



Constraints on Higgs Self-coupling via $HH \rightarrow b\bar{b}\gamma\gamma$ and Joint Interpretation of Single- and Double-Higgs Analyses Using Data Collected with ATLAS Detector at $\sqrt{s} = 13$ TeV

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DECLARATION

I hereby declare that the thesis entitled “*Constraints on Higgs Self-coupling via $HH \rightarrow b\bar{b}\gamma\gamma$ and Joint Interpretation of Single- and Double-Higgs Analyses Using Data Collected with ATLAS Detector at $\sqrt{s} = 13$ TeV*” submitted by me, for the award of the degree of *Doctor of Philosophy* to Shanghai Jiao Tong University is a record of bona fide work carried out by me under the supervision of Prof. Haijun Yang from School of Physics and Astronomy, Shanghai Jiao Tong University, and Dr. Giovanni Marchiori from APC in Paris and Université Paris Cité.

I further declare that the work reported in this thesis has not been submitted and will not be submitted, either in part or in full, for the award of any other degree or diploma in this institute or any other institute.

Place: Shanghai, China

Date: November 25, 2024

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ABSTRACT

This thesis presents measurements of the Higgs (H) boson self-coupling λ derived from a search for Higgs boson pair (HH) production in the $b\bar{b}\gamma\gamma$ final state, as well as from a joint interpretation of various searches for Higgs boson pair production and measurements of single-Higgs boson production. The measurements utilize 140 fb^{-1} of proton-proton collisions at a center-of-mass energy of $\sqrt{s} = 13 \text{ TeV}$ collected with the ATLAS detector at the Large Hadron Collider during 2015–2018. Limits are presented on the cross-section of the Higgs boson pair production, and on multiplicative modifiers of the Higgs boson self-coupling (κ_λ) and the quartic $VVHH$ ($V = W, Z$) vertex coupling (κ_{2V}). In addition, the thesis presents an optimization work of the algorithm used by the ATLAS experiment to identify photon candidates through their electromagnetic shower shapes, in order to improve the algorithm’s robustness against pile-up in the harsh environment of the LHC.

Photon identification algorithms are crucial in collider experiments to distinguish prompt photons from candidates arising from collimated photon pairs from decays of neutral mesons. These algorithms typically rely on shower shapes reconstructed with an electromagnetic calorimeter. In the ATLAS experiment at the LHC, the large level of pile-up (additional inelastic pp collisions) leads to additional energies deposited in the calorimeter that impact the shower shape distributions. In this thesis, improvements in the ATLAS photon identification algorithm are studied by optimizing the selection criteria on the shower shapes as a function of pile-up. A new set of criteria for the identification of photons is proposed that leads to significantly higher prompt photon identification at high pile-up.

The Higgs boson self-coupling induces leading-order Feynman diagrams for Higgs boson pair production in proton-proton collisions. The process $HH \rightarrow b\bar{b}\gamma\gamma$ is one of the most sensitive channels for searching Higgs boson pair production due to the clean diphoton signature and low irreducible backgrounds. Events are selected and classified in orthogonal categories with different signal-to-background ratio using machine learning techniques to distinguish signal from background. An unbinned maximum likelihood fit is performed to the diphoton invariant mass distribution of the selected events to extract constraints on the signal strength (i.e. ratio between measured and predicted values, μ_{HH}) of Higgs boson pair production and on κ_λ and κ_{2V} . No significant deviation from the expected background predicted by Standard Model processes has been observed. The observed upper limit on the signal strength of the Higgs boson pair production is $\mu_{HH} < 3.96$ at 95% confidence level (CL). The observed 95% CL constraints for the coupling modifiers are $-1.44 < \kappa_\lambda < 6.92$ and $-0.48 < \kappa_{2V} < 2.68$, where the other coupling modifiers are fixed to their SM predictions in the interpretations.

The trilinear Higgs boson vertex induced by the Higgs boson self-coupling also modifies the leading-order predictions for single-Higgs boson production cross-sections and branching ratios through next-to-leading order electroweak corrections. The Higgs boson self-coupling can thus be constrained more precisely from a joint interpretation of searches for Higgs boson pair production in various final states ($b\bar{b}\gamma\gamma$, $b\bar{b}\tau^+\tau^-$, $b\bar{b}b\bar{b}$) and of measurements of single-Higgs boson production in many decay channels ($\gamma\gamma$, WW^* , ZZ^* , $\tau^+\tau^-$, $b\bar{b}$). A crucial advantage of this approach is that single-Higgs boson data constrains the values of the modifiers of the Higgs

boson to other particles (such as to the top quark) that also affect Higgs boson pair production and that would otherwise need to be fixed to some reference value (typically the SM prediction) in the interpretation of Higgs boson pair data alone. The results of this work are as follows. The combination of searches for Higgs boson pair production in three decay channels yields an upper limit on the HH signal strength $\mu_{HH} < 2.4$ at 95% CL. The joint interpretation of single- and di-Higgs analyses constraints the Higgs boson self-coupling to $-0.4 < \kappa_\lambda < 6.3$ at 95% CL, assuming all other coupling modifiers are fixed to their SM predictions, and to $-1.4 < \kappa_\lambda < 6.1$ when the other main coupling modifiers (to top and bottom quarks, W and Z bosons and τ leptons) are floated. The results provides significant insights into the fundamental properties of the Higgs boson and its interactions, and represents an important milestone towards the observation of Higgs boson pair production and of the Higgs boson self interaction.

Keywords: Standard Model, ATLAS experiment, Higgs boson, Higgs self-coupling, Diphoton and Di-bottom quarks

TITRE

Contraintes sur l’auto-couplage du Higgs avec $HH \rightarrow b\bar{b}\gamma\gamma$ et interprétation conjointe des analyses simple- et double-Higgs à l’aide de données collectées avec le détecteur ATLAS à $\sqrt{s} = 13$ TeV

RÉSUMÉ

Cette thèse présente des mesures de l’auto-couplage du boson de Higgs (H), noté λ , obtenues à partir de la recherche de production de paires de bosons de Higgs (HH) dans l’état final $HH \rightarrow b\bar{b}\gamma\gamma$, ainsi que d’une interprétation conjointe des recherches sur la production de paires de bosons de Higgs et des mesures de production de boson de Higgs unique. Les mesures exploitent 140 fb^{-1} de collisions proton-proton à 13 TeV, recueillies par le détecteur ATLAS au LHC entre 2015 et 2018. Des limites sont présentées sur la section efficace de la production de paires de bosons de Higgs et sur les modificateurs multiplicatifs de l’auto-couplage κ_λ et du couplage quartique κ_{2V} du vertex $VVHH$ ($V = W, Z$). La thèse propose également une optimisation de l’algorithme d’identification des photons utilisé par ATLAS pour améliorer sa robustesse face au pile-up.

L’identification des photons est cruciale pour distinguer les photons prompt des paires de photons collimés issus de la désintégration de mésons neutres. Ces algorithmes s’appuient sur les formes de gerbes électromagnétiques reconstruites avec un calorimètre. Le fort pile-up dans ATLAS génère des dépôts d’énergie supplémentaires dans le calorimètre, modifiant les distributions de gerbes. Un nouveau jeu de critères d’identification des photons est proposé, augmentant la sensibilité des mesures de processus avec photons prompt.

L’auto-couplage du boson de Higgs induit des diagrammes de Feynman de premier ordre pour la production de paires de bosons de Higgs dans les collisions proton-proton. Le processus $HH \rightarrow b\bar{b}\gamma\gamma$ est l’un des plus sensibles pour cette recherche. Les événements sont classés en catégories orthogonales avec différents rapports signal/bruit de fond, utilisant des techniques d’apprentissage automatique pour distinguer le signal du bruit de fond. Un ajustement à la distribution de masse invariante des diphotons contraint la force du signal de la production de paires de bosons de Higgs ainsi que κ_λ et κ_{2V} . Aucune déviation significative par rapport au bruit de fond prévu par le Modèle Standard n’est observée. La limite supérieure observée sur la section efficace, normalisée à la prédiction du Modèle Standard, est $\mu_{HH} < 3.96$ à 95% CL. Les contraintes à 95% CL sur les modificateurs de couplage sont $-1.44 < \kappa_\lambda < 6.92$ et $-0.48 < \kappa_{2V} < 2.68$, les autres modificateurs étant fixés aux valeurs du Modèle Standard.

Le vertex trilineaire du boson de Higgs, induit par l’auto-couplage, modifie aussi les prédictions des sections efficaces de production de bosons de Higgs uniques et des rapports d’embranchement via des corrections électrofaibles. L’auto-couplage peut ainsi être mieux contraint par une interprétation conjointe des recherches sur les paires de bosons de Higgs et des mesures de production de bosons de Higgs uniques. Un avantage de cette approche est que les données sur le boson de Higgs unique contraignent les modificateurs de couplage du boson de Higgs aux autres particules, qui affectent aussi la production de paires de bosons de Higgs. Cela permet d’éviter de

fixer ces valeurs à une référence, typiquement celle du Modèle Standard, lors de l'interprétation des données de production de paires seules. La combinaison des recherches sur trois canaux de désintégration de paires de bosons de Higgs donne une limite supérieure sur la force du signal HH , $\mu_{HH} < 2.4$ à 95% CL. L'interprétation conjointe des analyses sur les bosons de Higgs uniques et les paires donne $-0.4 < \kappa_\lambda < 6.3$ à 95% CL, avec les autres modificateurs de couplage fixés à leurs valeurs du Modèle Standard, et $-1.4 < \kappa_\lambda < 6.1$ lorsque ces modificateurs sont flottants. Les résultats offrent des informations cruciales sur les propriétés fondamentales du boson de Higgs et ses interactions, et constituent une étape clé vers l'observation de la production de paires de bosons de Higgs et de l'auto-interaction du boson de Higgs.

Mots clefs : modèle standard, expérience ATLAS, boson de Higgs, interaction auto-couplée, états finaux à deux photons et à deux quarks bas

RÉSUMÉ DÉTAILLÉ

Cette thèse présente des mesures de l'auto-couplage du boson de Higgs (H), noté λ , obtenues à partir de la recherche de production de paires de bosons de Higgs (HH) dans l'état final $HH \rightarrow b\bar{b}\gamma\gamma$, ainsi que d'une interprétation conjointe des recherches sur la production de paires de bosons de Higgs et des mesures de production de boson de Higgs unique. Les mesures exploitent 140 fb^{-1} de collisions proton-proton à 13 TeV, recueillies par le détecteur ATLAS au LHC entre 2015 et 2018. Des limites sont présentées sur la section efficace de la production de paires de bosons de Higgs et sur les modificateurs multiplicatifs de l'auto-couplage κ_λ et du couplage quartique κ_{2V} du vertex $VVHH$ ($V = W, Z$). La thèse propose également une optimisation de l'algorithme d'identification des photons utilisé par ATLAS pour améliorer sa robustesse face au pile-up pour les futures phases de prise de données du LHC. Les annexes décrivent certaines contributions à la recherche et développement sur les détecteurs en vue de la future mise à niveau à haute luminosité du LHC (en particulier la fabrication de prototypes pour les détecteurs à gaz dans le cadre de la mise à niveau du détecteur à muons d'ATLAS) ainsi que pour le Circular Electron-Positron Collider (CEPC), notamment la conception et les tests de l'électronique de lecture pour un calorimètre hadronique semi-digital (SDHCAL) destiné à un détecteur du CEPC.

Atténuation de la Dépendance au Pile-up dans l'Algorithme d'Identification des Photons

L'identification des photons est essentielle pour de nombreuses analyses physiques de l'expérience ATLAS au LHC (*Large Hadron Collider*), comme les études concernant les désintégrations du boson de Higgs, la production de photon + jet, et les processus électrofaibles. L'identification des photons est basée sur un algorithme de reconstruction et de sélection qui utilise plusieurs variables de la forme du shower, extraites du calorimètre électromagnétique (*ECAL*). Ces variables sont conçues pour distinguer les photons prompts, qui proviennent directement de la collision, des photons de fond ou des jets mal identifiés comme des photons.

Le problème du Pile-up

Au LHC, chaque collision proton-proton est accompagnée de plusieurs autres collisions, appelées *pile-up*. À mesure que la luminosité augmente, le nombre d'événements de pile-up s'accroît, ce qui nuit à l'identification des photons en introduisant des dépôts d'énergie supplémentaires dans le calorimètre, rendant plus difficile la distinction entre les photons prompts et ceux de fond. Ce *pile-up* introduit du bruit dans le signal et réduit l'efficacité de l'algorithme d'identification des photons.

La sélection *tight*, utilisée dans de nombreuses analyses clés, est particulièrement sensible au pile-up. Alors que des critères de sélection plus stricts réduisent le fond, ils rendent également l'algorithme d'identification plus vulnérable aux effets du pile-up, ce qui entraîne une détérioration significative de l'efficacité d'identification des photons lorsque le pile-up augmente.

Stratégie d'Identification des Photons

Le cadre d'identification des photons dans *ATLAS* utilise des algorithmes basés sur des coupures à trois niveaux de précision :

- **Loose** : Haute efficacité mais pureté relativement faible.
- **Medium** : Un compromis entre pureté et efficacité.
- **Tight** : Haute pureté avec une efficacité plus faible.

La sélection *tight* fait usage de plusieurs *variables de la forme du shower* issues du calorimètre, telles que la distribution d'énergie dans la deuxième couche de l'ECAL et la fuite d'énergie dans le calorimètre hadronique. Ces variables sont optimisées pour des conditions avec un pile-up minimal.

Stratégies d'Atténuation de la Sensibilité au Pile-up

Afin d'atténuer la dépendance au pile-up de l'algorithme d'identification des photons *tight*, deux stratégies potentielles ont été explorées :

1. Introduire de nouvelles variables discriminantes, moins sensibles aux effets du pile-up. Ces variables permettraient d'améliorer la séparation entre le signal et le fond.
2. Ré-optimiser les critères de sélection actuels sur les variables de forme du shower déjà utilisées. Cela implique de resserrer ou d'assouplir les coupures sur des variables spécifiques afin de maintenir l'efficacité dans des conditions de pile-up élevé.

Cette thèse se concentre sur la deuxième approche : *ré-optimiser les variables actuelles*.

Ré-optimisation de l'Algorithme d'Identification des Photons

Le processus de ré-optimisation visait à réduire la dépendance au pile-up en ajustant les valeurs des coupures sur plusieurs variables clés, en particulier celles liées à la forme du shower électromagnétique. La ré-optimisation a consisté à évaluer la performance de ces variables dans différentes conditions de pile-up, dans le but de minimiser la dégradation de l'efficacité tout en préservant la capacité de rejet des photons de fond.

Résultats de l'Étude

La ré-optimisation des coupures de sélection sur les variables de forme du shower a montré les améliorations suivantes :

- **Stabilité dans différentes conditions de pile-up** : L'efficacité d'identification des photons s'est avérée plus stable, même avec un nombre moyen croissant d'interactions de pile-up. Cela est crucial pour les prochaines phases de prise de données à haute luminosité du *LHC*, où le pile-up représentera un défi majeur.
- **Amélioration de la séparation signal/fond** : En resserrant les coupures sur certaines variables de forme du shower, la séparation entre le signal (photons prompts) et le fond (jets mal identifiés) a été améliorée, notamment dans des scénarios avec un pile-up élevé.

- **Performance constante dans les analyses du Higgs** : Dans les analyses où les photons sont essentiels, telles que l'étude des désintégrations du boson de Higgs en deux photons ($H \rightarrow \gamma\gamma$), l'algorithme optimisé a montré des performances constantes en termes d'identification des photons, offrant une meilleure sensibilité pour ces analyses physiques.

Défis et Considérations Supplémentaires

Malgré les améliorations, certains défis demeurent :

- **Équilibre entre efficacité et pureté** : L'augmentation de la rigueur des critères de sélection peut entraîner des taux de rejet plus élevés pour les photons mal identifiés, mais elle pourrait également réduire l'efficacité globale pour les vrais photons prompts. Cet équilibre doit être soigneusement géré, notamment dans les analyses nécessitant une efficacité élevée.
- **Efficacité dans des conditions de pile-up extrême** : Bien que la ré-optimisation se soit révélée efficace dans les niveaux actuels de pile-up, les futures phases de prise de données du *LHC*, en particulier le *HL-LHC* (*High-Luminosity LHC*), connaîtront des niveaux de pile-up encore plus élevés. Des études supplémentaires pourraient être nécessaires pour garantir que l'algorithme reste robuste dans ces conditions.

Conclusion

Cette étude montre que l'algorithme d'identification des photons ré-optimisé améliore significativement la résistance aux effets du pile-up. En ajustant soigneusement les critères de sélection pour les variables clés de la forme du shower, l'algorithme atteint un meilleur équilibre entre efficacité et rejet des photons de fond dans des environnements à fort pile-up. Ces améliorations profiteront aux analyses futures au *LHC*, en particulier dans des conditions de haute luminosité, où le pile-up devrait être encore plus prononcé.

Les résultats de ce travail joueront un rôle essentiel dans le maintien des capacités scientifiques du détecteur *ATLAS*, garantissant que les analyses basées sur les photons restent sensibles à des processus clés comme la production du boson de Higgs et d'autres recherches de nouvelle physique.

Recherche de la production de paires de bosons de Higgs dans l'état final $b\bar{b}\gamma\gamma$

Comprendre la forme du potentiel du champ de Higgs et la nature de la rupture de symétrie électrofaible spontanée nécessite une mesure précise du modificateur de l'auto-couplage du Higgs, κ_λ . Cette mesure est essentielle pour sonder d'éventuelles nouvelles physiques affectant l'auto-interaction du champ de Higgs. L'approche la plus directe pour étudier l'auto-interaction du champ de Higgs est la production de paires de bosons de Higgs au *LHC*, principalement via les processus $ggFHH$ et $VBFHH$. De plus, $VBFHH$ sert d'excellent probe pour l'interaction au vertex $VVHH$, κ_{2V} . Parmi tous les modes de désintégration HH , l'état final $b\bar{b}\gamma\gamma$ est l'un des plus sensibles.

Stratégie d'analyse : Stratégie de référence vs Analyse alternative

Cette these présente les résultats d'une recherche de production de paires de bosons de Higgs dans l'état final à deux jets de b et diphotons, en utilisant deux stratégies d'analyse : la stratégie de référence utilisée pour la publication officielle de l'ATLAS et une stratégie alternative. Les deux stratégies utilisent des techniques d'apprentissage automatique pour classer les événements signal et bruit de fond, améliorant ainsi le rapport signal/bruit. Les résultats attendus des deux stratégies sont cohérents, tandis que les résultats observés sont dérivés de la stratégie de référence.

Résultats de l'étude

Les derniers résultats dans ce canal à 95% CL sont les suivants. Les limites supérieures observées (attendues) de la force du signal μ_{HH} sont de 3.96 (5.03) fois les prédictions du SM. La limite supérieure μ_{HH}^{VBF} est de 100 (131) fois les prédictions du SM. Le modificateur de l'auto-couplage du Higgs est contraint dans la plage $-1.44 < \kappa_\lambda < 6.92$ ($-2.84 < \kappa_\lambda < 7.82$). Le modificateur de couplage du vertex VVHH est contraint dans la plage $-0.48 < \kappa_{2V} < 2.68$ ($-1.11 < \kappa_{2V} < 3.31$). Ces résultats sont conformes aux prédictions du SM, sans excès significatif observé dans les données sous l'hypothèse de bruit de fond seul. L'incertitude dominante provient des limitations statistiques, avec des incertitudes systématiques significatives résultant des échelles de renormalisation et de factorisation, ainsi que de la résolution d'énergie des photons.

