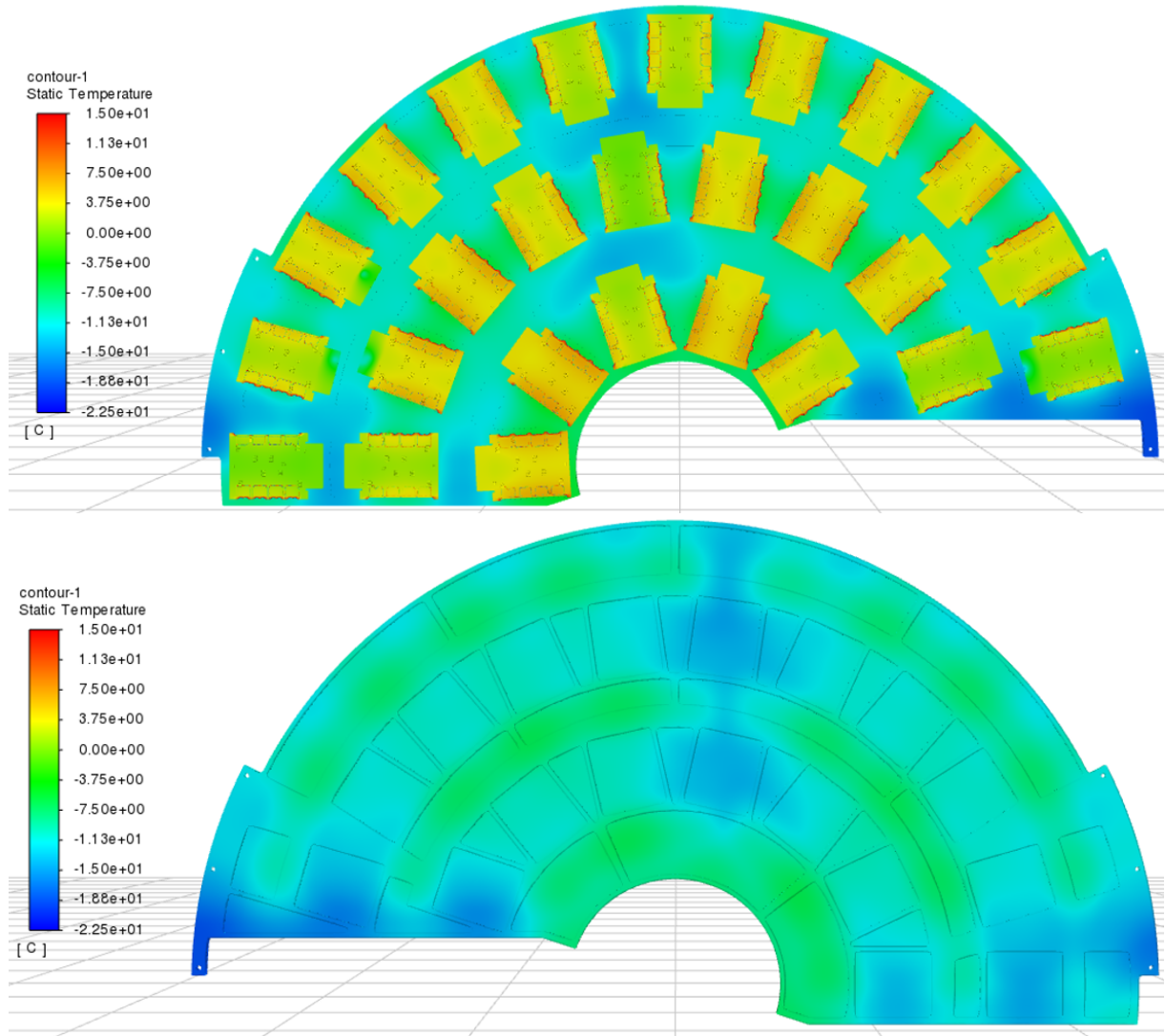


Figure 7.20: Front side (top) of the simulated dee prototype under 9.6 W thermal load per module. Back side (bottom) of the simulated dee prototype under 9.6 W thermal load per module. Although there are no modules on the back, one can see warmer regions caused by the modules on the front side.

solution is providing sufficient and uniform cooling along the dee. Fig. 7.20 also shows the cooler unpopulated backside of the dee. Even though the backside features no modules, one can see warmer regions caused by the modules on the front side.

Fig. 7.21 shows the temperatures along a transversal cut through the dee at the position of the center module of ring 1 allowing us to draw several conclusions. Firstly, one can clearly see the effect of the lower thermal conductivity of the glue compared to the K9 carbon foam as the glue-filled trench is much colder. Additionally, the effect of the low thermal conductivity of the glue used can be seen by the temperature jump between the K9 carbon foam and the CFK. This suggests that the use of a more thermally conductive glue would most likely increase the cooling performance significantly, as the transition between these two materials is a bottleneck for heat flow.

Secondly, one can observe a similar effect at the transition between CFK and the copper plate. Due to the air gap between the two, the heat flow is severely diminished which can be seen by the large temperature jump between the two materials. Similar to the connection between the CFK and the K9 carbon foam, this indicates that the cooling performance could be

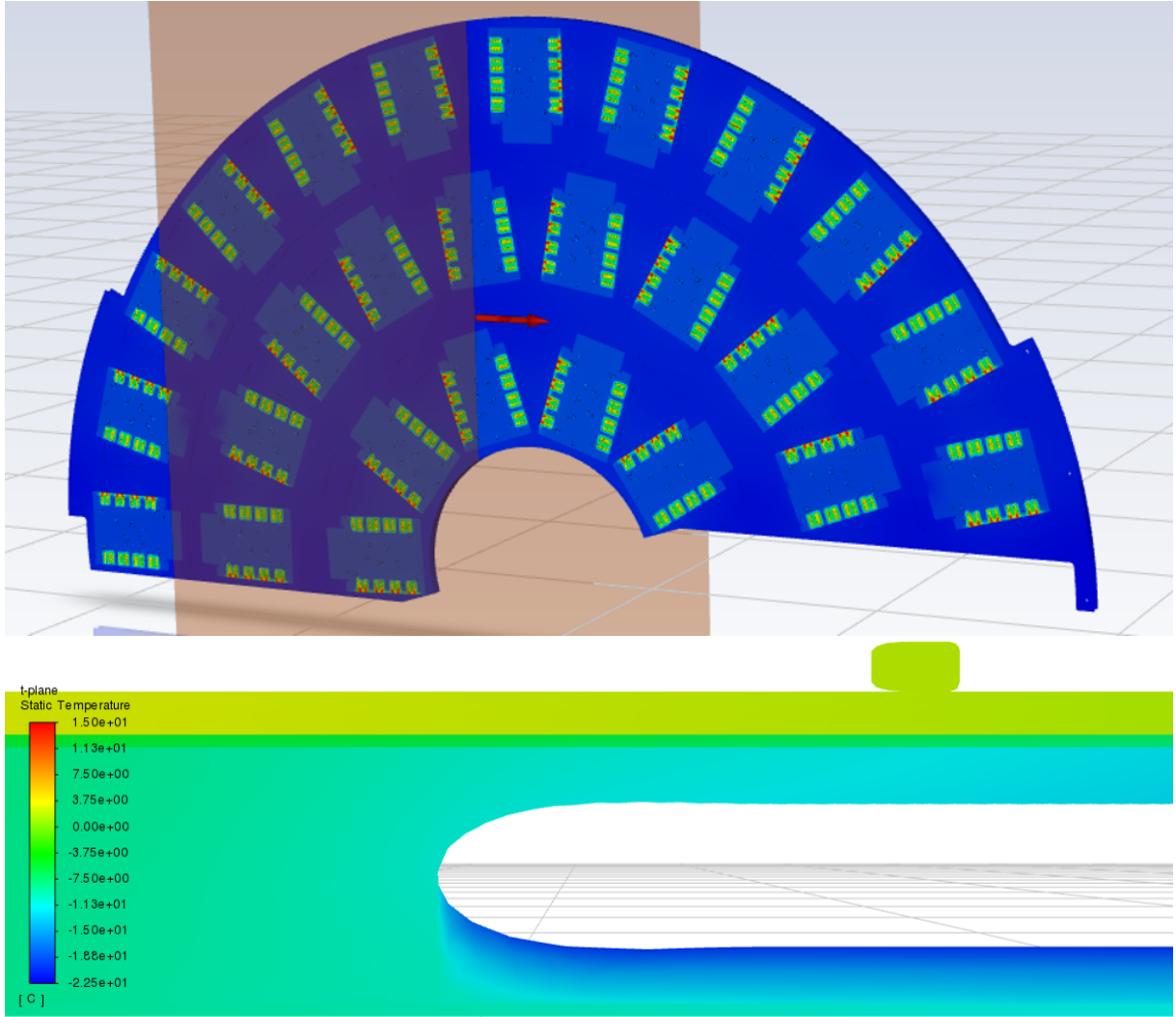


Figure 7.21: The figure on top shows the transversal plane on which the figure below is based on. The figure below shows the temperature along the transversal cut through the dee at the location of the module in the innermost ring (ring 1).

significantly improved by introducing a material such as thermal paste between the CFK and the copper plate to improve the thermal contact¹.

Table 7.4: This table shows the results of a measurement with a thermal load of 9.6 W per module in °C. The first four columns show the simulated input and output temperatures of the cooling pipes. The next six columns show the temperatures of the modules and the temperature of the CFK next to the module.

T_{In1}	T_{Out1}	T_{In2}	T_{Out2}	T_{M13}	$T_{M13,CFK}$	T_{M35}	$T_{M35,CFK}$	T_{M57}	$T_{M57,CFK}$
-22.5	-22.5	-22.5	-22.5	8.5	-2.3	6.5	-2.3	8.3	-2.3

Tab. 7.4 shows the results of the FEA using similar conditions to the dee prototype test. One difference between the FEA and the measurements is that in the FEA we assume a constant coolant temperature along the tubes and the same coolant temperature in both tube circuits. However, as the temperature difference between the sides and between the inlet and outlet is small, we assume this effect to be negligible.

¹In the final assembly of the TEPX disk, a layer of thermal paste is planned between the CFK and the modules.

7.3.6 Comparison FEA and Prototype

The comparison between the measured temperatures of the experimental setup and the corresponding temperatures of the FEA model can be seen in Tab. 7.5, and follows from the results presented in Tab. 7.3 and 7.4.