Conclusion et perspectives

Les techniques d'apprentissage automatique sont très efficaces pour distinguer les signaux des bruits de fond, et des avancées supplémentaires dans ces techniques pourraient améliorer la précision de classification. Les améliorations potentielles incluent une meilleure performance dans la sélection des jets de b et des objets photon. Une perte de rendement substantielle se produit en raison des inefficacités de sélection des jets de b , soulignant la nécessité d'améliorations dans ce domaine pour améliorer le rapport signal/bruit. De plus, des améliorations de la résolution d'énergie des photons pourraient être réalisées grâce à des algorithmes de calibration et de reconstruction raffinés. Augmenter la taille du jeu de données est la stratégie la plus efficace pour améliorer la sensibilité de la recherche de production de paires de bosons de Higgs dans ce canal, avec des prises de données dans Run-3 actuellement en cours. La luminosité intégrée ciblée sera plus du double de celle de Run-2, tandis que la future phase de haute luminosité du LHC apportera une augmentation supplémentaire d'un facteur dix de la luminosité intégrée, rendant très probable l'observation de la production de HH et la contrainte des auto-interactions du boson de Higgs.

Contraintes sur l'Auto-couplage du Boson de Higgs à partir d'Analyses Conjointes de Production de Bosons de Higgs et de Paires de Bosons de Higgs

L'étude de l'auto-couplage du boson de Higgs, représenté par le paramètre de couplage λ_{HHH} , fournit des informations essentielles sur la nature de la rupture de symétrie électrofaible.

Ce couplage contribue à la production de paires de bosons de Higgs ainsi qu'aux corrections électrofaibles dans la production de bosons de Higgs uniques. En combinant les analyses des bosons de Higgs simples et doubles, la sensibilité à ce couplage peut être considérablement améliorée. En plus d'améliorer la sensibilité, une analyse combinée permet la variation libre d'autres couplages qui influencent la production de paires de bosons de Higgs, tels que κ_t et κ_V , qui étaient auparavant fixés. Ces facteurs peuvent désormais être contraints directement par les données.

Stratégie d'analyse

Cette analyse utilise les études effectuées avec l'ensemble complet des données du Run 2 d'ATLAS, en examinant les résultats de mesures de production et désintégration d'un seul boson de Higgs ainsi que les recherches de production de paires de bosons de Higgs dans les canaux $b\bar{b}\gamma\gamma$, $b\bar{b}b\bar{b}$ et $b\bar{b}\tau^+\tau^-$. En combinant ces résultats, une compréhension plus complète de l'auto-couplage du boson de Higgs est atteinte.

L'interprétation utilise un modèle statistique basé sur l'approche de vraisemblance profilée. Les interprétations en termes d'auto-couplage du boson de Higgs sont d'abord effectuées en utilisant uniquement les mesures de production d'un seul boson de Higgs, puis uniquement des recherches de production de paires de bosons de Higgs, puis les deux au même temps. Pour la combinaison, les chevauchements possibles entre les espaces de phase sélectionnés par les différentes analyses sont étudiés en détail, ainsi que le modèle statistique de corrélation entre les incertitudes systématiques dans différentes analyses.

Résultats de l'étude

Les principaux résultats sont les suivants :

- pour la combinaison des mesures de production du boson de Higgs, les valeurs d'ajustement optimales observées (attendues) de κ_λ sont $2.497^{+4.595}_{-3.941}$ ($0.963^{+7.048}_{-3.816}$). Les intervalles de confiance unidimensionnels CL à 68% et 95% pour κ_λ sont respectivement $[-1.4, 7.1]$ ($[-2.8, 8.0]$) et $[-4.0, 10.3]$ ($[-5.2, 11.5]$). Les résultats sont cohérents avec les prédictions SM.
- la combinaison des résultats des recherches de production de paires de boson de Higgs, notamment dans les états finaux $b\bar{b}\gamma\gamma$, $b\bar{b}b\bar{b}$ et $b\bar{b}\tau^+\tau^-$, mènent à des limites supérieures observées et attendues de la section efficace HH respectivement de 78.48 et 94.83 fb à 95% CL. Les résultats indiquent qu'aucun excès significatif n'est observé dans les données par rapport au bruit de fond attendu.

Des analyses la fonction de vraisemblance profilée sont effectuées pour déterminer les contraintes attendues et observées à 68% et 95% CL pour κ_λ et κ_{2V} . Deux minima locaux pour la fonction de vraisemblance profilée attendu en fonction de κ_λ sont observés en raison des effets d'interférence entre divers diagrammes de Feynman contribuant à la production de HH . Ces processus contraignent κ_λ à $-0.6 < \kappa_\lambda < 6.6$ et κ_{2V} à $0.1 < \kappa_{2V} < 2.0$ à 95% CL, lorsque les autres modificateurs de couplage sont fixés à l'unité. La valeur d'ajustement optimale observée de $(\kappa_\lambda, \kappa_t)$ est (1.22, 0.13). La combinaison HH fournit

des contraintes plus strictes sur κ_λ que le Higgs simple mais des contraintes beaucoup plus lâches sur κ_t . En particulier, la sensibilité des données expérimentales à κ_t diminue à des valeurs plus élevées. La valeur d'ajustement optimale de (κ_V, κ_{2V}) est observée comme étant (0.33, 0.06).

- l'interprétation conjointe des deux analyses conduit aux contraintes les plus fortes, maximisant la sensibilité à λ_{HHH} . Dans l'ensemble, ces résultats montrent que les données observées sont cohérentes avec les prédictions de SM dans le niveau actuel d'incertitude. À 95% CL, les contraintes observées (attendues sous l'hypothèse SM) pour la combinaison sont $-0.4 < \kappa_\lambda < 6.3$ ($-1.9 < \kappa_\lambda < 7.6$) lorsque les autres modificateurs de couplage sont fixés à un, principalement déterminés par l'analyse di-Higgs. La valeur de meilleur ajustement de κ_λ est $3.0^{+1.8}_{-1.9}$. Lorsque les autres modificateurs de couplage sont profilés, la plage autorisée observée (attendue) pour κ_λ à 95% CL est $-1.4 < \kappa_\lambda < 6.1$ ($-2.2 < \kappa_\lambda < 7.7$). Comme prévu, le modèle générique fournit des contraintes plus lâches sur κ_λ par rapport au modèle avec seulement κ_λ flottant en raison du plus grand nombre de degrés de liberté autorisés à flotter dans l'ajustement. Cependant, l'effet est plutôt faible. En plus de contribuer à la sensibilité à κ_λ , l'analyse de Higgs unique permet des hypothèses plus souples concernant les autres modificateurs de couplage de Higgs. En raison des contraintes strictes sur κ_t issues des mesures de Higgs simples, les ajustements avec κ_t fixé à la valeur SM ou profilé en fonction des données produisent des contraintes similaires sur κ_λ , dès que les données de Higgs simples sont incluses. Fixer les autres couplages à l'unité ou les profiler a peu d'impact dans ce cas.

R&D détecteurs

Chambres à plaques résistives en verre pour le future système à muons d'ATLAS

Dans le futur, le détecteur ATLAS sera amélioré pour faire face à la luminosité instantanée plus élevée et aux doses accrues fournies par la phase de haute luminosité du LHC (HL-LHC), qui commencera vers 2030, après un long arrêt suivant la fin de Run-3. Le HL-LHC fournira dix fois plus de données que les précédentes périodes de fonctionnement du LHC, augmentant considérablement le potentiel physique du LHC. Pour le HL-LHC, le spectromètre à muons du détecteur ATLAS subira une mise à niveau majeure, incluant le remplacement des chambres à muons et de l'électronique de déclenchement et de lecture.

Durant ma thèse de doctorat, j'ai contribué à la R&D des prototypes pour les détecteurs à gaz (chambres à plaques résistives en verre, GRPC) dans le cadre de la mise à niveau du détecteur à muons d'ATLAS. Des GRPCs ont été fabriqués et simulés avec différentes structures et tailles, et leur efficacité a été testée à l'aide des rayons cosmiques.

Mécanisme des Chambres à Plaques Résistives

Les chambres à plaques résistives (RPCs) sont des détecteurs gazeux largement utilisés en physique des hautes énergies, en particulier pour la détection de muons et de rayons cosmiques, grâce à leur excellente résolution temporelle et leur faible coût. Typiquement, un RPC se compose de deux plaques résistives parallèles séparées par un mélange de gaz, comme l'argon,

le fréon et l'iso-butane. Lorsqu'une particule chargée traverse la chambre, elle ionise le gaz, produisant des paires électron-ion, qui sont détectées sous un champ électrique élevé.

Simulation du Flux de Gaz

Une simulation du flux de gaz a été réalisée pour optimiser la distribution uniforme du mélange de gaz dans la chambre GRPC. La simulation a utilisé des modèles de dynamique des fluides numérique (CFD) pour analyser les motifs d'écoulement, les variations de pression et la distribution des gaz en fonction de différentes configurations d'entrée et de sortie. Les résultats ont montré qu'un flux de gaz optimisé assurait une ionisation uniforme et réduisait les zones mortes, améliorant ainsi les performances du détecteur. L'étude a également identifié la conception d'entrée de gaz la plus efficace, générant le moins de turbulence et maintenant un échange de gaz stable dans la chambre, ce qui a conduit à une efficacité de détection plus uniforme sur l'ensemble de la surface du détecteur.

Performances et Résultats

Les GRPCs subissent un processus de formation de haute tension, où la tension est progressivement augmentée de 2 kV à 8 kV pour conditionner les chambres à un fonctionnement efficace. La courbe courant-tension (IV) d'une chambre GRPC de $35 \times 50 \times 0.12 \text{ cm}^2$ montre des niveaux de courant stables dans la plage de 6 kV à 8 kV, mais au-delà de 8 kV, la chambre approche de la défaillance, entraînant une augmentation importante du courant.

Les résultats de détection des muons cosmiques ont indiqué une amplitude de signal d'environ 10 mV avec un temps de montée dans la plage des nanosecondes. L'efficacité du détecteur, définie comme le rapport entre les muons détectés et les muons passant les deux scintillateurs, a augmenté avec des tensions plus élevées, atteignant plus de 95% d'efficacité à 7 kV.

Conception d'un système de lecture électronique à synchronisation rapide pour un calorimètre hadronique semi-digital pour CEPC

À plus long terme, le Circular Electron-Positron Collider (CEPC) est un collisionneur de particules à haute énergie proposé pour être construit en Chine. Le CEPC est conçu pour faire entrer en collision des électrons avec des positrons à des énergies très élevées (environ 240 GeV), offrant une plateforme pour la recherche avancée en physique des particules. Les principaux objectifs du CEPC incluent l'étude des propriétés du boson de Higgs, l'exploration des particules et forces fondamentales de l'univers, et l'amélioration de notre compréhension des lois fondamentales de la nature, avec un niveau de précision sans précédent. La construction et l'exploitation du CEPC devraient contribuer de manière significative aux connaissances de la communauté scientifique mondiale en physique des particules.

Un calorimètre hadronique semi-digital (SDHCAL) a été conçu pour l'un des détecteurs proposés du CEPC, et testé avec des faisceaux au CERN. Dans le SDHCAL, l'information temporelle sera exploitée pour discriminer les gerbes de hadrons neutres de celles des hadrons chargés. Pour cette raison, des chambres multi-plaques résistives (MRPC), avec une meilleure résolution temporelle, sont utilisées à la place de chambres RPC simples, ainsi que de l'électronique rapide.

Dans le cadre de cette thèse, la carte électronique de lecture frontale (FEB) utilisant la puce ASIC *PETIROC2B* de OMEGA et la carte d'interface (DIF) ont été conçues et testées. La version préliminaire du système d'acquisition de données (DAQ) a été développée sur la base

de la carte FPGA ZCU102 de Xilinx avec une logique programmable (PL) et un système de traitement (PS). En combinant la FEB et le DAQ, la chaîne complète de mesure des informations temporelles provenant des RPC a été mise en œuvre et testée en injectant un signal depuis le générateur.

Cette these fournit une analyse détaillée de la carte d'interface numérique (DIF) et de ses sous-systèmes, incluant l'alimentation, la distribution d'horloge et les performances temporelles.

Structure du DIF

La carte DIF est composée de 8 couches, conçues pour assurer l'intégrité du signal, une bonne mise à la terre et une distribution efficace de la puissance. Les couches supérieure et inférieure sont des plans en cuivre pour le routage des signaux, tandis que les couches intermédiaires incluent des plans d'alimentation et de masse, fabriqués en matériau FR-4 pour l'isolation. Les plans de masse (GND1, GND2, GND3) aident à réduire le bruit et les interférences électromagnétiques (EMI), assurant une transmission stable des signaux.

Architecture d'Alimentation

L'architecture de l'alimentation utilise le convertisseur DC-DC LTM4644 pour fournir une alimentation stable et régulée au système, délivrant jusqu'à 4A par canal avec un total de quatre canaux. Il fournit du 3.3V et du 2.5V à différents sous-systèmes comme l'ASIC PETIROC, avec une régulation supplémentaire pour des composants spécifiques comme le nettoyeur de gigue (Si5345) à 1.8V. Des domaines d'alimentation analogiques et numériques séparés minimisent le bruit entre domaines, améliorant ainsi les performances du système.

Distribution d'Horloge

Le système de distribution d'horloge est contrôlé par le nettoyeur de gigue Si5345, qui garantit des signaux d'horloge précis et stables. Le système fonctionne avec une horloge de 40 MHz, distribuée à divers sous-systèmes, assurant un minimum de gigue et de bruit.

Génération d'Impulsions et Performances Temporelles

Les performances temporelles du système ont été testées avec une impulsion de 20 kHz, avec un temps de montée de 1 μ s et un temps de descente de 2 ns, avec un cycle de service de 95%. La résolution temporelle a été évaluée via des coups voisins et des coups en coïncidence, atteignant une résolution de 50 ps RMS pour les coups voisins et de 75 ps pour les coups en coïncidence. La résolution temporelle intrinsèque du système a été estimée à environ 36 ps, indiquant une résolution temporelle meilleure que 100 ps, validant ainsi la performance du PETIROC2B.

Plans Futurs

Les prochaines étapes incluent la conception d'une carte frontale (FEB) de plus grande taille pour les chambres à plaques résistives à multi-fentes (MGRPCs) et le développement supplémentaire du système d'acquisition de données pour le Time-SDHCAL.

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INTRODUCTION

The Standard Model (SM) represents the essence of the current human comprehension of the natural world at the microscopic level. The discovery of the Higgs Boson in 2012 by the ATLAS and CMS experiments with the data from the Run-1 (2011–2012) of the Large Hadron Collider marked a pivotal moment for particle physics, with all fundamental particles predicted by the SM finally observed in collider experiments. Since then, many of the Higgs properties have been well studied, and found in agreement with the SM predictions. However, one of the key features of the Higgs sector of the SM, the shape of the Higgs potential and the related Higgs self-coupling, remains unknown. This thesis focuses mainly on constraining the Higgs boson self-coupling through the search for Higgs boson pair production in the $b\bar{b}\gamma\gamma$ final state, and from the combination between searches of Higgs boson pair production and measurements of single Higgs boson production. The full Run-2 data collected with ATLAS detector during 2015-2018 at the LHC was used.

Additional properties of the Higgs boson that are currently tested with low precision are the branching ratios of its rarest decays, such as that to the $Z\gamma$ final state. Recently, evidence for this decays by combining ATLAS and CMS searches with the full LHC Run-2 data was obtained. In the context of this thesis, some preparatory work was performed to improve the acceptance and sensitivity of the analysis in view of the LHC Run-3 data taking (2022–2025).

In Run-3 the number of additional inelastic (pile-up) collisions between protons accelerated by the LHC taking place at the same time as the interaction of interest is significantly larger than in the two previous runs. The efficiency of the photon identification algorithms used by ATLAS is thus significantly degraded, as additional energy from pile-up modifies the distribution of the shower shape variables reconstructed in the ATLAS electromagnetic calorimeter and used to discriminate prompt photons from background photons for instance from decays of neutral pions. To maintain a high prompt photon efficiency with good background rejection, needed for both searches of Higgs decays to $Z\gamma$ and photon pairs, the photon identification algorithm was re-optimized during this thesis, mitigating significantly the impact from pile-up.

In the future, the ATLAS detector will be upgraded in order to cope with the higher instantaneous luminosity and dose provided by the high-luminosity phase of the LHC (HL-LHC) that will start around 2030, after a long shutdown following the end of Run-3. The HL-LHC will deliver ten times more data than the previous LHC runs, increasing significantly the physics potential of the LHC. For the HL-LHC the muon spectrometer of the ATLAS detector will undergo a major upgrade, including replacements of the muon chambers and of the trigger and readout electronics. During my Ph.D. thesis I contributed to the fabrication of prototypes for the gas detectors for ATLAS Muon detector upgrade.

On a longer timescale, the Circular Electron-Positron Collider (CEPC) is a high-energy particle collider proposed to be built in China. The CEPC is designed to collide electrons with positrons at very high energies (240 GeV), providing a platform for advanced research in particle physics. The primary goals of the CEPC include studying the properties of the Higgs boson, exploring the fundamental particles and forces in the universe, and advancing our understanding of the fundamental laws of nature, with an unprecedented level of accuracy. The construction

and operation of the CEPC are expected to contribute significantly to the global scientific community’s knowledge in particle physics. A semi-digital hadronic calorimeter (SDHCAL) was designed for one of the proposed CEPC detectors, and tested with beams at CERN. In SDHCAL, timing information will be exploited to discriminate showers of neutral hadrons from those of charged hadrons. For this reasons, multi-resistive plate chambers (MRPC) with better time resolution are used instead of single RPC, together with fast electronics. In the context of this thesis, the front-end readout electronics board (FEB) using the ASIC chip *PETIROC2B* from OMEGA and the interface board (DIF) are designed and tested. The preliminary version of data acquisition system (DAQ) is developed on basis of Xilinx FPGA ZCU102 with programmable logic (PL) and processing system (PS). Combining the FEB and the DAQ, the full-chain of measuring the time information from RPC is implemented and tested through injecting a signal from the generator.

The thesis is organized as follows. In chapter 1, the Standard Model and the Higgs boson are described. In chapter 2, the LHC and the ATLAS detector are introduced. In chapter 3, the reconstruction of particle candidates with the ATLAS detector is presented. Chapter 4 describes the work that I performed to re-optimize the photon identification algorithm to mitigate the impact of pile-up on its efficiency and background rejection. The new photon identification “tight” working point provides a photon identification efficiency that does not decrease at large pile-up, while maintaining an acceptable level of background photon rejection. In chapter 5, the search for Higgs boson pair production with the full ATLAS Run-2 data in the $b\bar{b}\gamma\gamma$ final state is detailed. This is one of the most sensitive channels to Higgs boson pair production. Constraints are set on both the Higgs boson self-coupling and the quartic coupling between two Higgs bosons and two vector bosons (W or Z). The results from the baseline analysis are reported. The chapter also outlines the innovative event selection strategy I proposed, which differs from the baseline approach, showing a promising prospects. The systematic and theoretical uncertainties I contributed to the analysis are thoroughly examined. Additionally, the final statistical interpretations I made are detailed within the chapter. In chapter 6, a combination of direct constraints on the Higgs boson self-coupling from searches of Higgs boson pair production with indirect constraints from single Higgs boson measurements arising from electroweak next-to-leading order corrections is performed. The correlation schemes of the systematic uncertainties are studied between single Higgs and double Higgs and helped prepare the implementation tool. The fitted results from the combined workspace are displayed. Finally, chapter 7 provides concluding remarks and an outlook to the future. Appendix A focuses on the fabrication of prototypes for the gas detectors for ATLAS Muon Phase-II Upgrade. Appendix B describes the hardware and the design and tests of its readout electronics for the SDHCAL for CEPC. Appendix C is devoted to the search for the rare Higgs boson decay to $Z\gamma$ and the work performed to improve its sensitivity with the analysis of ATLAS Run-3 data.

C H A P T E R

Standard Model of Particle Physics and Higgs Boson Phenomenology at the LHC

The intrinsic nature of the universe and the laws that govern it have long stimulated human curiosity and propelled investigations into the natural world. This culminated in the Standard Model of particle physics, a monumental achievement grounded in quantum mechanics and special relativity, which illuminates the microscopic structure of matter and its interactions. This chapter aims to outline the theoretical foundations of the Standard Model, with a particular emphasis on Higgs physics and double Higgs processes at the Large Hadron Collider, which are the main subjects of investigation of this thesis.

1.1 Standard Model Theory

The Standard Model (SM) represents the modern understanding of the fundamental particles and forces that constitute the universe and their interactions in the natural world [1, 2]. Developed during the 1970s and 1980s, the Standard Model is based on quantum field theory (QFT) and special relativity, and its validity has been confirmed through numerous experiments. It is a comprehensive framework categorizing all known elementary particles into “families” with similar properties, and describing three fundamental forces between these particles (electromagnetic, weak, and strong interactions) – all the fundamental interactions that seem to govern the universe at the microscopic scale, where the fourth one, gravity, not explained by the SM, plays a negligible role. Its development unfolded over the second half of the 20th century, propelled by the collaborative efforts of many scientists, with the final formulation receiving a crucial experimental validation by the discovery of W and Z bosons (1983) [3]. Subsequent observations of the top quark (1995) [4], tau neutrino (2000) [5], and Higgs boson (2012) [6, 7] have further substantiated the Standard Model.

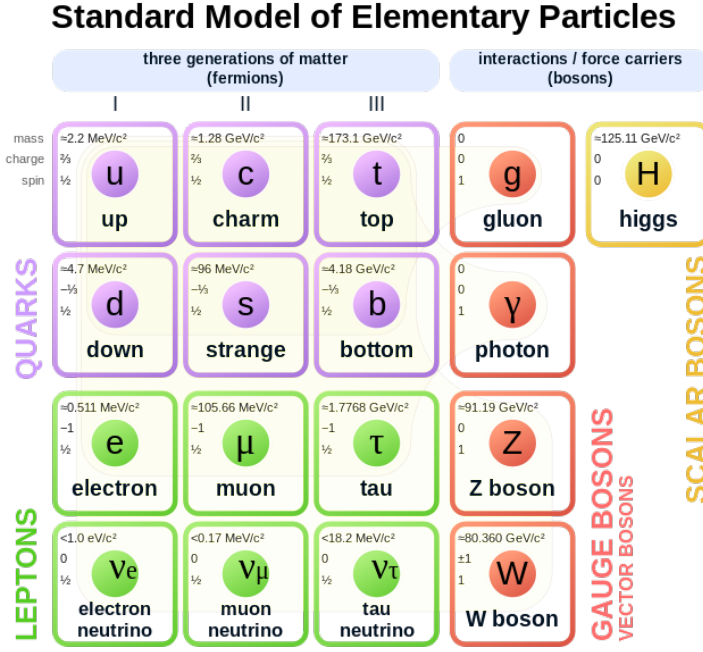


Fig. 1.1 The elementary particles in the standard model. Fermions and bosons with their mass, charge and spin are shown. Credits: [Particle Data Group](#).

The Standard Model is a quantum field theory based on the gauge symmetry group $SU(3)_C \otimes SU(2)_L \otimes U(1)_Y$, which is the direct product of the color group $SU(3)_C$ and the electroweak group $SU(2)_L \otimes U(1)_Y$. The $SU(3)_C$ group corresponds to the gauge symmetry of Quantum Chromodynamics (QCD), which describes the strong interaction between quarks and gluons. The $SU(2)_L \otimes U(1)_Y$ group corresponds to the gauge symmetry of the electroweak interaction, which is the unified theory of electromagnetic and weak interactions. The SM Lagrangian can be expressed as

$$\mathcal{L}_{SM} = \mathcal{L}_{EW} + \mathcal{L}_{QCD} + \mathcal{L}_{Higgs} + \mathcal{L}_{Yukawa} \quad (1.1)$$

$\mathcal{L}_{EW}$ is the Lagrangian of the electroweak interactions (EW), $\mathcal{L}_{QCD}$ is the Lagrangian of the strong interactions (QCD), $\mathcal{L}_{Higgs}$ is the Higgs Lagrangian and $\mathcal{L}_{Yukawa}$ characterizes the interactions of the Higgs field with the elementary fermions. The various terms are described in the following: the EW and QCD Lagrangians in Section 1.1.2, while the other two terms in Section 1.1.3.

1.1.1 Elementary Particles and Mediators

In the SM, the elementary particles are divided into two categories: fermions and bosons, which are distinguished by their spin quantum number and the statistics that they obey. All the identified elementary particles in the SM are summarized in Figure 1.1.

The elementary fermions have half-integer spin ($\frac{1}{2}$) and obey the Fermion-Dirac statistics. They are the building blocks of matter. The fermions are further divided into two categories: quarks (u, d, c, s, t, b) and leptons ($e^-, \nu_e, \mu^-, \nu_\mu, \tau^-, \nu_\tau$). Both of them are categorized into

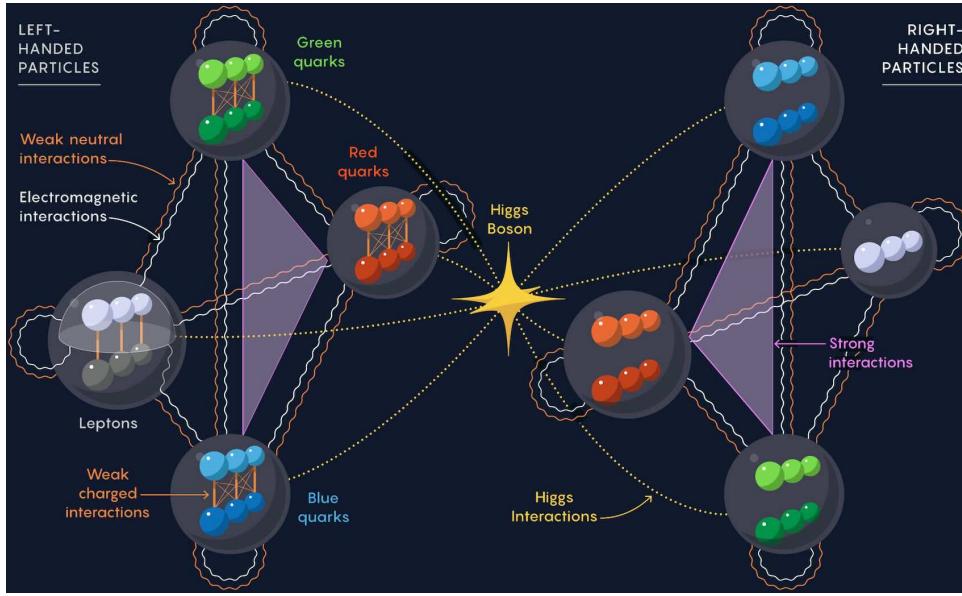


Fig. 1.2 The interaction map between the fundamental particles in the standard model.
Credits: [Quanta Magazine](#).

three generations, which are identical in their quantum numbers but differ in their masses. The quarks carry electric and color charge and are the constituents of hadrons via strong interaction, while the leptons are the elementary matter particles that do not participate in the strong interaction. The weak interaction is *chiral*: only the left-handed fermions and right-handed anti-fermions participate in the weak interaction. In SM, neutrinos are massless and only left-handed.

The elementary bosons have integer spin and follow the Bose-Einstein statistics. They are the carriers (or mediators) of the fundamental forces between the elementary particles. The massless photon (γ) mediates the electromagnetic interaction, massive vector bosons ($W^\pm$ and Z^0) carry the weak interaction, and gluons (g) are responsible for the strong interaction. They all have spin equal to one. There are eight gluons in the QCD, which are massless and carry the color charge (*red, green, blue*). Finally, a hypothesized graviton (G) with integer spin (2) would be the mediator of the gravitational force.

The Higgs boson is the only elementary scalar particle (boson with spin equal to zero) in the SM. It is responsible for the mass generation of the elementary particles through the Higgs mechanism. In a nutshell, the interaction map between the fermions and bosons is shown in Figure 1.2.

1.1.2 Electroweak and Quantum Chromodynamics

The electromagnetic interactions are described by the quantum electrodynamics theory (*QED*). The weak interactions, responsible for nuclear reactions such as beta decays of radioactive elements and fusion of nuclei in the core of the stars, were first described by Fermi with an effective Lagrangian approach, as a contact interaction. In the SM, these two forces are encompassed within a unified “electroweak” theory, developed during the 1960s. The elec-

electroweak interaction corresponds to the $SU(2)_L \otimes U(1)_Y$ symmetry group [8–10]. In Equation 1.1, the electroweak Lagrangian can be written as the sum of gauge boson and fermion terms as:

$$\mathcal{L}_{EW} = \mathcal{L}_{\text{gauge}} + \mathcal{L}_{\text{fermion}} \quad (1.2)$$

where $\mathcal{L}_{\text{gauge}}$ and $\mathcal{L}_{\text{fermion}}$ are as follows.

Gauge Term: The gauge term describes the propagation of the gauge bosons and their interactions. The Lagrangian can be expressed as:

$$\mathcal{L}_{\text{gauge}} = -\frac{1}{4}W_{\mu\nu}^a W_a^{\mu\nu} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} \quad (1.3)$$

where $W_{\mu\nu}^a$ ($a = 1, 2, 3$) stands for the field strength tensors of the $SU(2)_L$ gauge group and $B_{\mu\nu}$ is the field strength tensor of the $U(1)_Y$ gauge group:

$$W_{\mu\nu}^a = \partial_\mu W_\nu^a - \partial_\nu W_\mu^a - g\varepsilon_{abc}W_\mu^b W_\nu^c \quad (1.4)$$

$$B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu \quad (1.5)$$

In these equations, the contributions comprising the partial derivatives represent the kinetic term, while the last term in Equation 1.5 is the self-interaction term of the gauge bosons. There, g means the gauge interaction coupling constant of $SU(2)_L$ and ε_{abc} is the anti-symmetric Levi-Civita tensor.

Fermions Term: The fermion term describes the propagation of the fermions and their interactions with the gauge bosons. The fermion fields (ϕ) can be divided into left-handed (ϕ_L) and right-handed (ϕ_R) components, which are the eigenstates of the chirality operator γ^5 :

$$\begin{aligned} \phi_L &= \frac{1}{2}(1 - \gamma^5)\phi, \\ \phi_R &= \frac{1}{2}(1 + \gamma^5)\phi. \end{aligned} \quad (1.6)$$

In the EW theory of SM, the left-handed fermions are weak-isospin doublets ψ_L , while the right-handed fermions are singlets ψ_R . The neutrinos are massless and only left-handed, while right-handed neutrinos are not included in the SM:

$$\begin{aligned} \psi_L &= \begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L, \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}_L, \quad \psi_R = e_R, \mu_R, \tau_R \\ \psi_L &= \begin{pmatrix} u \\ d \end{pmatrix}_L, \begin{pmatrix} c \\ s \end{pmatrix}_L, \begin{pmatrix} t \\ b \end{pmatrix}_L, \quad \psi_R = u_R, d_R, c_R, s_R, t_R, b_R \end{aligned} \quad (1.7)$$

The Lagrangian for free fermions, ignoring interactions with gauge bosons and the Higgs field, can be written as:

$$\mathcal{L}_{\text{free, fermion}} = \bar{\psi}_L i\gamma^\mu \partial_\mu \psi_L + \bar{\psi}_R i\gamma^\mu \partial_\mu \psi_R \quad (1.8)$$

In order to maintain the gauge invariance of the theory, the partial derivative ∂_μ of the free fermion field Lagrangian $\bar{\psi}i\gamma^\mu \partial_\mu \psi$ in Equation 1.8 is replaced by a covariant derivative D_μ , which is the partial derivative plus the gauge boson fields:

$$\begin{aligned} D_{L,\mu} &\equiv \partial_\mu + ig' \frac{Y}{2} B_\mu + ig \frac{\vec{\sigma}}{2} \cdot \vec{W}_\mu \\ D_{R,\mu} &\equiv \partial_\mu + ig' \frac{Y}{2} B_\mu \end{aligned} \quad (1.9)$$

Here, g and g' are the gauge coupling constants of weak-isospin and hypercharge (Y), while $\vec{\sigma}$ are the Pauli matrices.

The fermion Lagrangian thus becomes:

$$\mathcal{L}_{\text{fermion}} = \bar{\psi}_L i\gamma^\mu D_{L,\mu} \psi_L + \bar{\psi}_R i\gamma^\mu D_{R,\mu} \psi_R \quad (1.10)$$

With respect to the Lagrangian describing the free propagation of fermions, there appears an additional Lagrangian term that describes the interaction between the fermions and four massless W and B fields, that are the gauge bosons associated with the $SU(2)_L$ and $U(1)_Y$ gauge groups, respectively:

$$\mathcal{L}_{\text{EW, interaction}} = \bar{\psi}_L \gamma^\mu \left(g W_\mu^a \frac{\sigma^a}{2} + g' B_\mu \frac{Y}{2} \right) \psi_L + \bar{\psi}_R \gamma^\mu g' B_\mu \frac{Y}{2} \psi_R \quad (1.11)$$

After electroweak symmetry breaking, as shown in Section 1.1.3, these will give rise to the weak and electromagnetic interactions.

QCD Term: Quantum chromodynamics is the gauge field theory of the strong interaction of quarks and gluons. The non-Abelian, i.e. non-commutative, $SU(3)_C$ symmetry group acts on the colored quark triplets and introduces eight colored force carrier, the *gluons*, that interact with the quarks and with themselves. The leptons are colorless and do not participate in the strong interaction. The Lagrangian of the free quarks, omitting the mass term, would be:

$$\mathcal{L}_{\text{free quark}} = \bar{\psi}_i i\gamma^\mu \partial_\mu \psi_i, \quad (1.12)$$

where ψ_i is the quark field and ∂_μ is the partial derivative with respect to the spacetime coordinates, representing the kinetic term. To make the Lagrangian gauge-invariant under $SU(3)$ transformation, the partial derivative is replaced with a covariant derivative D_μ :

$$D_\mu \equiv \partial_\mu - ig_s T^a G_\mu^a. \quad (1.13)$$

Here, g_s is the strong coupling constant, $T^a = \lambda^a/2$ indicates the eight generators of the $SU(3)$ group known as Gell-Mann matrices, and G_μ^a is the gluon field. The QCD interaction between quarks and anti-quarks with gluons is described by the term:

$$\mathcal{L}_{\text{QCD, interaction}} = -\frac{g_s}{2} \bar{\psi} \lambda_a \gamma^\mu G_\mu^a \psi \quad (1.14)$$

The gluon field strength tensor $G_{\mu\nu}^a$ consists of the kinetic term and the self-interaction term of the gluons, is given by:

$$G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a - g_s f^{abc} G_\mu^b G_\nu^c \quad (1.15)$$

Finally, the QCD Dirac Lagrangian can be written as:

$$\mathcal{L}_{QCD} = \bar{\psi} i\gamma^\mu D_\mu \psi - \frac{1}{4} G_a^{\mu\nu} G_{\mu\nu}^a \quad (1.16)$$

1.1.3 Electroweak Spontaneous Symmetry Breaking

In the Lagrangian of the EW theory (Equations 1.3, 1.10, and 1.16), the mass terms of the gauge bosons and of the fermions cannot be introduced because they are not $SU(2)$ gauge invariant. This is inconsistent with the experimental observation that weak bosons, quarks and charged leptons are massive. In 1964, Peter Higgs, Robert Brout, and François Englert proposed a solution to this problem through the spontaneous breaking of the electroweak symmetry via a process known as *BEH mechanism* or *Higgs mechanism* [11, 12]. The electroweak spontaneous symmetry breaking (EWSSB) is the cornerstone of the SM, leading to a decoupling of EW and Higgs interactions, massive EW bosons and fermion mass terms. The Higgs mechanism is associated with the presence of the Higgs field, which permeates space. As particles interact with this field, they experience resistance, akin to moving through a medium, resulting in the manifestation of mass. The Higgs field is a complex scalar doublet expressed as:

$$\Phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix} \quad (1.17)$$

where ϕ^+ and ϕ^0 are the charged and neutral components of the Higgs field.

Higgs Term: the Higgs Lagrangian can be written as:

$$\mathcal{L}_{Higgs} = T(\Phi) - V(\Phi) = (D_\mu \Phi)^\dagger (D^\mu \Phi) - V(\Phi), \quad (1.18)$$

where D_μ is the covariant derivative and $V(\Phi)$ is the Higgs potential, which are given by:

$$D_\mu \equiv \partial_\mu + ig \frac{\vec{\sigma}}{2} \cdot \vec{W}_\mu + ig' \frac{Y}{2} B_\mu$$

$$V(\Phi) = -\mu^2 \Phi^\dagger \Phi + \lambda (\Phi^\dagger \Phi)^2 = -\frac{1}{2} \mu^2 \left(\sum_{i=1}^4 \phi_i^2 \right) + \frac{1}{4} \lambda \left(\sum_{i=1}^4 \phi_i^2 \right)^2. \quad (1.19)$$

Here, $\vec{\sigma}$ represents Pauli matrices, μ^2 is the mass term and λ is the self-interaction coupling constant. The condition $\lambda > 0$ is necessary to ensure the stability of the potential. Such potential is invariant under $SU(2) \otimes U(1)$ and renormalizable. In the case of $\mu^2 \leq 0$, the potential will have a minimum value at zero doublet, which is invariant under the symmetry of the Lagrangian. For $\mu^2 > 0$, the potential has a set of equivalent states for which it is minimum: all doublets with norm $\langle 0 | \phi | 0 \rangle = \sqrt{\mu^2 / \lambda} = 246.2 \text{ GeV}/c^2$, called *Vacuum Expectation Value* (VEV). However, the Universe will be in just one of these equivalent minimum states, effectively breaking the electroweak symmetry. The VEV defines the electroweak scale, which is the energy scale at which the electroweak symmetry breaking occurs. In general, the possible shape of the Higgs potential is shown in Figure 1.3.

The scalar sector Lagrangian, as presented in Equation 1.18, can be expanded around its ground state, i.e. one of the equivalent minima of the potential. This expansion involves the radial degree of freedom, multiplied by an exponential that incorporates the generators of the broken gauge symmetry. The Higgs field is then:

$$\Phi = \frac{1}{\sqrt{2}} e^{i \frac{\sigma_i}{2} \theta^i(x)} \begin{pmatrix} 0 \\ v + h \end{pmatrix}, \quad (1.20)$$

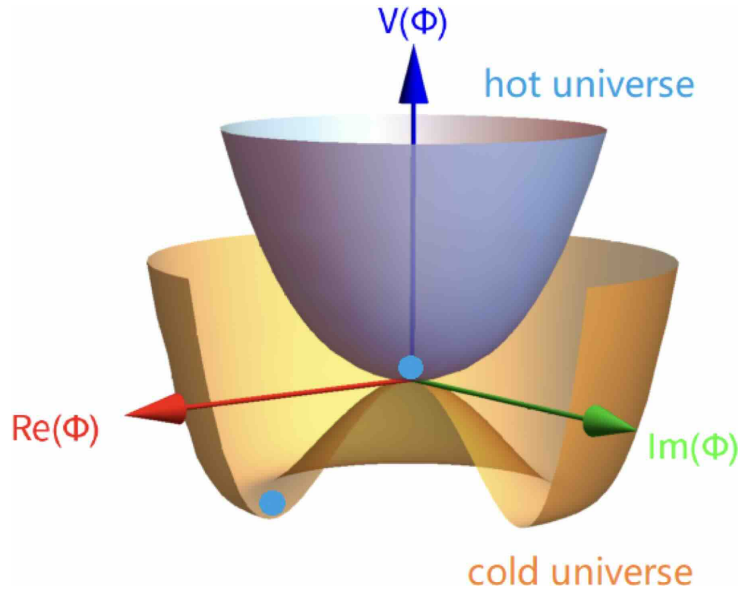


Fig. 1.3 The potential shape of the Higgs field at early hot ($\mu^2 \leq 0$) and cold ($\mu^2 > 0$) universe [13].

where h is the physical scalar boson Higgs, and $\theta^i(x)$ are the pseudoscalar Nambu-Goldstone bosons [14–16], which are the massless scalar bosons that are absorbed by the massive gauge bosons ($W^\pm, Z^0$) and become their longitudinal components. The unitary gauge can be chosen to eliminate the Nambu-Goldstone bosons, and the scalar field can be rewritten as:

$$\Phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h \end{pmatrix} \quad (1.21)$$

After expansion, the Lagrangian of the Higgs boson becomes:

$$\mathcal{L}_{Higgs} = \frac{1}{2} \partial_\mu h \partial^\mu h - \frac{1}{4} v^2 g^2 W_\mu^+ W^{-\mu} \left(1 + \frac{h}{v}\right)^2 + \frac{1}{8} v^2 (g^2 + g'^2) Z_\mu Z^\mu \left(1 + \frac{h}{v}\right)^2 - V(h), \quad (1.22)$$

where there appear four physical gauge bosons: $W^\pm, Z^0$ and $A(\gamma)$ that are related to those of the EW theory W^1, W^2, W^3 and B by:

$$\begin{aligned} W^\pm &= \frac{1}{\sqrt{2}} (W^1 \mp iW^2), \\ Z &= W^3 \cos \theta_W - B \sin \theta_W, \\ A &= W^3 \sin \theta_W + B \cos \theta_W. \end{aligned} \quad (1.23)$$

Here, θ_W is the weak mixing angle, defined as $\tan(\theta_W) = g'/g$.