Table 7.5: This table shows a comparison of the values presented in Tab. 7.3 and 7.4 in °C. First, the difference between the coolant input and output temperature is shown. Then the difference between the module temperature and the CFK next to the module is shown. Finally, the difference between the module temperature and the coolant temperature is shown.

	$dT_{In1,Out1}$	$dT_{In2,Out2}$	$dT_{M13,CFK}$	$dT_{M35,CFK}$	$dT_{M57,CFK}$	dT_{M13,CO_2}	dT_{M35,CO_2}	dT_{M57,CO_2}
Lab	1.5	0.7	9.1	12.1	12.1	29.2	28.7	29.0
FEA	0.0	0.0	10.8	8.8	10.6	30.9	28.9	30.8

Tab. 7.5 shows good agreement between the FEA results and the prototype measurements. The temperature difference between the coolant and the modules as well as the modules and the CFK show a good level of agreement.

The results show a good match between our assumptions and the mechanical prototype. Therefore, we can conclude, that the thickness of the glue layer between the cooling pipes and the carbon foam as well as the glue layer between the carbon foam and the CFK are approximately in line with the assumptions made in the FEA.

Similarly, the good agreement between the temperature difference between the module and the CFK indicates that the assumptions on the thickness of the air gap between these two parts also accurately reflect the real case.

Overall, the good agreement between the dee prototype and the FEA increases our confidence that many of the assumptions made for the TEPX dee prototype are indeed valid for the real case and that the FEA results will accurately reflect the actual TEPX dee in future tests.

7.4 Summary

The upgrade of the CMS IT in regards of the HL-LHC poses significant mechanical and technical challenges. The TEPX section of the IT was presented with a particular focus on the thermal design.

The studies presented show that the application of a parylene layer to the modules for electrical insulation will result in a module temperature increase of about 2.0°C. Furthermore, several design choices (e.g. cooling pipe layout) were tested and their optimal configuration was selected, resulting in an improved thermal design of the TEPX dees. It was shown, that according to the results of the FEA performed, the material choice of the cooling tubes between SS and Ti has no significant effect on the cooling performance

Additionally, measurements of a first TEPX dee prototype were presented and compared to a FEA of said prototype. A good agreement between the measurements and the FEA was achieved, which increases our confidence in the mechanical assumptions made for the final design. Further studies involve a TEPX prototype dee populated with CROC modules to test its performance with CROC modules instead of dummy modules. Also more specialized tests still need to be performed, like for example scenarios, where one module breaks in way that results in more voltage applied to the remaining modules connected in series. Finally, studies to examine the properties of the dees under thermal cycling still need to be performed.

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A Optimal Transport for a Novel Event Description at Hadron Colliders

The work presented in this section is a copy of the published paper [189]. The analysis was performed in collaboration with the involvement of the researchers below:

- L. Gouskos, (CERN, Switzerland; Brown University, USA)
- F. Iemmi (Institute of High Energy Physics, China)
- B. Maier (CERN, Switzerland; Karlsruhe Institute of Technology, Germany)
- V. Mikuni (National Energy Research Scientific Computing Center, Berkeley Lab)
- H. Qu (CERN, Switzerland)

My main contribution to this project was the development of the complete technical framework together with F. Iemmi. Additionally, I was also lightly involved in the studies performed with the neural network.

A.1 Introduction

At the High Luminosity-LHC (HL-LHC), up to 200 proton collisions will take place simultaneously. This poses an unprecedented challenge to the reconstruction algorithms of experiments such as ATLAS and CMS, hindering their ability of searching for new physics with highest sensitivity if collision products are not disentangled properly. A performant rejection of particles from subordinate proton collisions (pileup) is therefore paramount to the success of the LHC physics program. Exploiting the excellent position resolution of tracking systems, charged particles from pileup collisions can be effectively mitigated [118, 190] by discarding particles not associated to the primary vertex. Contributions from neutral particles (photons and neutral hadrons), however, can only be reconstructed using the calorimeter systems with comparably poor spatial resolution. To this end, dedicated algorithms based on a physics-motivated, rule-based selection were developed to obtain a set of per-particle probabilities indicating whether neutral particles originate from the leading primary vertex or not. For instance, the PUPPI algorithm is the state-of-the-art at the CMS experiment [125, 191].

The complexity of the pileup mitigation task motivated the proposition of machine learning (ML)-based algorithms: the PUMML algorithm [192] relies on image recognition techniques to identify particles stemming from pileup vertices; other algorithms, e.g., in Refs. [193, 194], exploit graph neural networks (GNNs) or transformers. In all cases, the ML-based approaches yield sizable improvements compared to rule-based algorithms.