In terms of these fields the electroweak interaction Lagrangian becomes

$$\begin{aligned} \mathcal{L}_{int} &= -e \sum_f q_f \bar{\psi}_f \gamma^\mu \psi_f A_\mu - \frac{g}{\sqrt{2}} \sum_{\text{fermions}} \left(\bar{\psi}_u \gamma^\mu \frac{1-\gamma_5}{2} \psi_d W_\mu^+ + \bar{\psi}_d \gamma^\mu \frac{1-\gamma_5}{2} \psi_u W_\mu^- \right) \\ &\quad - \frac{g}{\cos \theta_W} \sum_f \bar{\psi}_f \gamma^\mu (g_V^f - g_A^f \gamma_5) \psi_f Z_\mu, \end{aligned} \quad (1.24)$$

$$(1.25)$$

where one can identify a term describing interactions between charged fermions and the field A , a second term describing chiral interactions between fermions and the W field, with the typical V-A structure of charged weak interactions, and a third term describing interactions between fermions (charged or neutral) and the Z field.

As one can see from Equation 1.22, the vector bosons ($W^\pm, Z^0$) acquire mass terms while the photon (γ) remains massless, and the interactions of gauge W and Z bosons with the Higgs boson are proportional to the square of their masses. Their masses are given by:

$$\begin{aligned} M_W &= \frac{1}{2}vg, \\ M_Z &= \frac{1}{2}v\sqrt{g^2 + g'^2} = \frac{M_W}{\cos\theta_W}, \\ M_\gamma &= 0. \end{aligned} \tag{1.26}$$

In the unitary gauge, the Higgs potential becomes:

$$V(\Phi) = \frac{\mu^4}{4\lambda} + \mu^2 h^2 + \lambda_3 v h^3 + \frac{1}{4}\lambda_4 h^4, \tag{1.27}$$

where the first two terms denote the vacuum energy and the mass of the Higgs boson. The third and fourth terms denote the triple and quartic Higgs self-interactions, respectively. These latter terms play a pivotal role in defining the configuration of the Higgs potential, an essential aspect in the theoretical understanding of the Higgs mechanism. The self-interaction couplings predicted in the SM are $\lambda_3 = \lambda_4 = \frac{m_H^2}{2v^2}$, so the measurements on triple and quartic Higgs coupling are significant to the understanding of the Higgs mechanism. The Higgs boson mass can be derived as

$$M_H = \sqrt{2\mu^2} = \sqrt{2\lambda}v \tag{1.28}$$

Yukawa Term: last but not least, the Yukawa interaction is the term that describes the mass generation of the fermions through the Higgs mechanism. The Yukawa Lagrangian can be written as

$$\mathcal{L}_{Yukawa} = -\sum_f y_f \bar{f}_L \Phi f_R + h.c. \tag{1.29}$$

where y_f is the Yukawa coupling constant, f is the fermion field, $\bar{f}_L$ and f_R are the left-handed and right-handed fermion fields. After the spontaneous symmetry breaking, the Yukawa term becomes:

$$\mathcal{L}_{Yukawa} = -\sum_f \frac{y_f v}{\sqrt{2}} \bar{f} f - \sum_f \frac{y_f v}{\sqrt{2}} \bar{f} f \frac{h}{v} = -\sum_f m_f \bar{f} f - \sum_f m_f \bar{f} f \frac{h}{v}, \tag{1.30}$$

where $m_f \equiv y_f v / \sqrt{2}$ denotes the mass of fermions that are produced after EWSSB, which implies that the Higgs couplings to fermions are proportional to their masses.

Within the framework of the Standard Model (SM), neutrinos are initially presumed to be massless, leading to a total of nine fermions that gain mass via the Yukawa interaction. This concept is built on the foundation that all particles in the SM are inherently massless, and it is through the Higgs mechanism that they acquire mass. Non-zero neutrino masses could be generated by assuming the existence of right-handed “sterile” neutrinos with zero isospin charge and hypercharge, and a very tiny Yukawa coupling leading to the small neutrino masses that

are observed. An additional possibility to generate neutrino masses is to assume that neutrinos are identical to antineutrinos. In that case a “Majorana” mass term could be introduced in the Lagrangian without breaking the gauge symmetry.

The landmark discovery of the Higgs boson, a critical component of the SM, marked a significant milestone in particle physics. This discovery, achieved by the ATLAS [6] and CMS [7] experiments at the LHC in 2012, confirmed the last elusive element of the SM.

1.2 Higgs Boson Physics at the LHC

The quest to detect the Higgs boson began with the Tevatron [17] and LEP [18] experiments. However, it wasn't until 2012 that the ATLAS and CMS experiments at the LHC announced the discovery of the Higgs boson with a mass close to 125 GeV. This section will cover the production, decay, and characteristics expected in the SM for a 125 GeV of Higgs boson in detail.

1.2.1 Higgs Boson Production

At the LHC collider, that will be introduced in detail in Section 2.1, the Higgs boson production occurs through the following mechanisms:

Gluon-Gluon Fusion [ggFH]: through a heavy quark loop (mainly *top* or *bottom* quarks), two gluons fuse to produce a Higgs boson ($gg \rightarrow H$). This represents the primary mode of Higgs boson production at the LHC ($\approx 87\%$ of the total cross-section). The leading-order Feynman diagram is displayed in Figure 1.4(a).

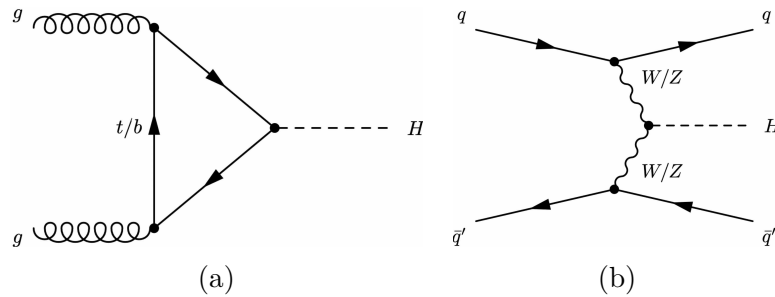


Fig. 1.4 Feynman diagrams illustrating Higgs boson production: gluon-gluon fusion (a) and vector boson fusion (b).

Vector Boson Fusion [VBF]: owing to the interaction between the Higgs boson and vector bosons, the fusion of two vector bosons originating from incoming quarks results in the formation of a Higgs boson ($q_1 q_2 \rightarrow q_3 q_4 H$). This mechanism constitutes the second most prevalent mode of Higgs boson production at the LHC ($\approx 7\%$). A notable characteristic of the Vector Boson Fusion (VBF) process is the emergence of two forward jets in the final state, originating from the quarks. It renders the VBF process distinct from other modes of Higgs boson production. The leading-order Feynman diagram is shown in Figure 1.4(b).

Associated Vector Boson Production [VH]: the Higgs boson is produced in association with a vector boson, $q\bar{q}' \rightarrow VH$, where V represents a W or Z boson. Additionally, $gg \rightarrow ZH$ could provide small contributions to the Higgs boson production at the LHC ($\approx 4\%$). The mode is

also called Higgs-strahlung and is the third most prevalent production mode. The leading-order Feynman diagrams are shown in Figure 1.5.

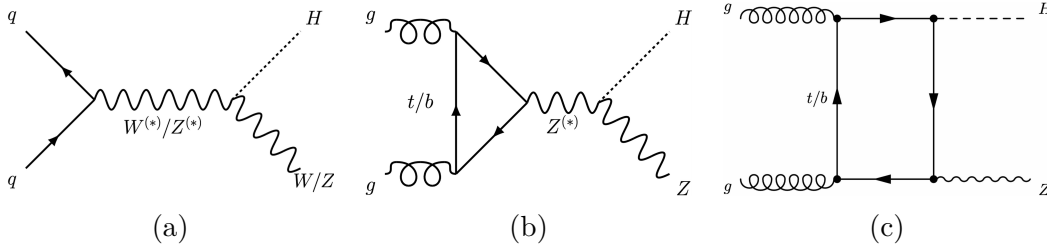


Fig. 1.5 Feynman diagrams showing Higgs boson production through associated vector boson production (a) $q\bar{q}' \rightarrow VH$ and $gg \rightarrow ZH$ (b, c).

Associated Top/Bottom Quark Pair Production [$t\bar{t}H$, $b\bar{b}H$]: the Higgs production is accompanied by a pair of bottom or top quarks ($gg, q\bar{q} \rightarrow t\bar{t}H, b\bar{b}H$). This is the 4th largest mode of production at the LHC ($\approx 1\%$ each). $t\bar{t}H$ is induced by the coupling between the Higgs boson and the *top* quark. $b\bar{b}H$ has production rate similar to $t\bar{t}H$ but produces rather soft b-jets and the kinematics is similar to that of the much larger ggF process. The leading-order Feynman diagram is exhibited in Figure 1.6.

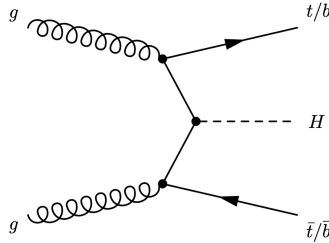


Fig. 1.6 Feynman diagram for Higgs production via *top/bottom* quark pair production.

Associated Single Top Quark Production [tHq , tHW]: the production of the Higgs boson occurs in conjunction with a single top quark ($qg \rightarrow tHq'$ as tHq and $gb \rightarrow tHW$ as tHW). This process has the lowest predicted production rate at the LHC (almost one order of magnitude smaller than $t\bar{t}H$). The tHq and tHW processes are sensitive to the top Yukawa coupling and Higgs-W coupling. The leading-order Feynman diagrams are shown in Figure 1.7.

Figure 1.8 shows the predicted cross-section of Higgs boson production as a function of the Higgs boson mass at $\sqrt{s} = 13$ TeV.

1.2.2 Higgs Boson Decays and Total Width

According to the Standard Model, the total decay width of the Higgs boson at $m_H = 125$ GeV is about 4.1 MeV [19]. As a consequence, once created, the Higgs boson exists for an absolutely short duration, approximately 10^{-22} seconds. Its detection can thus be achieved only indirectly through the observation of final states resulting from the decay of Higgs boson. The individual partial decay widths of the Higgs boson depend on the coupling strengths between the Higgs boson and the respective particles participating in the decay. Since the Higgs boson couplings are proportional to fermion masses and gauge boson squared masses, this leads to two distinct cases:

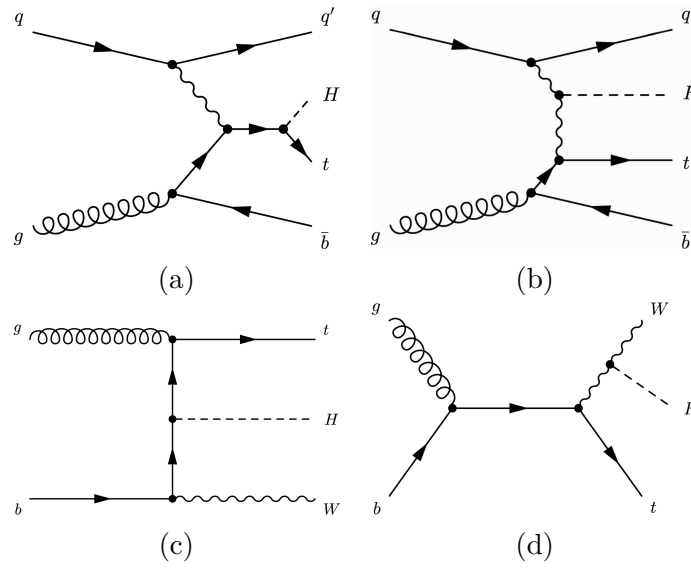


Fig. 1.7 Feynman diagrams for Higgs production in conjunction with top quark production: tHq (a, b) and tHW (c, d).

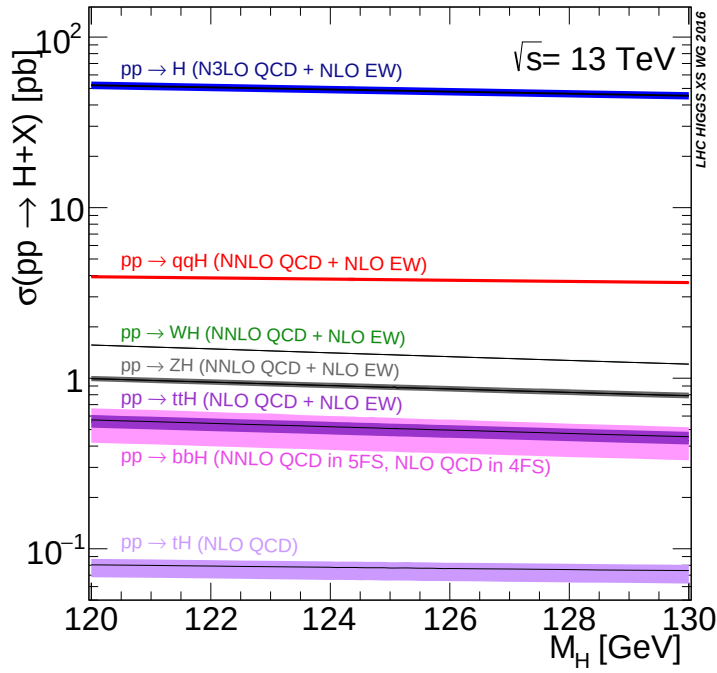


Fig. 1.8 Cross-section for Higgs boson production in the Standard Model as a function of the Higgs boson mass at $\sqrt{s} = 13$ TeV. The thickness indicates the scale and PDF uncertainty. Credits: LHC Higgs Working Group

the Higgs boson undergoing decay into massive fermions and bosons via tree-level processes as shown in Figure 1.9 (a,b), or decaying into massless bosons through loop-induced mechanisms as shown in Figure 1.9 (c, d, e).

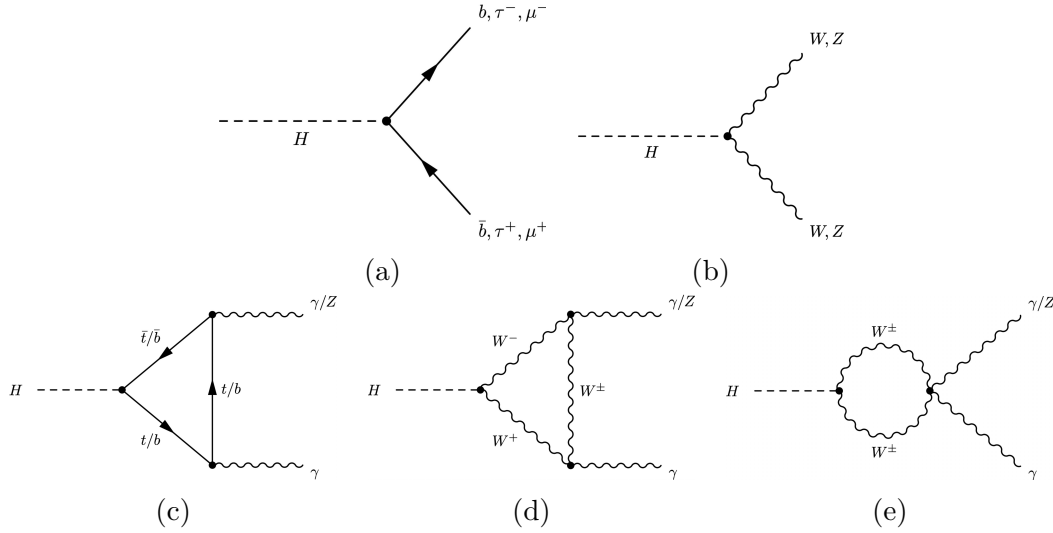


Fig. 1.9 Feynman diagrams illustrating Higgs decaying into fermions and gauge bosons: tree-level decay (a, b) and loop-induced decay (c, d, e).

Figure 1.10 shows the branching ratios (BRs) for various decay channels of the Higgs boson [19], as predicted by the Standard Model, inclusive of their theoretical uncertainties for a mass $m_H = 125$ GeV. The most prominent decay channel is into a pair comprising a bottom quark and its corresponding anti-quark ($H \rightarrow b\bar{b}$) with a branching ratio of 57.5%. This is followed by the decay process wherein the Higgs boson transitions into a W boson and its associated virtual counterpart, denoted as $H \rightarrow WW^*$, with a branching ratio of 21.6%. The third most dominant decay channel ($H \rightarrow gg$) with a branching ratio of 8.56% is impossible to distinguish from the multi-jets production, by the LHC experiments that have no gluon tagging. The fourth leading decay channel ($H \rightarrow \tau\tau$) with a branching ratio of 6.3% could measure the coupling of Higgs boson to leptons and the tau tagging was developed by ATLAS and CMS Collaboration [20]. $H \rightarrow c\bar{c}$ has a branching ratio of 2.90%, probing the coupling of Higgs boson to charm quarks. The decay $H \rightarrow ZZ^*$ has a branching ratio of 2.67%, the two Z bosons could decay to electrons or muons, the so-called *golden channel* due to its clean signatures. The Higgs boson decays with the smallest BRs are those to $\gamma\gamma$ (0.227%), $Z\gamma$ (0.155%) and $\mu\mu$ (0.022%). Despite the lower frequency of Higgs boson decay into $\gamma\gamma$, the ATLAS detector could provide clean trigger due to remarkable photon identification, which played a pivotal role in the initial discovery of the Higgs boson mode. The rare decay modes of the Higgs boson, specifically $H \rightarrow Z\gamma$ and $H \rightarrow \mu\mu$, have not yet been observed with $> 5\sigma$ statistical significance, but a 3σ evidence has been obtained for both [21, 22]. The $H \rightarrow Z\gamma$ decay will be briefly discussed in Chapter C.

The Higgs boson properties are extremely important for testing the SM. The mass of the Higgs boson is not predicted by SM theory and is a free parameter. The latest ATLAS measurement of the Higgs boson mass yields: $m_H = 125.11 \pm 0.09$ (stat) ± 0.06 (syst) GeV $= 125.11 \pm 0.11$ GeV [23] and its measured total width is $4.5^{+3.0}_{-2.5}$ MeV [23] to be compared with the SM expectation of $4.1^{+3.2}_{-3.5}$ MeV [19] at $m_H = 125$ GeV. The spin and charge-parity (CP) of the Higgs boson are also critical parameters of interest. The SM-hypothesis is that the Higgs

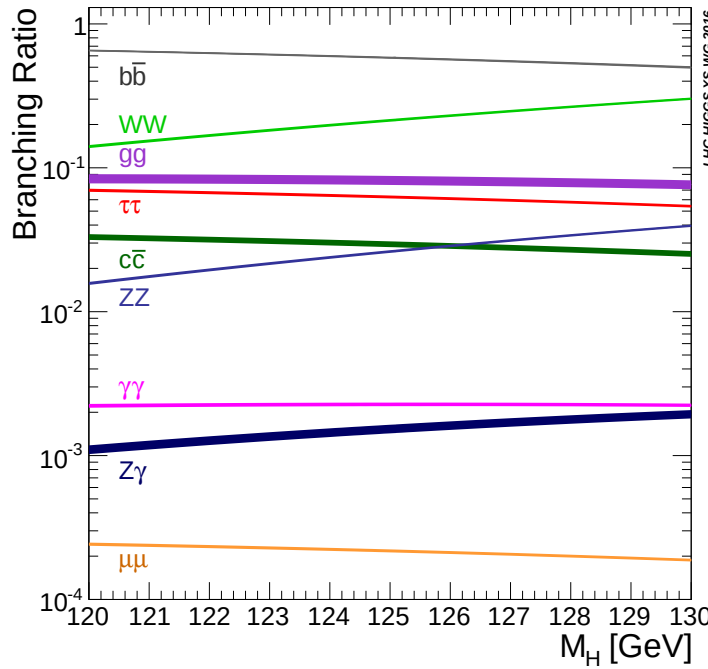


Fig. 1.10 The branching ratios and total uncertainties for various decay channels of the Higgs boson at Higgs mass around 125 GeV. Credits: LHC Higgs Working Group

boson is a neutral scalar particle with a spin zero and a positive CP. The Higgs bosons from extended Higgs sectors could be a mixed state including both positive and negative CP states. Both the spin and CP could be measured through analyzing the angular distributions of decay products of the Higgs boson and some decay channels are studied by the ATLAS and CMS experiments: $H \rightarrow \gamma\gamma, ZZ^*, W^\pm W^\pm, \tau\tau$ [24–27]. The couplings of the Higgs boson to massive gauge bosons or fermions are also essential to test the spontaneous symmetry breaking mechanism and their latest results [28] from ATLAS Run-2 are shown in Figure 1.11.

1.2.3 Higgs Boson Self-coupling from Single Higgs Productions and Decays

The Higgs boson self-coupling is theoretically fundamental as it determines the precise contours of the Higgs potential, a pivotal element for grasping the Higgs mechanism. As elucidated in Section 1.3.2, Higgs boson pair production offers a direct avenue to measure this self-coupling. However, the notably low production rate of these pairs presents a significant obstacle in accurately measuring the Higgs self-coupling. The single Higgs process, to a certain degree, offers a supplementary role in contributing insights into the Higgs self-coupling [29–31]: via Higgs self-energy loop and additional diagrams contributes to the Next-to-Leading Order (NLO) EW correction, whose Feynman diagrams are shown in Figure 1.12.

Theoretically, the association between the Higgs boson production cross-section and the trilinear Higgs coupling is expressed as: 1.31 [29].

$$\mu_i(\kappa_\lambda, \kappa_i) = \frac{\sigma^{\text{BSM}}}{\sigma^{\text{SM}}} = Z_H^{\text{BSM}}(\kappa_\lambda) \left[\kappa_i^2 + \frac{(\kappa_\lambda - 1)C_1^i}{K_{\text{EW}}^i} \right] \quad (1.31)$$

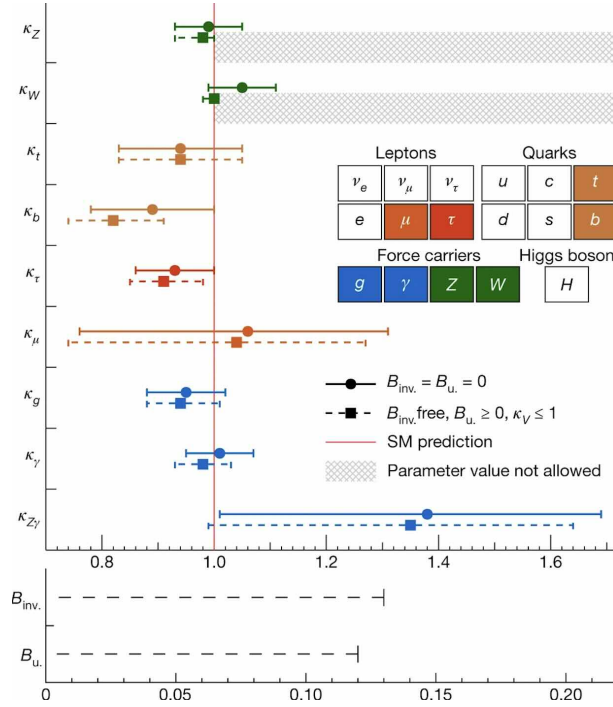


Fig. 1.11 The coupling strengths of the Higgs boson to particles with effective photon, $Z\gamma$, gluon couplings and the associated uncertainties [28].

where κ_λ is the ratio of the Higgs self-coupling to its SM value. The wavefunction renormalization factor $Z_H^{\text{BSM}}(\kappa_\lambda)$ is given by:

$$Z_H^{\text{BSM}}(\kappa_\lambda) = \frac{1}{1 - (\kappa_\lambda^2 - 1) \delta Z_H}, \text{ with } \delta Z_H = -1.536 \times 10^{-3} \quad (1.32)$$

The $\kappa_i^2 = \sigma_{\text{LO},i}^{\text{BSM}} / \sigma_{\text{LO},i}^{\text{SM}}$ with $\kappa_\lambda = 1$ are the modifiers of the coupling strength for the i th process. The C_1^i is the kinematic-dependent linear coefficient of the i th production process. The denominator $K_{\text{EW}}^i = \sigma_{\text{NLO}}^{\text{SM},i} / \sigma_{\text{LO}}^{\text{SM},i}$ represents the EW correction factor, which accounts for the NLO EM correction of the production cross-section for the i th process under the SM hypothesis ($\kappa_\lambda = 1$). The aforementioned description elucidates the contribution of Higgs production to the self-coupling of the Higgs boson.

The branching ratios could provide some sensitivities on the trilinear coupling, through the relation:

$$\mu_f(\kappa_\lambda, \kappa_f) = \frac{\text{BR}_f^{\text{BSM}}}{\text{BR}_f^{\text{SM}}} = \frac{\kappa_f^2 + (\kappa_\lambda - 1) C_1^f}{\sum_j \text{BR}_j^{\text{SM}} [\kappa_j^2 + (\kappa_\lambda - 1) C_1^j]} \quad (1.33)$$

where $\sum_j$ loops over all Higgs decay channels, BR_j^{SM} is the branching ratio of Higgs decay to the j th final state. The term C_1^f is defined identically to C_1^i , however, it pertains specifically to the f th decay channel. κ_f is the branching fraction modifier of the f th decay process and $\kappa_j^2 = \text{BR}_{\text{LO},j}^{\text{BSM}} / \text{BR}_{\text{LO},j}^{\text{SM}}$.

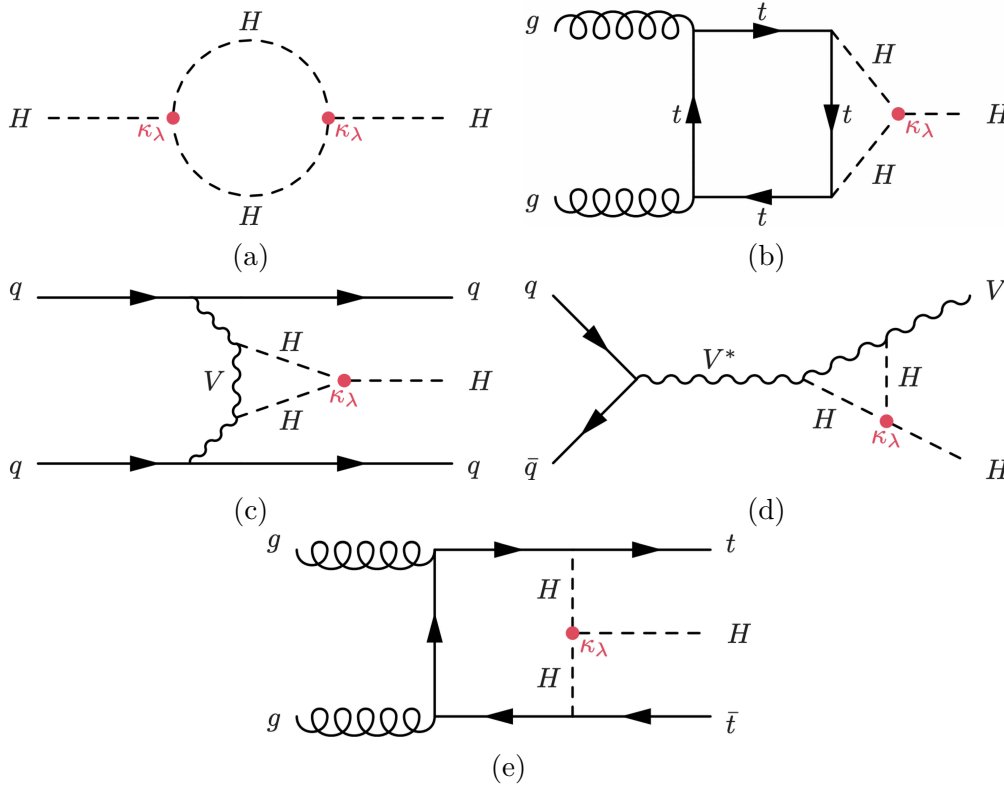


Fig. 1.12 One-loop diagrams illustrating the Higgs self-coupling noted as κ_λ from the contribution of single Higgs in the NLO EW correction. (a) Higgs self-energy loop, (b, c, d, e) for ggH , $VBFH$, VH , $t\bar{t}H$ process.

1.3 Higgs Boson Pair Production at the LHC

The amplitudes of the leading-order Feynman diagrams of Higgs boson pair production shown in Figure 1.14 and 1.15 are proportional to the self-coupling denoted as κ_λ , which could be directly measured from the Higgs boson pair production.

1.3.1 Higgs Boson Pair Production Modes and Decays

The cross-section of the Higgs boson production is approximately $\mathcal{O}(60\text{pb})$ at $\sqrt{s} = 13\text{ TeV}$, as shown in Figure 1.8. The di-Higgs boson cross-section as a function of the center-of-mass energy is shown in Figure 1.13. The SM Higgs boson pair production is extremely rare with a cross-section of $\mathcal{O}(30\text{fb})$, which is a thousandfold less than that of Higgs boson production. The measurement of the Higgs boson self-coupling is thus incredibly challenging. The section below focuses on the two HH production modes with the largest cross-section: gluon-gluon fusion and vector boson fusion. The contributions from other modes will not be considered due to their small cross-section and low production rate at the LHC.

Gluon-Gluon-Fusion [ggFHH]: among the various production mechanisms, gluon-gluon fusion stands out as the most significant route leading to the Higgs boson pair production. At the lowest perturbative order, this process involves two main Feynman diagrams, which are illustrated in Figure 1.14. However, the destructive interference between those diagrams suppresses the cross-

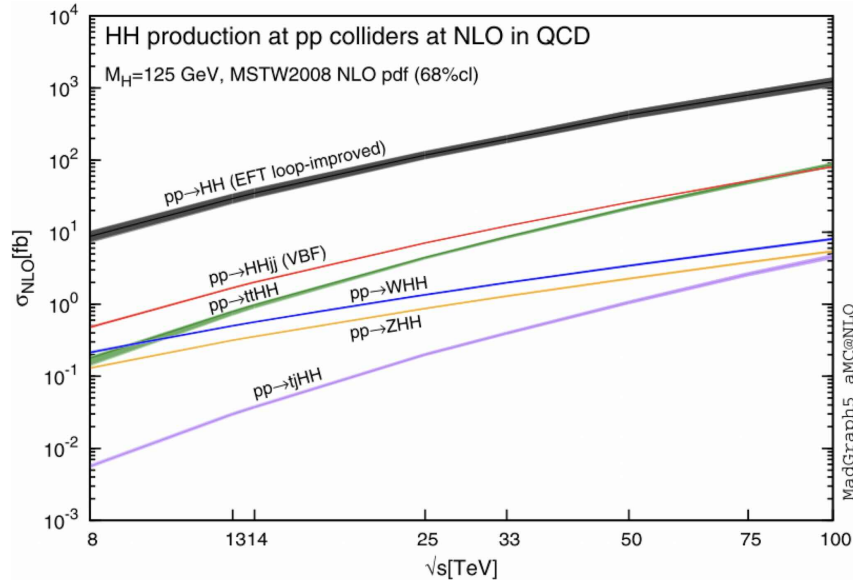


Fig. 1.13 Total cross-section at NLO in QCD from pp colliders with six largest production modes contained. The scale and PDF uncertainties are shown as the thickness [32].

section of the Higgs boson pair production. At $\sqrt{s} = 13$ TeV and $m_H = 125$ GeV, the calculation of the ggFHH cross-section at the next-to-next-to-leading order (NNLO) accuracy in the finite top-quark mass approximation (FTapprox) leads to the prediction:

$$\sigma_{HH}(\text{ggF}) = 31.05^{+6\%}_{-23\%}(\text{Scale} + m_{\text{top}}) \pm 3.0\%(\alpha_s + \text{PDF})\text{fb} \quad (1.34)$$

where $\text{Scale} + m_{\text{top}}$ quantifies the uncertainty from the effect of the finite order of the QCD calculation and the top-quark mass scheme, $\alpha_s + \text{PDF}$ indicates the uncertainty from the strong coupling constant and parton distribution functions (PDF) [33–35]. As displayed in Figure 1.14, the ggF HH cross-section depends on both the Higgs self-coupling strength modifier (κ_λ) and the interaction between the Higgs boson and the top quark (κ_t).

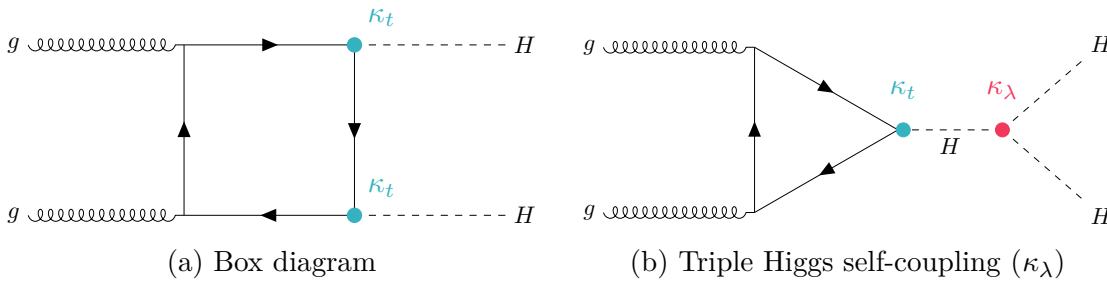


Fig. 1.14 The leading-order Feynman diagrams of the Higgs pair production in the gluon-gluon fusion process. The total cross-section calculated by summing these two diagrams and the destructive interference between them. Two vertexes denoted as κ_λ and κ_t could be constrained. Credits: DiHiggs Group.

Vector Boson Fusion [VBFHH]: this is the second-largest production mode, and its cross-section is calculated at the next-to-next-to-next-to-leading orders (N³LO) QCD accuracy with the renormalization and factorization scales set to the individual virtuality of the t-channel vector bosons. The predicted value of the cross-section is:

$$\sigma_{HH}(\text{VBF}) = 1.726^{+0.03\%}_{-0.04\%}(\text{Scale}) \pm 2.1\%(\alpha_s + \text{PDF})\text{fb} \quad (1.35)$$

where the uncertainties included the scale term and the $\alpha_s + \text{PDF}$ uncertainty based on the PDF4LHC15nnlmc set [36]. As illustrated in Figure 1.15, which showcases three Feynman diagrams pertinent to the VBF channel, the manifestation of two forward jets could be the most salient signature, facilitating the distinct identification of VBF HH events in contrast to other occurrences. Moreover, beyond the pivotal role in constraining the Higgs self-coupling, the VBF mode exhibits considerable sensitivities towards elucidating the $HHVV$ (κ_{2V}) coupling modifiers. This channel emerges as a unique investigative tool for probing the interactions at the vertex involving two vector bosons and two Higgs bosons denoted as κ_{2V} .

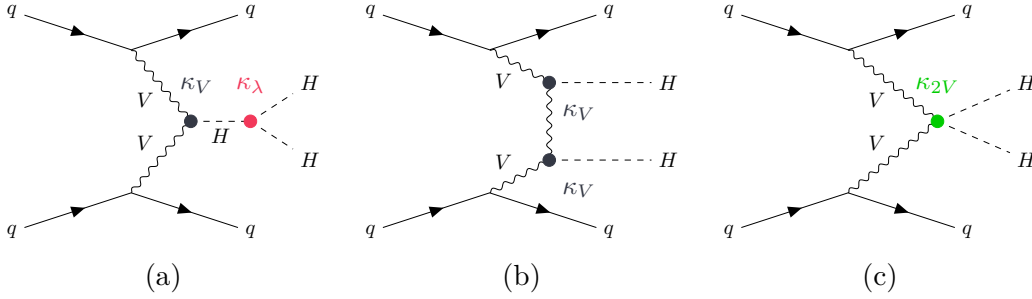


Fig. 1.15 The leading-order Feynman diagrams of the Higgs boson pair production in the vector-boson fusion process. Credits: DiHiggs Group.

In comparison to the decay of a single Higgs boson, the decay involving Higgs boson pairs (also referred to as di-Higgs candidates) exhibits greater abundance and diversity, as delineated in Figure 1.16. The decay mode with the most pronounced branching ratio (34%) is the $b\bar{b}b\bar{b}$ mode. However, the final state of the $b\bar{b}b\bar{b}$ decay suffers from those sophisticated QCD backgrounds, which pose a significant challenge in signal identification. The $b\bar{b}\tau^+\tau^-$ final state also provide some sensitivity due to its large BR but low signal over background ratio, while other channels with tiny BRs and large background contributions from other SM processes leads to worse sensitivities. In contrast, the $b\bar{b}\gamma\gamma$ channel, despite its relatively low branching ratio, is considered to be more advantageous due to its cleaner trigger and a background that is relatively smaller and more thoroughly understood.

1.3.2 Higgs Boson Self-coupling from Higgs Boson Pair Productions

The theoretical cross-section of Higgs boson pair production as a function of the Higgs boson self-coupling is shown in Figure 1.17. When $\lambda = \lambda_{SM}$, the effect of destructive interference is quite seizable, resulting in a lower cross-section that is without the box diagram, while beyond Standard Model (BSM) values $\lambda \neq \lambda_{SM}$ could potentially enhance the Higgs boson pair production cross-section. ggFHH and VBFHH modes represent approximately 95% of the total Higgs boson pair production cross-section at $\sqrt{s} = 14$ TeV for $m_H = 125$ GeV.

	bb	WW	$\tau\tau$	ZZ	$\Upsilon\Upsilon$
bb	34%				
WW	25%	4.6%			
$\tau\tau$	7.3%	2.7%	0.39%		
ZZ	3.1%	1.1%	0.33%	0.069%	
$\Upsilon\Upsilon$	0.26%	0.10%	0.028%	0.012%	0.0005%

Fig. 1.16 The branching ratio of the Higgs pair production in the double Higgs decay process. Credits: DiHiggs Group.