One of the main limitations of these ML algorithms is, that they require a sound definition of a ground truth, i.e., the assignment of a label to each particle, indicating if it originates from the leading primary vertex or not, to train a fully-supervised ML model. Such labels are available in simplified detector simulations, such as the ones implemented in Delphes [195]. However, due to merged energy deposits and the much more complex event reconstruction, an

unambiguous ground truth definition for neutral particles is intractable in data and in the full-scale simulations based on Geant4 [157] that are used by experiments such as ATLAS and CMS. Therefore, per-particle target labels based on human annotation are very hard to obtain and exhibit insufficient sharpness, rendering fully supervised strategies suboptimal. Thus, none of the previously described ML-based solutions can be implemented in a straightforward manner by the experiments at the LHC. Recently, it has been proposed in [196] to train a semi-supervised network using charged particles, whose provenance can be obtained under the assumption of perfect tracking, and to extrapolate the results to neutral particles. While this approach would allow to train on full-scale simulations and on data, it only works in a central detector region where tracking is available, whereas pileup is predominant in the forward regions of the detectors. Therefore, our primary motivation to develop the algorithm for Training Optimal Transport with Attention Learning (TOTAL) in this article is to address these bottlenecks. We achieve this by employing metrics inspired by optimal transport (OT) [197] problems as the cost function of a self-supervised, attention-based GNN, whose architecture closely follows the development in [198]. This network is used to assimilate two simulated samples, one containing only the particles arising from the primary interaction and the other containing also contributions from pileup. By training in a self-supervised fashion, i.e., not relying on per-particle truth labels from human annotation, our approach can be realistically implemented in full-scale simulations and does not rely on any kind of extrapolation. Following this strategy, we are able to derive an event description that is straightforward to implement and that exhibits greatly improved precision, yielding a global sensitivity enhancement for SM measurements and searches alike, explained as follows.

A.2 Sliced Wasserstein Distance

Instead of relying on truth labels for reconstructed particles, we design an alternative objective that transforms the entire set of particles from multiple simultaneous interactions into the same collision event containing only the primary interaction. Borrowing from concepts of OT, we are interested in finding the transport function that leaves particles with similar features between sets unchanged while removing contributions from additional interactions. The Wasserstein distance [199] can leverage geometric information in the probability space to estimate the distance between probability measures. Given two probability measures $\alpha \in P(X)$ and $\beta \in P(Y)$, both defined in the set of probability measures $P(\Omega)$, we identify the q -Wasserstein distance problem as the determination of the transportation plan $\gamma \in \Gamma(\alpha, \beta)$ that satisfies:

$$\text{OT}_q(\alpha, \beta) = \left(\inf_{\gamma \in \Gamma(\alpha, \beta)} \int_{\Omega \times \Omega} c(\mathbf{x}, \mathbf{y})^q d\gamma(\mathbf{x}, \mathbf{y}) \right)^{1/q}, \quad (\text{A.1})$$

where c is the cost function evaluated over observations $\mathbf{x}, \mathbf{y}$ drawn from the sets X, Y and the order q can be chosen to give the q -th root of the total cost incurred. In high-dimensional spaces, solving the OT problem becomes computationally expensive since only the one-dimensional case allows a closed-form solution [200]. This observation motivates the formulation proposed in [200, 201] to introduce the sliced Wasserstein distance (SWD) as an integral over one-dimensional transport problems:

$$\text{SWD}(\alpha, \beta) = \int_{\mathcal{S}^{d-1}} \text{OT}_q(\mathcal{R}_\theta(\alpha), \mathcal{R}_\theta(\beta)) d\theta. \quad (\text{A.2})$$

The term $\mathcal{R}_\theta$ represents the linear operation that projects (or “slices”) the probability measures over the one-dimensional space and is integrated over a uniform measure θ in the unit sphere $\mathcal{S}^{d-1} \in \mathbb{R}^d$. The dimensionality d corresponds to the number of particle features considered. Since the integral is intractable, we can instead use a Monte Carlo approach to replace it with multiple random projections. In this formulation, the optimal coupling is the one that minimizes the cost function evaluated over one-dimensional, sorted projections, thus replacing the expensive OT problem by several (one for each projection), yet simple, sorting problems.

Accordingly, we denote the set of particles in the sample with pileup as $x_p \in \mathbb{R}^{N \times d}$, while the same particle collision in the set without pileup is denoted as $x_{np} \in \mathbb{R}^{N \times d}$. Since the set of particles without pileup is considerably smaller than the one with, we keep the overall number of particles N fixed by zero-padding as necessary. Given M projections with permutations μ and ν that sort N particles of the sets $\mathcal{R}_{\theta_m}(x_p)$ and $\mathcal{R}_{\theta_m}(x_{np})$, the SWD is calculated as:

$$\text{SWD}(x_p, x_{np}) = \frac{1}{M} \sum_j^M \sum_i^N c(\mathcal{R}_{\theta_j}(x_{p, \mu(i)}), \mathcal{R}_{\theta_j}(x_{np, \nu(i)}})) , \quad (\text{A.3})$$

where the cost function $c(\mathbf{x}, \mathbf{y}) \equiv |\mathbf{x} - \mathbf{y}|^2$ is used in the following studies.

Our method aims to train a neural network to output a set of weights $\omega \in [0, 1]$, for each particle, that removes particles from pileup collisions. While the network is trained using a larger set of features, the SWD calculation in Eq. A.3 is carried out using only the four-vector (p_x, p_y, p_z, E) for each particle. The weights ω are learned by minimizing $\text{SWD}(x'_p, x_{np})$, with the weighted set $x'_p = \omega x_p$. By multiplying the four-vector with a single weight, we are able to re-scale the magnitude of the momentum vector while preserving the direction in the calculation.

As a result, particles created from pileup collisions increase $\text{SWD}(x'_p, x_{np})$ and should populate ω values closer to zero, whereas particles from the primary collision are assigned $\omega \approx 1$.