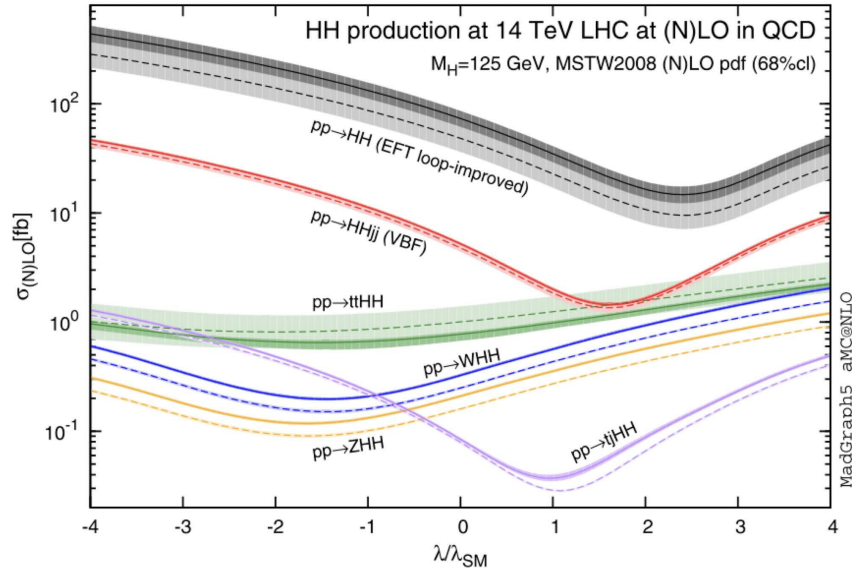


Fig. 1.17 The total cross-section at the QCD (N)LO for Higgs pairs at $\sqrt{s} = 14$ TeV and $m_H = 125$ GeV as a function of the Higgs self-coupling. The dash and solid lines respectively indicate the LO and NLO results, while the deep and light color bands represents the scale and PDF uncertainties. $\kappa_\lambda = \lambda/\lambda_{SM} = 1$ corresponds to the SM predictions [32].

1.4 Physics Beyond the Standard Model

The Standard Model of particle physics, despite its remarkable success in explaining a wide range of phenomena, encounters several significant problems and limitations:

- **Dark Matter and Dark Energy:** These constituents represent the most enigmatic aspects of the universe's composition. Dark matter, elusive to electromagnetic interaction, is estimated to constitute approximately 27% of the universe's mass-energy content, inferred primarily through gravitational influences on visible matter. Dark energy, which comprises about 68% of the mass-energy content, is posited as the driving force behind the universe's accelerated expansion. The Standard Model does not encompass particles that could constitute dark matter, nor does it elucidate the nature of dark energy [37, 38].
- **Gravity:** As a fundamental force, gravity remains conspicuously absent from the Standard Model. It is currently described by the classical framework of general relativity, a non-quantum theory. The integration of gravity into the quantum realm of the Standard Model is a significant objective in theoretical physics, leading to efforts towards a unified theory or a theory of everything [39].
- **Neutrino Mass:** Contrary to the initial assumptions of the Standard Model that neutrinos are massless, experimental observations, particularly those pertaining to neutrino oscillations, have demonstrated that neutrinos possess a minute mass. The underlying mechanism for mass acquisition in neutrinos, potentially involving physics beyond the Standard Model, remains an area of active investigation [40, 41].
- **Matter-Antimatter Asymmetry:** The prevailing cosmological models suggest an equal formation of matter and antimatter in the early universe. However, the observable universe predominantly consists of matter. This discrepancy is not adequately addressed by the Standard Model, presenting a significant anomaly in our understanding of the universe's evolution [42].
- **Hierarchy Problem:** This issue pertains to the stark disparity in the magnitude of gravitational force compared to other fundamental forces, specifically the weak nuclear force. The enigma revolves around the unexpectedly low mass of the Higgs boson relative to theoretical predictions, necessitating a fine-tuning of the Standard Model's parameters to align with empirical observations [43, 44].
- **Strong CP Problem:** The strong force, integral to the stability of atomic nuclei, is theoretically expected to violate charge-parity (CP) symmetry. However, empirical evidence suggests that the strong force maintains CP symmetry, in stark contrast to the weak force, which does exhibit CP violation. The Standard Model does not adequately account for this discrepancy [45].
- **Inclusion of All Particle Masses and Forces:** The Standard Model, in its current form, does not provide an intrinsic explanation for the specific values of fundamental particle masses, nor does it elucidate the basis for the relative strengths of the fundamental forces. These parameters are derived from experimental measurements and integrated into the model, yet their foundational significance remains elusive.

Each of these domains represents a forefront of contemporary physics research, with theoretical and experimental endeavors aimed at extending or supplementing the Standard Model to resolve these fundamental questions. Addressing these issues remains a central focus in modern physics, and various extensions of the Standard Model, like supersymmetry, string theory, and

others, have been proposed to tackle these challenges.

1.4.1 Higgs Boson Pair Production in Beyond-Standard-Model Scenarios

As previously discussed, the SM Higgs boson pair production has an extremely low cross-section at the LHC. However, BSM scenarios can significantly enhance the Higgs boson pair production rate, particularly in cases where there are substantial deviations in the Higgs boson self-coupling from the SM prediction, as illustrated in Figure 1.17. Possible SM extensions leading to enhanced Higgs boson pair production include models with extended scalar sectors, Supersymmetry (SUSY), and extra-dimensional theories. Each predicts distinctive experimental signatures, providing measurable deviations in Higgs pair production that could reveal the nature of fundamental interactions.

- **Extended Scalar Sector Models:** Adding scalar fields, like singlets or doublets, enhances Higgs boson pair production through resonant processes. A gauge singlet, for instance, can mix with the SM Higgs, forming mass eigenstates where the heavier one decays into Higgs pairs if its mass is sufficiently large. Models such as the Two-Higgs-Doublet Model (2HDM) [46], introduce additional Higgs states that decay into Higgs boson pairs, often showing interference effects in the gluon-gluon fusion production mode. Such interference, combined with modified self-couplings, makes scalar extensions promising for new physics searches.
- **Supersymmetry Theory (SUSY):** SUSY [47, 48] extensions, like Next-to-Minimal Supersymmetric Standard Model (NMSSM) [49], introduce new scalar and fermionic states that influence Higgs pair production through resonant and non-resonant processes. Additional particles, such as top squarks and extra Higgs bosons, contribute through loop effects and decays, altering the effective coupling between Higgs pairs and gluons. SUSY models thus support a broad range of Higgs pair production signatures, offering rich phenomenological implications for collider experiments.
- **Extra-Dimensional Models:** Theories with extra dimensions, such as Randall-Sundrum (RS) models [50], predict Kaluza-Klein (KK) gravitons, which can mediate resonant Higgs pair production. These models, addressing the electroweak hierarchy problem, predict a series of KK states that interact with the Higgs sector, producing unique di-Higgs signatures through resonant and cascade decays. This distinct interplay between gravity and Higgs physics complements scalar and EFT-based searches.

Deviations from the SM can also be described in a model-independent way through an effective field theory (EFT) framework [51, 52]. By incorporating higher-dimensional operators, EFT captures potential modifications to Higgs interactions from heavy states without specifying a complete model. Key operators alter the Higgs self-coupling and gluon interactions, modifying both production rates and kinematic distributions. Potential deviations from the SM predictions that could be observed in e.g. the Higgs boson self-coupling would constrain the Wilson coefficients of the EFT Lagrangian. These would then be recast as constraints on the couplings of concrete BSM models.

CHAPTER 2

Large Hadron Collider and ATLAS detector

Particle physics experiments explore the subatomic realm to understand the universe's elementary constituents and their fundamental interactions. The Heisenberg uncertainty principle [53] implies that these experiments require higher energy to probe finer scales. The Large Hadron Collider (LHC) [54–57], built at CERN, is the world's highest-energy particle accelerator, enabling proton-proton collisions at multi-TeV center-of-mass energies. The ATLAS detector [58–61], crucial for collecting and reconstructing the signals from the particles produced in the LHC collisions, has been taking data since 2010. Together with the other LHC experiments, it has been instrumental in advancing particle physics since its inception. This thesis analyzes data collected by the ATLAS detector during the second phase of LHC data taking (Run-2). The following sections discuss the design and operation of both the LHC accelerator and of the ATLAS detector.

2.1 Large Hadron Collider

The *Large Hadron Collider* is a circular particle accelerator situated 50 to 175 meters beneath the surface in a tunnel that was previously built for the Large Electron-Positron Collider (LEP). It is the last element of an accelerator chain shown in Figure 2.1 and is located on the border between France and Switzerland, near Geneva. The LHC was designed to accelerate protons or heavy nuclei to close to the speed of light and make them collide. It encompasses a 27-kilometer circumferential arrangement of superconducting magnets, integrated with numerous accelerating modules that systematically elevate the kinetic energy of the particles throughout their trajectory within the ring. The designed maximum center-of-mass energy of proton-proton collision is $\sqrt{s} = 14$ TeV and of heavy ion collision is $\sqrt{s} = 2.3$ TeV per nucleon. Four crossing points along the accelerator ring are equipped with four major physics detectors: ATLAS [58–61], CMS [62], ALICE [63], and LHCb [64]. ATLAS and CMS are the two largest general-

purpose particle physics experiments in the world, with a broad physics programme including QCD, electroweak, top, flavour, Higgs boson physics and searches for signatures of physics beyond the Standard Model. ALICE stands as a dedicated experiment to explore the quark-gluon plasma through heavy nuclei (lead) collisions, while LHCb is a specialized experiment for the detailed examination of flavour physics in the quark sector.

2.1.1 Layout and Parameters of Accelerator Design

The LHC is designed in to reach a proton-proton center-of-mass energy of up to 14 TeV, allowing the exploration of physics processes produced in parton collisions with energy up to a few TeV, thus above the electroweak symmetry breaking scale. The rate of events of a given process produced at the LHC is defined as $dN_{\text{event}}/dt = L\sigma_{\text{event}}$, where L is the accelerator's instantaneous luminosity in units of $cm^{-2}s^{-1}$ and σ_{event} is the production cross-section of the physics process under study in area units. The instantaneous luminosity quantifies the number of beam particles crossing each other per unit area and time, while the cross-section is a measure of the probability that these particles will interact and produce the process of interest. The design peak luminosity of the LHC is $10^{34} cm^{-2}s^{-1}$ for proton-proton collisions. It depends on the beam parameters, and under the assumption of *Gaussian beam distribution*, it can be written as [56]:

$$L = \frac{N_b^2 n_b f_{\text{rev}} \gamma_r}{4\pi \varepsilon_n \beta^*} F \quad (2.1)$$

Here, N_b denotes the number of particles per bunch, n_b signifies the number of bunches per beam, f_{rev} stands for the frequency of the revolution, γ_r represents the relativistic gamma factor, ε_n indicates the normalized transverse beam emittance, and β^* corresponds to the beta function at the collision point. F refers to the geometric reduction factor due to the crossing angle at the interaction point (IP) [56]:

$$F = \left(1 + \left(\frac{\theta_c \sigma_z}{2\sigma^*} \right)^2 \right)^{-1/2}, \quad (2.2)$$

where θ_c is the full crossing angle at the IP, σ_z and σ^* is the RMS of the longitudinal bunch and the transverse beam size at the IP, respectively. In order to maximize the production rate of rare physics events, i.e. with small cross-sections, a high luminosity is needed, requiring high beam intensities (large number of particles per bunch, large crossing frequency of the bunches i.e. small separation between each bunch) and excellent beam focusing (small emittance, small beta function at the IP). Table 2.1 displays the main design parameters of the LHC accelerator at the peak luminosity and the maximum beam energy.

As depicted in Figure 2.1, the CERN acceleration complex employs a series of multi-stage accelerators specifically engineered to accelerate protons or heavy ions to their designated energy levels. Initially, hydrogen anions (H^-) undergo acceleration within the *linear accelerator 4* (LINAC4), during which process the electrons enveloping these anions are stripped away, resulting in the formation of protons (H^+) possessing an energy of 50 MeV. Subsequently, these protons are conveyed to the *BOOSTER* apparatus, where their energy is increased to 1.4 GeV. Following this stage, the protons are advanced to the *Proton Synchrotron* (PS), achieving an energy threshold of 25 GeV. The journey continues as the protons are then directed to the *Super*

Design parameters	Number
Circumference	26.659 km
Nominal beam energy at collision	7 TeV
Nominal beam energy at injection	450 GeV
Peak luminosity	$10^{34} \text{ cm}^{-2}\text{s}^{-1}$
No. of protons per bunch (N_b)	1.15×10^{11}
No. of bunches per proton beam (n_b)	2808
Circulating current per beam	0.54 A
Revolution frequency (f_{rev})	11245 Hz
Frequency of main RF system	400.8 MHz
Bunch spacing time	24.95 ns
Beam lifetime	10 h
Total crossing angle at collision point (θ_c)	300 μrad
Peak magnetic dipole field	8.33 T
Bending radius	2.804 km
Dipole operating temperature	1.9 K (-271.3°C)
Nominal emittance (ε_n)	3.75 $\mu\text{m rad}$
Beta function at IP (β^*)	0.55 m

Tab. 2.1 Design parameters of the LHC accelerator [56, 57].

Proton Synchrotron (SPS) and their energy is further augmented to 450 GeV. Culminating the acceleration process, the protons are introduced into the LHC, where they are accelerated to reach the peak collision energy of 7 TeV per proton beam [56, 57].

Within the LHC, two beams of particles fly nearly at the speed of light in opposite directions within two separate and vacuum-sealed tubes, and each proton beam contains 2808 bunches with a bunch spacing of 24.95 ns, each bunch containing 1.15×10^{11} protons. The beams are directed around the accelerator's circular path by the magnetic field generated by superconducting electromagnets cooled to -271.3°C (1.9 K), a temperature even colder than the vacuum of space.

During the first data-taking phase of the LHC (Run-1), from 2010 to 2012, the proton-proton center-of-mass energy was 7 TeV (2010-2011) or 8 TeV (2012) [65, 66]. The LHC was then shut down during two years (2013-2014) for maintenance and upgrades, and the center-of-mass energy was then increased to 13 TeV in the second data-taking phase (Run-2) in 2015-2018 [66]. The peak luminosity in Run-1 was surpassed by a factor of two at the end of Run-2, reaching to a value higher than the design peak luminosity [67]. In July 2022 a new phase of LHC data taking started (Run 3), after more than three years spent on accelerator and detector upgrades and maintenance works. During Run 3 the LHC will operate for about four years, reaching an unprecedented center-of-mass energy of 13.6 TeV [68] and delivering more integrated luminosity than that collected in the two previous LHC runs. The increased data samples and higher collision energy in Run-3 will further expand the already diverse LHC physics programme.

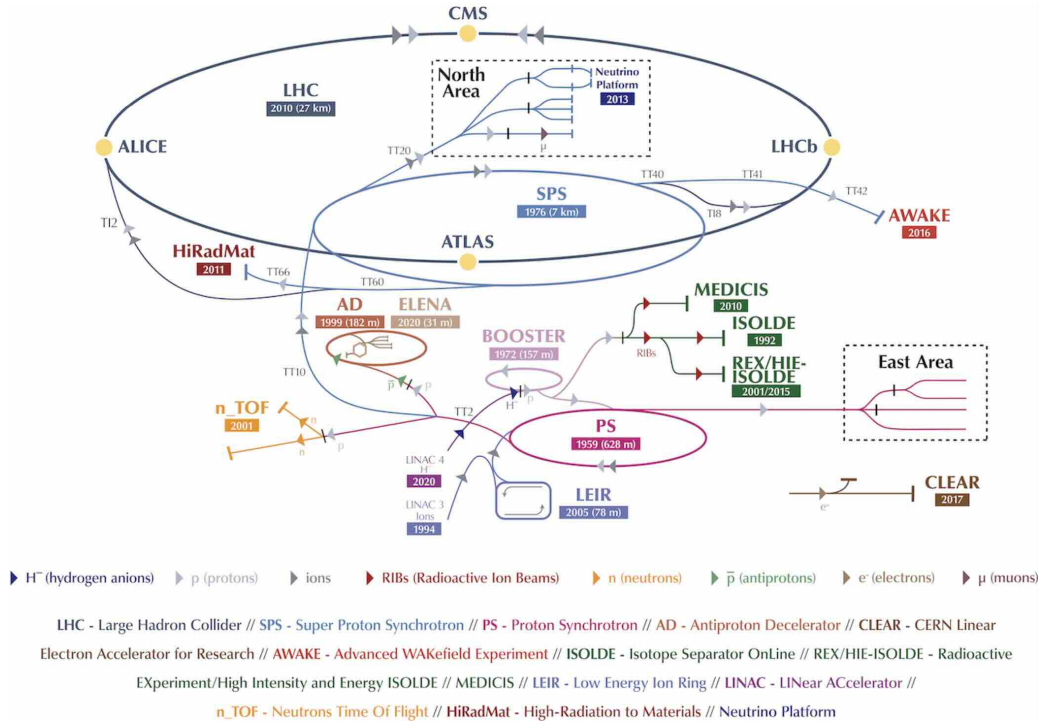


Fig. 2.1 The CERN accelerator complex and the Large Hadron Collider. Credits: CERN

2.1.2 Performance and Operational Insights from Run-2

The number of events of a given process produced during a given amount of LHC running time is given by:

$$N_{\text{events}} = L_{\text{int}} \sigma_{\text{event}}, \quad L_{\text{int}} = \int L dt, \quad (2.3)$$

where L_{int} is the so called integrated luminosity. Broadly speaking, the integrated luminosity depends on the effective turnaround time of the LHC. The total integrated luminosity recorded during the LHC's Run-1 [66] was 28 fb^{-1} , while in Run-2, the LHC achieved a total integrated luminosity of 156 fb^{-1} , as shown in Figure 2.2(a). Detector (in)efficiency and good data quality requirements reduce a bit the amount of collision data available for physics analysis. In particular, during Run-2, the ATLAS detector recorded 147 fb^{-1} of luminosity, and 140 fb^{-1} of this was certified as good-quality for physics analysis, with an associated uncertainty of 0.83% [69], as illustrated in Figure 2.2(b). In Run-3, the integrated luminosity has surpassed on September 1st 2024 that of Run-2, and could reach 190 fb^{-1} by the end of the year. The core findings presented in this thesis are derived from the analysis of the integrated luminosity data accumulated by the ATLAS detector during the Run-2 phase.

In the LHC, protons collide near the nominal interaction points. While the cross-sections of the main processes of interest for the ATLAS programme are sufficiently small, compared to the instantaneous luminosity, that there is at most one of these events per bunch crossing, the large inelastic proton-proton cross-section leads to *pile-up*, i.e. additional, soft interactions that occur alongside the primary collision of interest, affecting the clarity of the resulting data. The average number of pile-up collisions per bunch crossing is $\mu = L_{\text{bunch}} \times \sigma_{\text{inel}} / f_r$ where L_{bunch}

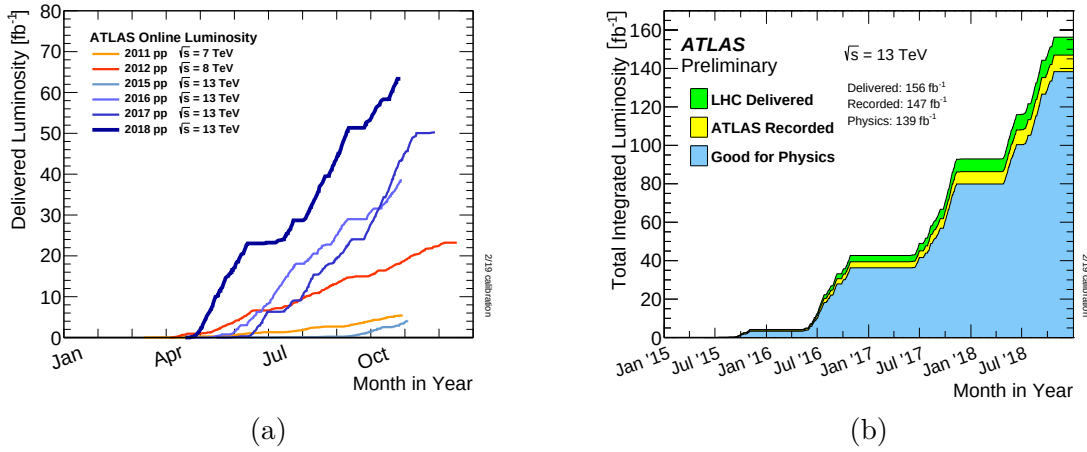


Fig. 2.2 Cumulative luminosity versus month in year: (a) Luminosity delivered to ATLAS for the stable beams and high energy pp collision in 2011-2018. (b) Integrated luminosity delivered to ATLAS (green), recorded by ATLAS (yellow) and verified to be good-data quality (blue) for physics analysis during Run-2. The luminosity determination was delivered by 140 fb^{-1} with a small uncertainty of 0.83% [69]. Credits: ATLAS

is the instantaneous luminosity per bunch, σ_{inel} is the inelastic cross section (around 80 mb for both 13 TeV and 13.6 TeV collisions), and f_r is the LHC revolution frequency. Increased instantaneous luminosity leads to higher pile-up, with the LHC's Run-2 experiencing an average of approximately 33.7 interactions per crossing, varying from 1 to over 70 in Figure 2.3. The upcoming High-Luminosity LHC, planned to start around 2030, aims for an instantaneous luminosity of 5-8 times the design LHC luminosity, at the price 140-200 interactions per crossing on average [70].