An extra term can be added to Eq. A.3 to control the energy scale of the events in the sample containing pileup. To that end, a constraint on the missing transverse momentum (p_T^{miss}) is introduced to the loss function as the mean square error (MSE) of the p_T^{miss} values between samples:

$$\mathcal{L} = \text{SWD}(x'_p, x_{np}) + \lambda \text{MSE}(p_T^{\text{miss}}(x'_p), p_T^{\text{miss}}(x_{np})). \quad (\text{A.4})$$

The parameter λ controls the strength of the regularization. In this letter, we present results for $\lambda = 0$ (no regularization), and for $\lambda = 10^{-3}$, resulting in the p_T^{miss} constraint to have the same order of magnitude as the SWD term.

We simulate proton collisions at a center-of-mass energy $\sqrt{s} = 14$ TeV employing the Pythia v8.244 event generator [202, 203]. The Delphes v3.4.3pre01 detector simulation [195] is used to obtain reconstructed particles with a detector layout resembling the Phase-II upgrade of the CMS detector. The simulated physics processes include jets produced via quantum chromodynamics (QCD); the production of a top quark-antiquark pair ($t\bar{t}$), where both W bosons decay leptonically; the vector boson fusion (VBF) production of a Higgs boson decaying into undetectable dark matter particles; the production of a heavy resonance (Z') decaying to $t\bar{t}$, where both W bosons decay hadronically; and the production of a W boson in association with at least one jet (W+jets). The former three processes are used for training and inference, while the Z' and W+jets processes are used to assess the performance on jet substructure and the robustness of the algorithm, respectively.

Starting from the same simulated hard interaction, we generate two event samples. The first one consists solely from particles produced during the hard interaction process. In the second

sample, we add contributions from pileup before reconstructing the event. The number of pileup interactions follows a Poisson distribution with a mean of 140 to match HL-LHC conditions.

The TOTAL algorithm accomplishes the task of pileup mitigation by taking the available properties of each particle as input features. These are the four-vector (p_T, η, ϕ, E) , the impact parameters in the transverse plane and along the beam axis, the particle ID, the electric charge, and the vertex identification for charged particles. The inputs are pre-processed so that the order of magnitude of all features is 1. We use the output weights $\omega \in [0, 1]$ to re-scale the four-vector of each particle in the slicing process. Per event, we consider the first 9000 particles (sorted by descending p_T and including zero-padding) and gather the 20 nearest neighbors in the η - ϕ plane for each particle when building the graph. The SWD in Eq. A.4 is computed taking 128 random projections per collision event. Different choices of number of projections were tested and changes in the results were found to be negligible when using more projections.

A.3 Results

The network trained with $\lambda = 0$ (cf. Eq. A.4) is evaluated on samples statistically independent from the ones used during training. The per-particle weights obtained from the evaluation process are used to re-scale the four-momenta of the particles in the event. We then use the FastJet software [124] to cluster two TOTAL jet collections using the anti- k_t algorithm [123] with small and large radius parameters of $R = 0.4$ and $R = 0.8$, respectively. The set of re-scaled particles is also used to compute p_T^{miss} . We evaluate the network on three benchmark processes: QCD multijet production, which is ubiquitous at hadron colliders and constitutes an important background to many measurements and searches; dileptonic $t\bar{t}$, which often enters analyses both as a signal or as a background process; and Z' , which is enriched in events with hadronically decaying top quarks merged in large-radius jets and is well suited to study jet substructure. These processes cover different physics scenarios, namely cases where sizable p_T^{miss} comes from detector and reconstruction inefficiencies, and events where genuine p_T^{miss} is caused by neutrinos.

To compare the performance of different pileup mitigation algorithms, a matching in $\Delta R = \sqrt{(\eta_i - \eta_j)^2 + (\phi_i - \phi_j)^2}$ is performed between reconstructed jets and generator-level jets. The latter are obtained by clustering only the particles coming from the leading primary vertex, before any detector and reconstruction effects. The following studies are based on generator-matched jets, namely reconstructed jets for which a generator-level jet is found within $\Delta R < 0.3$.

We define the response for a given observable x as the difference between the reconstructed and generator-level values, divided by the generator-level value $(x_{\text{reco}} - x_{\text{gen}})/x_{\text{gen}}$. In Figure A.1 we show the distributions for different kinematic variables and the corresponding response functions in the $t\bar{t}$ and Z' samples. The spread of the response is indicative of the experimental resolution of the reconstruction algorithms. We define the resolution in an observable as the spread in its response, given by

$$\frac{q_{75\%} - q_{25\%}}{2}, \quad (\text{A.5})$$

where $q_n\%$ represents the n -th percentile of the response distribution. Lower resolutions result in a better reconstruction and increased power of kinematic variables such as invariant masses or p_T^{miss} .