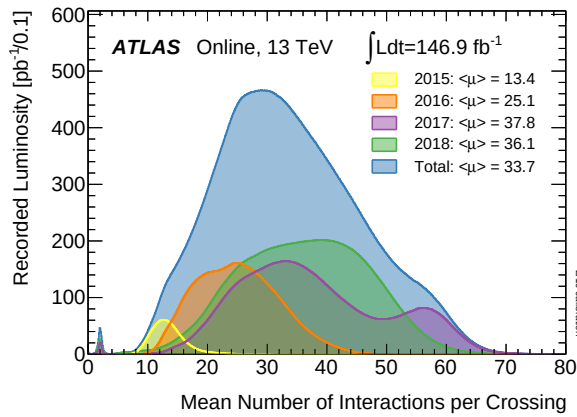


Fig. 2.3 The luminosity-weighted distribution of the mean number of interactions per crossing during Run-2 pp collisions at $\sqrt{s} = 13$ TeV. Credits: ATLAS

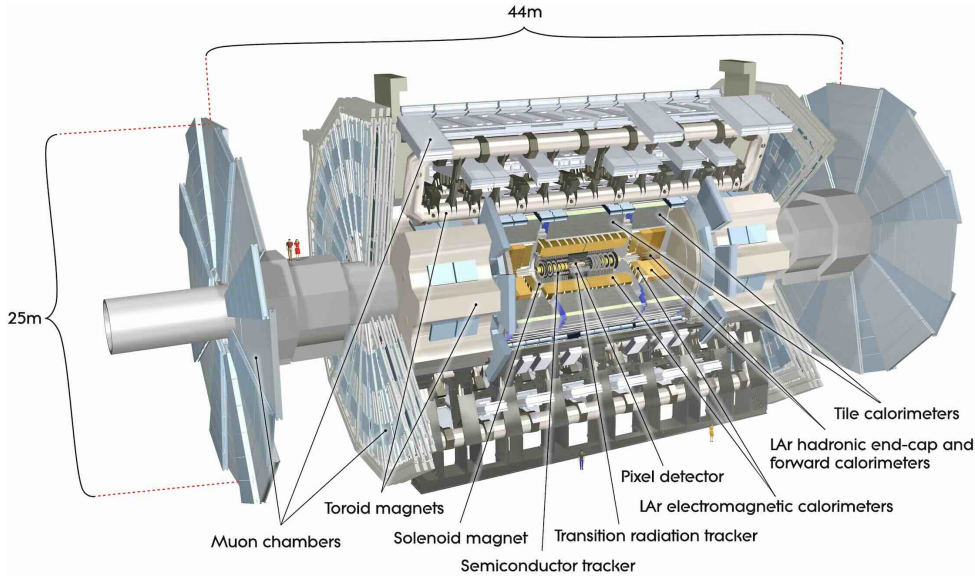


Fig. 2.4 Cut-away schematic of the whole ATLAS detector showing its various sub-detectors. Credits: [ATLAS](#)

2.2 ATLAS Detector

The ATLAS (A Toroidal LHC ApparatuS) detector [58] is one of the two general-purpose detectors at the LHC at CERN. Designed to investigate a wide range of physics phenomena, from the search for the Higgs boson to dimensions beyond the visible universe, ATLAS stands as a marvel of modern physics and engineering. Its complex structure, equipped with various layers of sensors and detectors, allows scientists to capture and analyze particles resulting from collisions at nearly the speed of light. This monumental instrument has played a crucial role in numerous groundbreaking discoveries, including the observation of the Higgs boson in 2012, providing insights into the fundamental building blocks of the universe and the forces that govern their interactions.

2.2.1 Overview of Design and Structure

The ATLAS detector is the largest particle physics detector in the world. It features a forward-backward symmetrical cylindrical design around the point of proton-proton collision and offers comprehensive coverage of nearly the entire 4π solid angle. Measuring about 44 meters in length and 25 meters in diameter, and weighing roughly 7000 tonnes, it resides within a cavern situated 100 meters underground. Its operational infrastructure is supported by an extensive network of cables stretching over 3000 km. An overview schematic of the detector is shown in Figure 2.4.

The ATLAS detector uses a right-handed *Cartesian* coordinate system, crucial for precision in analyzing particle trajectories and interactions, with the z-axis along the beam pipe, the x-axis pointing towards the LHC's center, and the y-axis upwards. This setup forms the basis for defining the azimuthal angle (ϕ) in the transverse (x-y) plane and polar angle (θ) from the beam

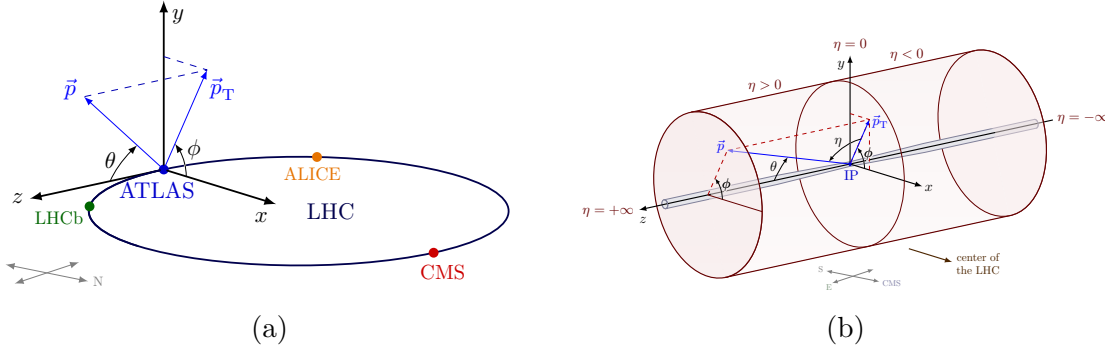


Fig. 2.5 The coordinate system of the ATLAS detector showing from the LHC perspective (a) and from the collision point perspective (b).

(z) axis. Two quantities that are used are the pseudo-rapidity (η) and rapidity (y), defined as:

$$\begin{aligned}\eta &= -\ln \left[\tan \left(\frac{\theta}{2} \right) \right] \\ y &= \frac{1}{2} \ln \left(\frac{E + p_z}{E - p_z} \right)\end{aligned}\tag{2.4}$$

Pseudo-rapidity is a quite good approximation of the rapidity for highly relativistic particles, where the total energy is much greater than their rest mass energy. Pseudo-rapidity is a function of the polar angle of the particle that is invariant under Lorentz boosts along the z-axis. The angular separation between two objects is quantified by:

$$\Delta R = \sqrt{\Delta \eta^2 + \Delta \phi^2}\tag{2.5}$$

where $\Delta \eta$ is the pseudo-rapidity difference and $\Delta \phi$ is the azimuthal angle difference, both of which are invariant under Lorentz boosts along the beam axis. The schematics illustrating the ATLAS coordinate system from the LHC perspective and the collision point perspective are presented in Figure 2.5.

As illustrated in Figure 2.4, ATLAS consists of multiple sub-detectors, each engineered to detect and analyze specific particles produced by the collisions in the LHC or by their interactions and decays, enabling the measurement of their characteristics. The primary sub-detectors of ATLAS include: the tracking system, the calorimeters, and the muon spectrometer. A magnet system provides the field needed for measuring the charged particles momenta. These systems are described in detail in the following sections.

The ATLAS detector can identify a wide range of particles, such as photons (γ), electrons (e), muons (μ), and hadronic jets (j) from decays of tau leptons or from the hadronization of quarks and gluons, which are significant for the Higgs boson and other fundamental BSM physics. The design of the detector is characterized by the following requirements and their corresponding parameters like resolution listed in Table 2.2:

- Radiation-resistant high-speed electronics to cope with the high-irradiation and high-frequency collision environments of the LHC.
- High timing resolution and calorimeter granularity to handle pile-up events.

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

Tab. 2.2 The design parameters of the ATLAS detector.

- Good energy resolution for the electromagnetic and hadronic calorimeters to identify the electrons, photons and jets as well as missing transverse energy (MET) from feebly or non-interacting particles (such as neutrinos).
- Excellent momentum resolution and reconstruction efficiency for the tracker and muon spectrometer.
- Large enough pseudo-rapidity acceptance to cover almost the full solid angle (4π).
- Efficient trigger systems to record the majority events of interest while discarding a large fraction of background events from low-energy collisions.

2.2.2 Magnet System

The ATLAS detector employs a sophisticated magnet system shown in Figure 2.6, designed to bend the paths of charged particles. This bending allows the experiment to measure the momenta of these particles with high precision from the curvature of their reconstructed trajectories. The magnet system of the ATLAS detector comprises four large magnets: a central solenoid situated around the inner detector, and three toroids, one barrel toroid surrounding the central part of ATLAS and two end-cap toroids extending into the forward regions. The solenoid and toroids are designed to operate in synergy to create a strong and uniform magnetic field where needed, while minimizing the field in regions requiring low magnetic interference.

The central solenoid provides a 2 Tesla (T) magnetic field with a length of 5.3 m, a diameter of 2.56 m and a thickness of 4.5 cm, crucial for the operation of the inner detector, which contains layers of tracking detectors that measure the position of particles as they fly out from the collision point.

The toroid magnets, consisting of eight coils in the barrel toroid and eight coils in each end-cap toroid, generate a toroidal magnetic field that envelops the muon spectrometer. They span 25.3 m in length and 20.1 m in diameter around the central part of the ATLAS detector. The field strength is up to 4 Tesla across the detector, allowing the spectrometer to accurately measure the momentum of high-energy muons that pass through the whole ATLAS detector. Muons are of particular interest in many physics analyses, including the search for new particles and the study of the Higgs boson, and can be easily distinguished from other particles and used for triggering, due to their ability to penetrate through several meters of material.

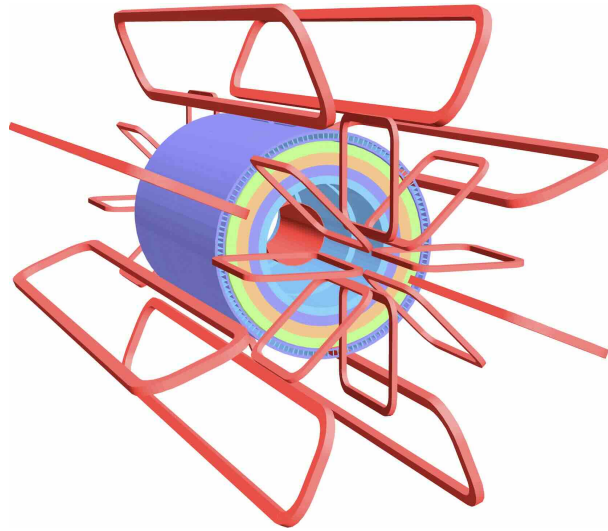


Fig. 2.6 The schematic of the ATLAS magnet system with the tile calorimeter steel. The eight barrel toroid coils, with the end-cap coils interleaved are visible. The solenoid winding lies inside the calorimeter volume. The tile calorimeter is modelled by four layers with different magnetic properties, plus an outside return yoke. Credits: [ATLAS](#)

All magnets are crafted from niobium-titanium (NbTi) and cooled to 4.5 Kelvin (K) to maintain superconductivity. The entire magnet system, weighing approximately 8300 tonnes, stores around 1.6 Gigajoules (GJ) of energy. It operates at superconducting temperatures thanks to a sophisticated cooling system that circulates liquid helium, essential for the functionality of the solenoid and toroids. Together, these magnets form an integral part of the ATLAS detector, enabling it to fulfill its role in probing the frontiers of particle physics.

2.2.3 Inner Detector

The Inner Detector (ID) is the main tracking system of ATLAS. It is a sophisticated system designed to track the paths of particles produced during high-energy collisions, contained within a cylindrical envelope of length ± 3512 mm and of radius 1150 mm. The ID covers a pseudo-rapidity acceptance of ± 2.5 and is immersed in a solenoidal magnetic field 2 T parallel to the beam axis. The system consists of several layers of detectors, each utilizing different technologies to maximize the balance between efficiency and accuracy in particle detection against number of readout channels and cost. At its core is the Pixel Detector, surrounded by the Semiconductor Tracker (SCT) and the Transition Radiation Tracker (TRT), as shown in Figure 2.7. These components work together to provide high-resolution measurements of the position of charged particles as they move through the detector, allowing for the precise determination of their momenta and the vertices from which they originated. Figure 2.8 shows the sensors and structural elements of the barrel and end-cap inner detectors that are traversed by charged tracks of $p_T = 10$ GeV.

One of the critical aspects of the detector architecture is its ability to operate in the extreme environment of the LHC, where it must withstand intense radiation and high particle fluxes

while maintaining exceptional performance. The use of advanced materials and electronics, coupled with innovative cooling systems, ensures the longevity and reliability of the detector. Additionally, the data collected by the trackers are processed by complex algorithms that filter and analyze the vast amounts of information to identify significant physical events among the millions of collisions that occur every second. Overall, the ATLAS tracker represents a pinnacle of engineering and physics research, enabling scientists to peel back the layers of the universe's deepest mysteries. Its contributions to discoveries, such as the Higgs boson, underscore its importance in the global effort to understand the fundamental constituents of matter and the forces that shape our universe.

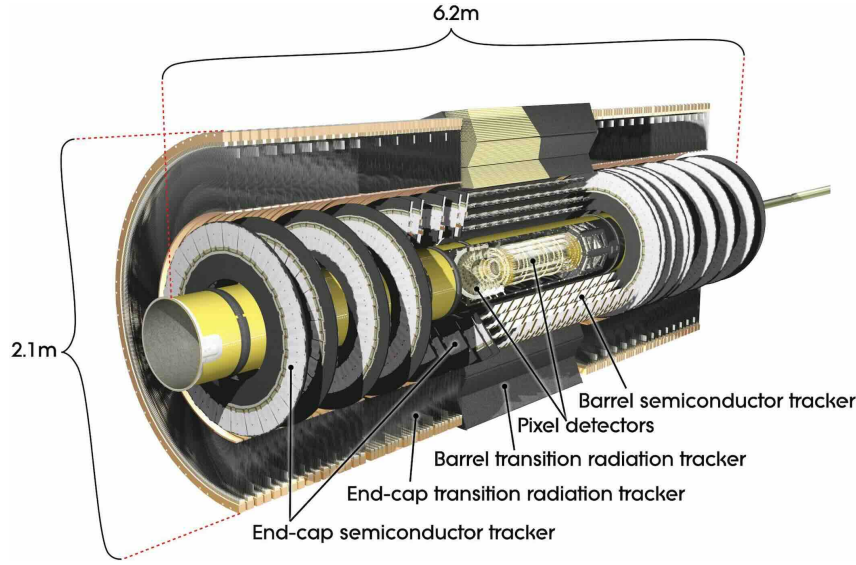


Fig. 2.7 Cutaway view of the ATLAS Inner Detector including pixel, SCT and TRT layers. Credits: [ATLAS](#)

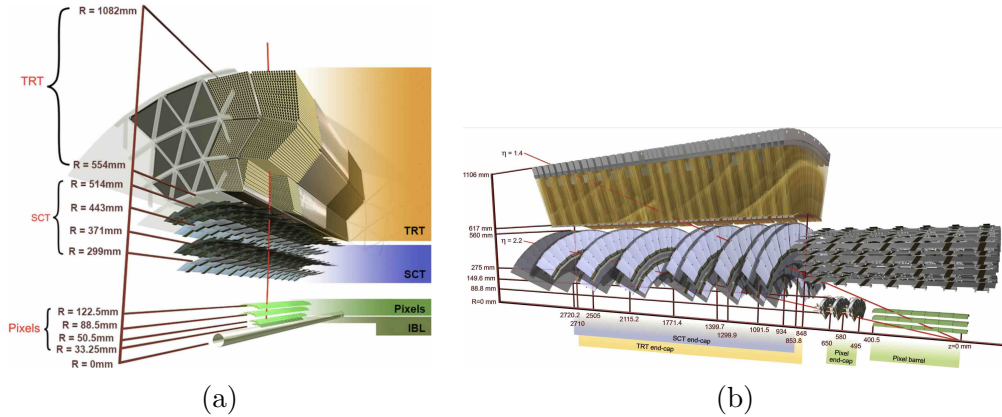


Fig. 2.8 Cutaway diagrams showing the sensors and structural elements: (a) traversed by a charged track of $p_T = 10$ GeV in the barrel inner detector ($\eta = 0.3$), (b) traversed by two charged tracks of $p_T = 10$ GeV in the end-cap inner detector ($\eta = 1.4$ and 2.2). Credits: [ATLAS](#)

2.2.3.1 Pixel Detector

The Pixel Detector, shown in Figure 2.8, represents the core component of the Inner Detector, comprising three concentric barrel layers positioned at radial distances of 50.5, 88.5, and 122.5 mm from the beam axis, accompanied by three disk assemblies orthogonal to the beam on both end-caps. This intricate detector contains a total of 1744 pixelated sensors along the $R-\phi$ and z planes, each corresponding to a silicon-based semiconductor device with an area of $50 \times 400 \mu\text{m}^2$. It boasts an approximate count of 67 million and 13 million readout channels respectively for barrel and end-caps, with each channel assigned to a single pixel, thereby achieving a spatial resolution in the transverse $R-\phi$ plane of about $10 \mu\text{m}$ and along the z -axis of $115 \mu\text{m}$ for charged particle position measurements.

The Insertable B-Layer (IBL) [71], integrated within the Pixel Detector's structure at a radius of 33.25 mm during the Long Shutdown (LS1) of the LHC between Run-1 and Run-2, consists of a dual-sensor configuration featuring both the conventional ATLAS pixel planar sensors and advanced 3D sensors, both having a pixel granularity of $50 \times 250 \mu\text{m}^2$. This layer exhibits a transverse impact parameter (d_0) resolution around 10-12 μm for high-momentum tracks, and longitudinal impact parameter (z_0) resolution ranging from approximately 200 to 800 μm for charged particles with transverse momentum between 0.4 and 20 GeV. The strategic inclusion of the IBL significantly enhances the precision of vertex reconstruction, thereby facilitating the identification and reconstruction of second displaced vertices arising from hadron decays with b -quarks and τ -leptons. The whole pixel detector is illustrated in Figure 2.9.