Figure A.2 shows the jet resolution in the transverse momentum p_T (jet energy resolution, JER) of generator-matched jets, computed as a function of p_T and η of the matched generator-level jet, for $t\bar{t}$ and QCD multijet events, respectively; and the large-radius jet resolution in τ_3/τ_2 , which is a variable that provides a handle on the substructure of the jet, as a function of

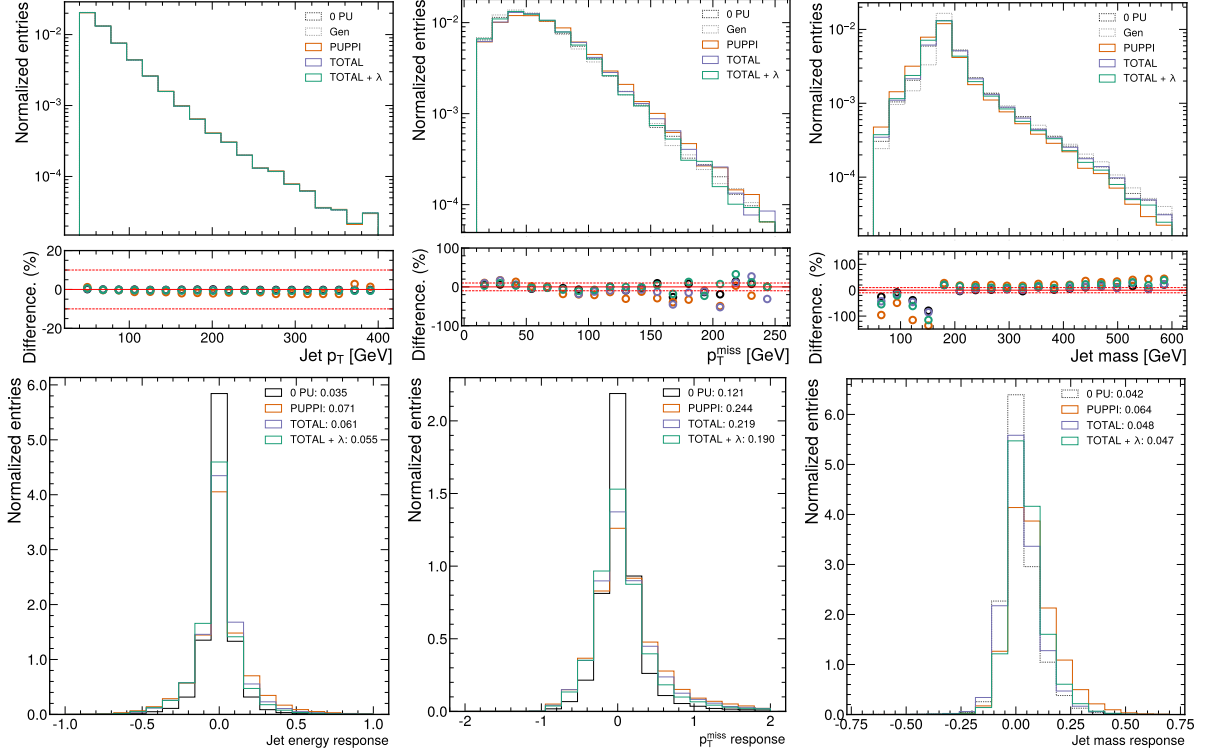


Figure A.1: Distributions of the jet p_T and missing transverse momentum p_T^{miss} for $t\bar{t}$ events and of the jet mass for Z' events (top row); and the respective response functions (bottom row). Numbers shown in the response function represent the resolution of the observable. We compare the TOTAL algorithm with (green) and without (violet) additional energy conservation, and the PUPPI algorithm (orange), with the ideal scenario of zero pileup interactions (black), and the distribution at generator level (gray). The ratio panels display the percentage difference in resolution of different algorithms compared to generator level events.

the p_T of the matched generator-level jet for Z' events. While truth labels for pileup particles are not always available, we investigate the differences in performance of the TOTAL algorithm with respect to a fully supervised network trained using the same strategy as the one used in [194]. Results are presented in the Appendix. A.5

Across the entire p_T spectrum considered, TOTAL jets are found to have a better JER than PUPPI jets, with improvements of $\sim 20\%$ at low p_T . The PUPPI parameters used for the comparison have been taken from [204]. We observe the convergence of all algorithms in the high- p_T regime, as expected due to the reduced effect of soft pileup particles in highly energetic jets. Similarly, we observe a better JER across all the considered η spectrum, with improvements of the order of 15% in the forward region of the detector ($|\eta| > 2.5$). The JER degrades in the forward region for all algorithms, due to a worse intrinsic performance of the instrumentation and higher levels of pileup. Finally, we observe a better performance in the τ_3/τ_2 variable with an improvement up to roughly 10%. The degradation of the τ_3/τ_2 resolution with increasing p_T is interpreted as the effect of particles becoming more collimated, resulting in a more challenging definition of the centers of the energy prongs. Finally, we observe that enforcing the energy conservation further improves the performance of TOTAL algorithm in all observables by up to 10%.

A robust pileup mitigation algorithm is required to show stable performance with respect to various physics processes and to the number of pileup interactions in a wide range of values, since pileup conditions can change during data-taking. To check the stability of our algorithm, we evaluate our model on W +jets events generated with a uniform distribution in the number

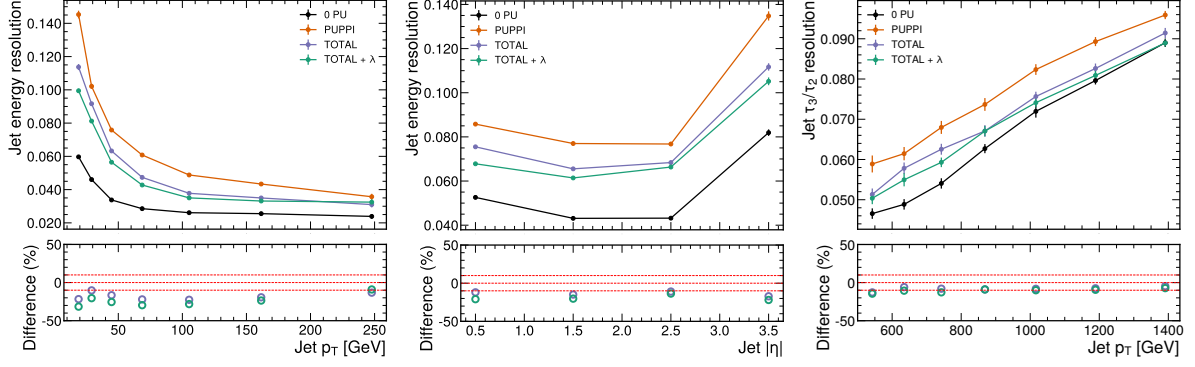


Figure A.2: JER as a function of the generator-level jet p_T for $t\bar{t}$ events (left); JER as a function of the generator-level jet η for QCD events (center); and large-radius jet τ_3/τ_2 resolution as a function of the generator-level jet p_T for $Z' \rightarrow t\bar{t}$ events (right). We compare the TOTAL algorithm with (green) and without (violet) additional energy conservation, and the PUPPI algorithm (orange) with the ideal scenario of zero pileup interactions (black). The ratio panels display the percentage difference in resolution of TOTAL compared to PUPPI.

of primary vertices, NPV, ranging from 0 to 200, and compute the JER as a function of the number of pileup interactions. In Fig. A.3, the performance of TOTAL is found to be stable and consistently better than PUPPI across the entire NPV spectrum. This testifies to the ability of the network to adapt to pileup scenarios and processes different from the ones experienced during training.

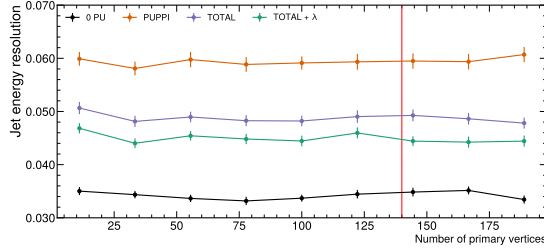


Figure A.3: Jet energy resolution as a function of the number of pileup interactions for W+jets events. We compare the TOTAL algorithm with (green) and without (violet) additional energy conservation, and the PUPPI algorithm (orange) with the ideal scenario of zero pileup interactions (black). The vertical line indicates the average number of PU collisions in the training.

Finally, to illustrate the benefit TOTAL brings to searches for new physics, we study its impact in a search for invisible Higgs boson decays, which is one of the essential search channels at the LHC. Such decays are highly suppressed in the Standard Model, rendering any observation of an enhanced decay rate an unambiguous sign for new physics. Here, the Higgs boson is assumed to be produced via the fusion of two vector bosons in association with two jets close to the beam axis. A predominant background in this search is the production (mediated by the strong interaction) of a Z boson decaying into neutrinos. In Fig. A.4, we demonstrate the improvement in significance $S/\sqrt{B}$, with S being the signal yield and B the background yield, as a function of a selection on a linear classifier constructed from p_T^{miss} and the dijet mass. We find the improvement from TOTAL to be in the order of 15% compared to PUPPI, consistent with the improvements in resolution for jets and p_T^{miss} . This would lead to a better sensitivity in the search for such decays and significantly improve the expected upper limit on the branching ratio of Higgs bosons to invisible particles quoted by the ATLAS and CMS collaborations [205, 206].

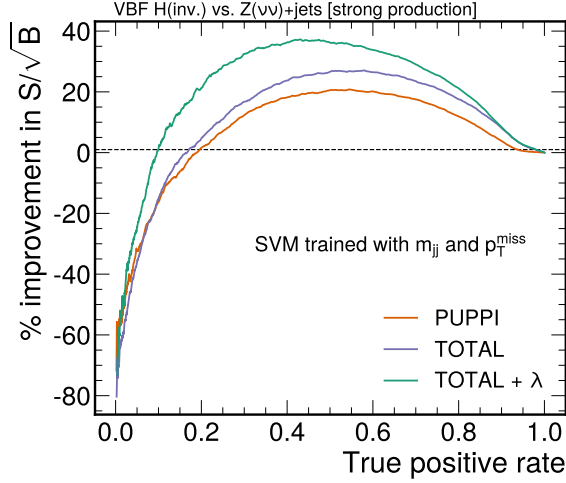


Figure A.4: A linear classifier (Support Vector Machine, SVM) trained with p_T^{miss} and the dijet mass results in a sizable improvement in $S/\sqrt{B}$ for the TOTAL algorithms over PUPPI.

A.4 Conclusions

We have presented a novel method to identify particles from the primary interaction and reject pileup particles in proton collisions at hadron colliders. Without relying on training labels, our self-supervised algorithm is able to morph an inclusive particle collection into a collection containing just the products of the primary interaction. Our algorithm provides a perspective for mitigating the impact of pileup at the High-Luminosity LHC, yielding an improvement over the current state-of-the-art of up to 25% in the resolution of key observables used in searches for new physics and in precision measurements. To the best of our knowledge, this is the first application of optimal transport concepts embedded into graph neural networks to solve a highly relevant problem of current and future particle collider experiments. Not relying on per-particle truth labels, our approach can be implemented in full-scale simulations of detectors such as ATLAS and CMS. Thus, we encourage our colleagues to test this strategy. Additionally, our approach can be applied to other problems inside and outside the field of high energy physics where de-noising is of great importance and where a realistic simulation of noise exists, even if the noise distribution is intractable. For instance, it could be used for shower reconstruction in highly granular calorimeters, or for mitigating noise in time series-based astronomical data. Future studies should focus on the expansion of the method to compare statistically independent samples with different noise levels. This would allow for a data-driven, global determination of pileup at the LHC, e.g., by comparing distributions obtained at the beginning of a given proton fill and towards the end, when less pileup is present in the data.

A.5 Appendix. Comparison with a Fully Supervised Network

The TOTAL algorithm is trained using a self-supervised setting to avoid the need of labels from human annotation that cannot perfectly be obtained in full simulation or in data. However, to compare our results with a fully supervised setting using perfect labels, which are available in the simplified reconstruction of the Delphes framework, we retrain the backbone architecture of TOTAL, ABCNET, using the same strategy presented in [194], with a regression objective that aims to learn the energy fraction of the primary collision carried by each individual particle and resulting in 0 labels for pileup interactions. Similarly, we also compare with the PUMA algorithm to check the differences in performance obtained by the use of different backbone

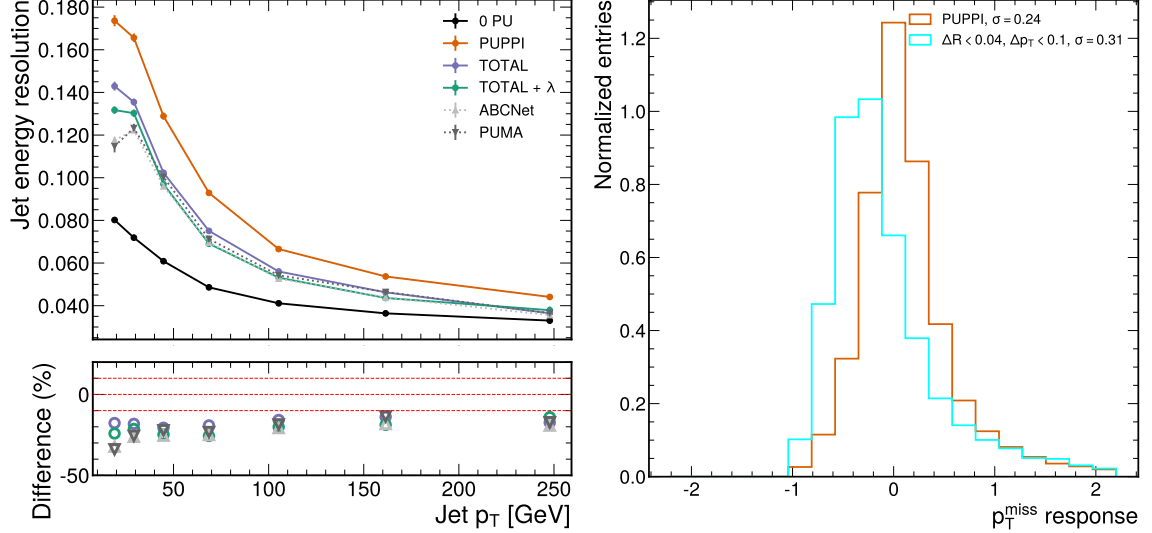


Figure A.5: Left: Jet energy resolution for QCD events as a function of the generator level p_T . We compare the TOTAL algorithm with (green) and without (violet) additional energy conservation, and the PUPPI algorithm (orange) with the ideal scenario of zero pileup interactions (black). Additional supervised results are shown for ABCNET (light gray) and PUMA (dark gray), both using unrealistic, perfect labels. Right: comparison of p_T^{miss} resolutions for PUPPI and for a human-annotation-based per-particle truth, where particles are labeled as coming from the primary interaction, if they can be matched to a particle in the same event without pileup overlaid, and from pileup otherwise. The poor resolution, when using truth definition, renders fully supervised algorithms relying on these targets inferior to our self-supervised strategy.

architectures. Results for the jet energy resolution versus the jet transverse momentum for QCD events are shown in Figure A.5. We observe the resolution obtained by TOTAL to be similar to the one obtained by the supervised training of both ABCNET and PUMA, with differences in performance below 10% in all generator level p_T intervals. Moreover, Figure A.5 demonstrates the performance of a truth definition obtained by matching (in angular separation and momentum difference) particles between the samples with and without pileup contributions to identify particles coming from the hard interaction. For the matching to be successful, particles have to be matched within $\Delta R = 0.04$ and have transverse momenta compatible within 10%. A successful matching of particles could then be used as truth labels for a fully supervised algorithm à la PUMA. However, as is visible from a comparison with even the classical benchmark PUPPI, the performance in p_T^{miss} resolution is severely degraded for such a truth definition even after cumbersome manual tuning of the matching parameters, rendering the application of fully supervised algorithms an arduous, if not impossible task, if one wants to achieve results competitive with our self-supervised approach.