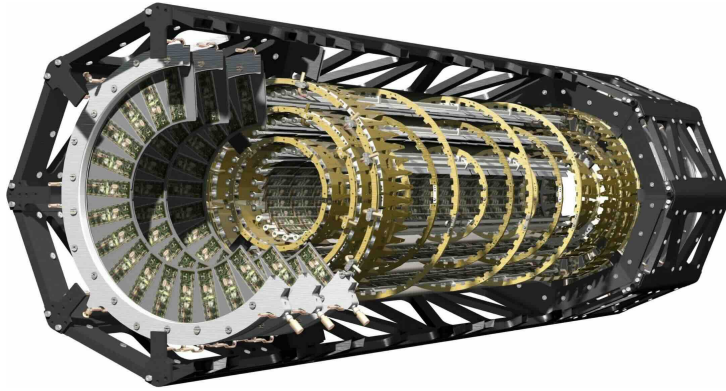


Fig. 2.9 The perspective cutaway view of the Pixel Detector. Credits: ATLAS

2.2.3.2 Semi-Conductor Tracker

The Semiconductor Tracker, situated externally to the Pixel Detector and serving as the central segment of the Inner Detector, encompasses an area of 61 square meters with silicon microstrip sensors and features 6.3 million channels for reading out data. It is structured into four concentric cylinders, having radii of 30.0, 37.3, 44.7, and 52.0 cm, along with nine disks placed at both ends of each end-cap. Spanning a length of 5.6 meters, the SCT's radius extends to 0.7 meters at the disk locations, which allows for the acquisition of four additional spatial measurements for each tracked object. In terms of precision, the SCT strip pitch achieves an approximate resolution of $16 \mu\text{m}$ in the $R-\phi$ plane and $580 \mu\text{m}$ in the z -axis direction.

2.2.3.3 Transition Radiation Tracker

Positioned as the most external component of the Inner Detector, the Transition Radiation Tracker operates on the principle of gas ionization for detecting particles. It incorporates straw tubes filled with Xenon, carbon dioxide (CO_2) and Oxygen (O_2), facilitating the generation of transition radiation when particles cross the interface of different radiator materials. Due to high cost of Xenon, other gases like Argon are considered as alternatives in portions of the TRT. The emitted radiation has an energy range of 5 to 30 KeV, directly proportional to the relativistic factor $\gamma = E/m$ of the incoming particle. This characteristic enables the differentiation of electrons from other similar momentum charged particles, such as pions and muons. The TRT consists of 52,544 straw tubes organized into 73 layers within the barrel section, and 122,880 straws arranged in 160 layers on each end-cap side, totaling 351,000 channels for data readout. With these straws, the TRT achieves measurement accuracy in the $R - \phi$ plane to about 170 μm per straw.

2.2.4 Calorimeters System

The calorimeters, positioned around the tracking and solenoidal magnet systems, are essential for measuring the energies of particles produced in high-energy proton-proton collisions. As particles traverse the calorimeter materials, they interact with atomic constituents, generating cascades of secondary particles that dissipate their energy and are ultimately absorbed within the detector. The core component of this system is a sampling calorimeter, designed with alternating layers of dense *absorber* material to stop incoming particles and an *active medium* to measure particle energies.

The ATLAS detector features two primary types of calorimeters: the electromagnetic calorimeter (ECAL) and the hadronic calorimeter (HCAL). The ECAL specializes in measuring the energies of electrons and photons, while the HCAL is calibrated to measure the energy of hadronic particles, such as protons and neutrons, which are composed of quarks. These instruments will be discussed in detail in subsequent sections.

Calorimeter systems effectively absorb most known fundamental particles with limited mean free paths, except for muons and neutrinos. The HCAL, due to its large scale, provides crucial data for jet reconstruction and the evaluation of missing transverse energy, derived from particle energy measurements.

A cross-sectional view of the ATLAS calorimeter systems is shown in Figure 2.10, illustrating the structural arrangement and operational domain of these critical components.

2.2.4.1 Electromagnetic Calorimeter

The ATLAS ECAL is a high-granularity sampling calorimeter employing lead as the absorber and liquid argon (LAr) as the active medium. Its accordion-shaped structure with a honeycomb pattern ensures continuous azimuthal (ϕ) coverage and rapid signal extraction. The ECAL is divided into the barrel (EMB) and two end-cap (EMEC) sections, covering a pseudo-rapidity range of $|\eta| < 3.2$ (Figure 2.10). A single ECAL module is illustrated in Figure 2.11.

A presampler module with fine granularity within $|\eta| < 1.8$ measures electron and photon energy dissipation before they enter the calorimeter. Composed of LAr, its thickness is 1.1 cm in the barrel and 0.5 cm in the end-caps.

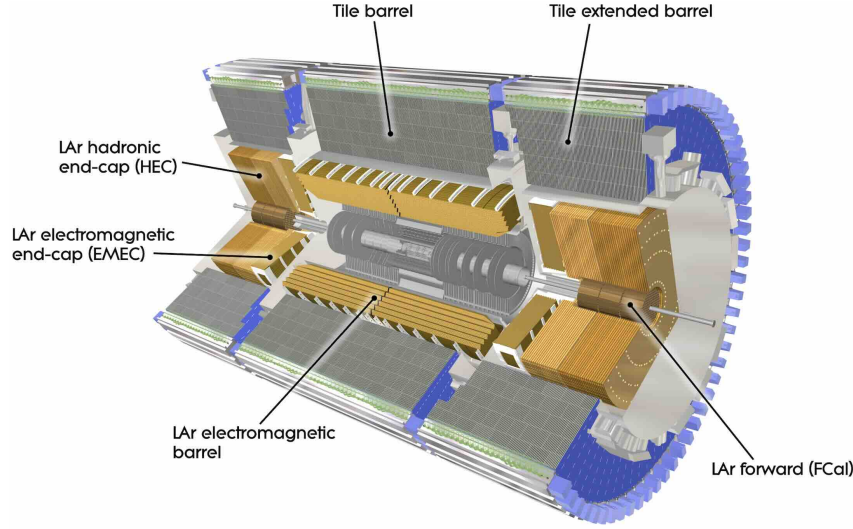


Fig. 2.10 Cutaway drawing of the ATLAS calorimeter. Credits: [ATLAS](#)

The calorimeter's longitudinal segmentation includes three layers for $|\eta| < 2.5$, reducing to two layers with coarser granularity for $2.5 < |\eta| < 3.2$. For $|\eta| < 2.5$, the first layer (L1) has a depth of 4.3 radiation lengths (X_0) and high granularity in η , chosen to facilitate the identification of prompt photons, leading to “strip” cells. The second layer (L2) has square cells and a depth of 16 X_0 , where most particle energy is deposited. The outer layer (L3) captures residual shower energy and has coarser granularity and a depth of 2 X_0 .

The typical energy resolution of the ECAL is

$$\frac{\sigma_E}{E} = \frac{10\%}{\sqrt{E}} \oplus 0.7\%. \quad (2.6)$$

The ECAL is surrounded by the cryostats that keep the LAr at low temperature (-184°C).

2.2.4.2 Hadronic Calorimeter

The ATLAS HCAL is constituted by two principal elements: the Tile Calorimeter (TileCal) and the Hadronic End-cap Calorimeter (HEC). The TileCal is designed to measure the energy emitted by hadrons and jets across the central pseudorapidity range of $|\eta| < 1.7$. It spans a diameter of 8 meters and extends along the beam axis for 12 meters. This component integrates steel plates for energy absorption and interspersed scintillating tiles as the active medium, which illuminate upon interaction with charged particles. The scintillation light is then captured by more than 9,500 photomultiplier tubes, converting the light emissions into electrical signals for precise energy measurement. The layout of TileCal features a central barrel covering $|\eta| < 1.0$ with a 5.8 meters length, and two extended barrels for the $0.8 < |\eta| < 1.7$ range, each extending 2.6 meters, subdivided into three distinct layers. The central barrel's layer thicknesses equate to approximately 1.5, 4.1, and 1.8 nucleon interaction lengths (λ), respectively, while the extended barrels' layers have thicknesses of 1.5, 2.6, and 3.3 λ . This configuration, along with its segmented arrangement in both azimuthal and pseudorapidity dimensions, facilitates the energy deposition localization.

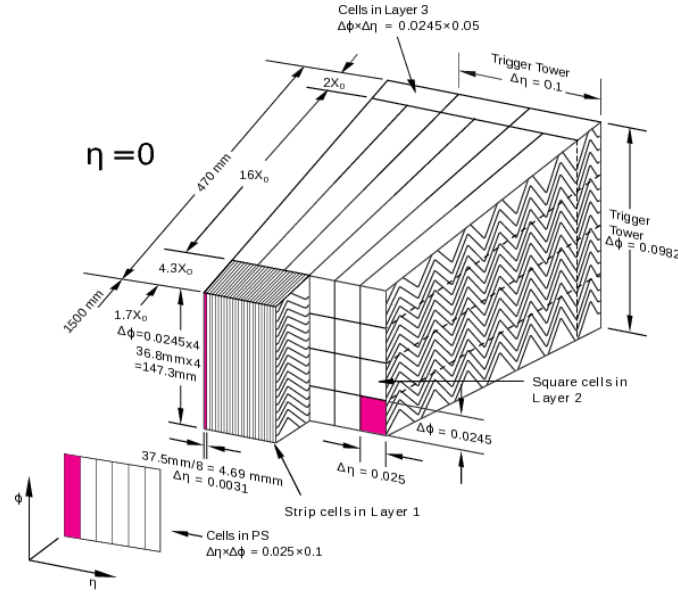


Fig. 2.11 Sketch of an EMB module where the different layers are visible. The granularity in η and ϕ of the cells of each of the three layers and of the trigger towers is also shown. Credits: [ATLAS](#)

Complementing the TileCal, the ATLAS HEC extends the hadronic energy measurement capabilities to a pseudorapidity range of $1.5 < |\eta| < 3.2$. Employing copper as the absorber and liquid argon (LAr) as the active medium, contained within cryostats to sustain cryogenic operation temperatures, LAr is selected for its superior ionization qualities, which assure a uniform response and high-resolution energy measurements. The HEC's architecture, offering granularity in both azimuthal and pseudorapidity dimensions, enhances the detector's efficiency in accurate energy deposit localization.

Finally, the Forward Calorimeter (FCal) further extends the ATLAS calorimetry system, enabling energy measurement in the extreme forward regions, spanning a pseudorapidity range of $3.1 < |\eta| < 4.9$. Comprising three modules, each 45 cm in depth, the FCal integrates dense materials for absorption: copper in the first module for electromagnetic measurements and tungsten in the subsequent modules focused on hadronic energy assessments, with LAr as the active medium across all modules. This design is specifically engineered to endure the high radiation levels and particle fluxes characteristic of the forward regions. The FCal's design, tailored for the detection and measurement of high-energy jets and particles in the forward direction, is indispensable for a comprehensive analysis of collision kinematics at the LHC.

The typical resolution of the HCAL is expressed as

$$\frac{\sigma}{E} = \frac{50\%}{\sqrt{E}} \oplus 3\%. \quad (2.7)$$

2.2.5 Muon Spectrometer

The Muon Spectrometer (MS) [73] is a critical and substantial component of the ATLAS detector, encompassing the calorimeters and designed to measure the momentum of muons

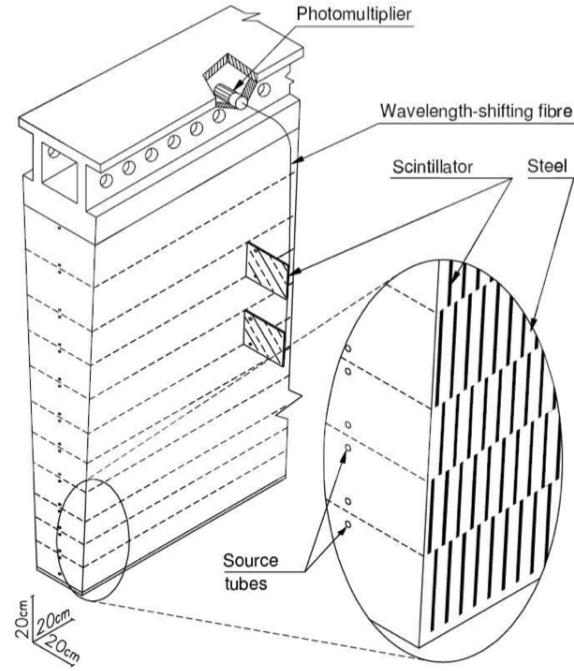


Fig. 2.12 Structure of a single module of the ATLAS tile calorimeter with the steel absorber and the scintillating tiles, as well as their PMTs readout through the wavelength shifting fibers [72].

within the range of $|\eta| < 2.7$. Muons, with their high penetrating power, traverse significant material without substantial absorption or deflection, making them vital for exploring new physics beyond the Standard Model. The MS operates within a strong magnetic field generated by superconducting toroidal magnets, with field intensities ranging from 1.5 to 5.5 T in the barrel and 1 to 7.5 T in the end-caps[60]. The MS comprises trigger chambers with fast response times and tracking chambers with excellent spatial resolution. It incorporates over 4000 muon chambers, including Monitored Drift Tubes (MDTs), Cathode Strip Chambers (CSCs), Resistive Plate Chambers (RPCs), and Thin Gap Chambers (TGCs). A cut-away view of the system is shown in Figure 2.13, and the chamber installation schematic is depicted in Figure 2.14(a).

2.2.5.1 Monitored Drift Tubes

The Monitored Drift Tubes are the primary components of the MS, and are responsible for the high-precision measurement of muon tracks in the barrel and end-cap regions of the detector. The basic module of the MDTs is a drift aluminum tube with a diameter of 30 mm and a thickness of 0.4 mm, filled with a gas mixture of Ar (93%) and CO₂ (7%) at 3 bar. When muons pass through the tubes, the gas mixture is ionized and then the electrons are transferred to and collected by the central Tungsten-Rhenium wire with a diameter of 50 μm under a high voltage of 3080 V. The barrel region ($|\eta| < 2.0$) holds three layers of MDTs distributed at various radii around 5 m, 7.5 m and 10 m, assembled in 16 sectors. A partial overlap among some chambers ensures good coverage over the full pseudo-rapidity range spanned by the system. The MDTs in the end-cap region ($2.0 < |\eta| < 2.7$) are mounted on three wheels perpendicular

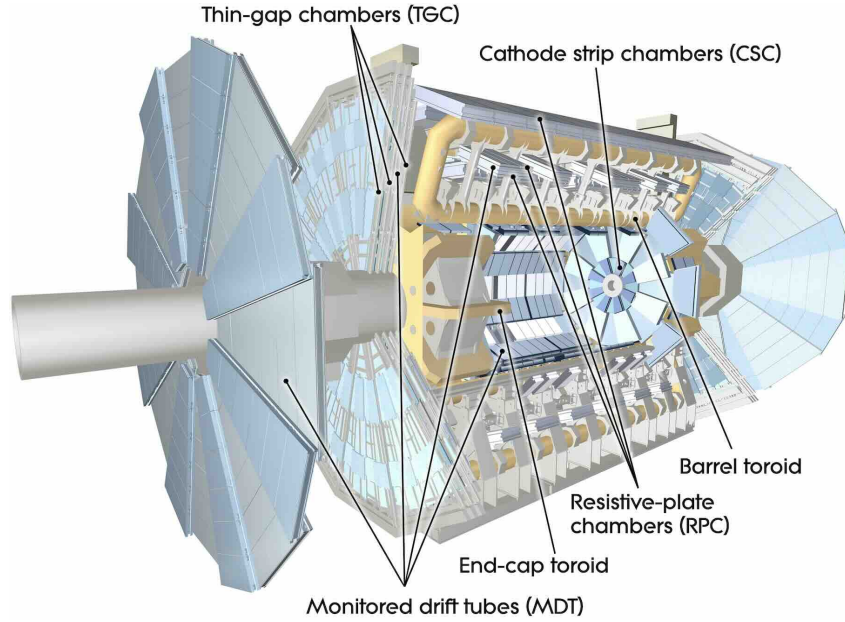


Fig. 2.13 Schematics of the Muon Spectrometer system in ATLAS. Credits: [ATLAS](#)

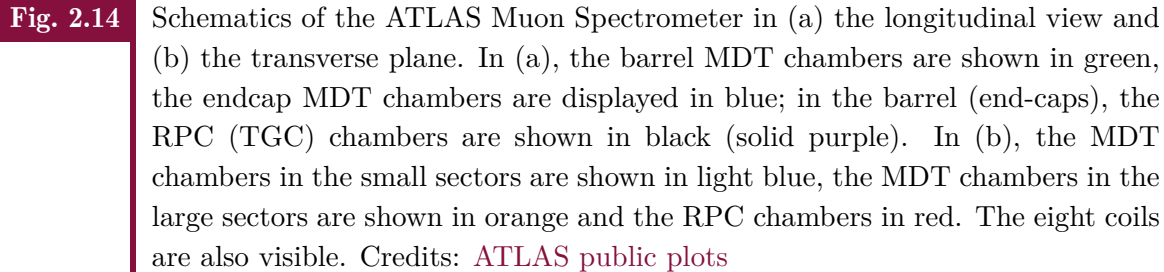
to the beam axis, positioned with $|z|$ at 7.5 m, 14 and 21 m. The tubes provide a space-point resolution of $80 \mu\text{m}$. The MDTs are exhibited in the cyan parts of Figure 2.14(a).

2.2.5.2 Cathode Strips Chamber

The Cathode Strip Chambers are specialized muon detectors situated in the forward regions ($2.0 < |\eta| < 2.7$) at $|z| = 7.4$ m, closest to the beam axis, where particle fluxes are highest. These detectors are designed to withstand the intense radiation and high particle rates characteristic of these areas. The CSCs feature a multi-layer structure, with each layer consisting of gas-filled chambers bordered by cathode plates segmented into strips and interspersed with anode wires. When muons pass through these chambers, they ionize the gas, and the resultant electrons drift toward the anode wires, inducing signals on the cathode strips. These signals are then processed to precisely determine the muons' paths. The spatial resolution of single chamber in the bending plane is about 40 to $60 \mu\text{m}$, while the resolution is about 5 mm in the second coordinate. The high granularity of the cathode strips, combined with the fast response of the gas ionization process, enables the ATLAS CSCs to provide accurate and reliable tracking information for muons even in the challenging conditions near the LHC beam line.

2.2.5.3 Resistive Plate Chambers

The Resistive Plate Chambers are the primary components to contribute to the muon identification and precise measurement of muon trajectories. They are essential for the ATLAS trigger system to select potentially interesting events for further analysis, providing a fast response to the high particle rates produced by the LHC. As shown in Figure 2.14(a), the RPCs are positioned in the barrel region ($|\eta| < 1.05$), sandwiched between other muon detectors like the MDTs and CSCs in regions of higher muon flux. The structure of individual RPC is gaseous detectors made from two parallel resistive plates, usually constructed from materials like bakelite or glass, with a gas-filled gap in between. The gas mixture typically includes components



2.2.5.4 Thin Gap Chamber

The Thin Gap Chambers in Figure 2.14(a) are crucial components of the MS, especially in the end-cap regions ($1.05 < |\eta| < 2.4$) where the magnetic field geometry and particle fluxes present unique challenges, ensuring comprehensive muon detection coverage across a wide range of angles. TGCs, like RPCs in the barrel section, are tasked with providing fast and accurate muon triggering and tracking capabilities. A TGC consists of a series of closely spaced parallel wire planes, with a thin gas gap between each plane. The wire planes are sandwiched between graphite-coated cathode planes. This design allows for a high-density, high-efficiency detection area within a relatively compact space. TGCs operate with a gas mixture that typically includes carbon dioxide (CO_2) and n-pentane (C_5H_{12}). This mixture is chosen for its properties that allow for fast drift times and efficient ionization by passing charged particles, such as muons. Their design enables them to maintain performance stability and reliability even under the intense bombardment of particles. The spatial resolution of TGCs is optimized for their role in the end-cap regions, providing the necessary precision for triggering decisions and initial trajectory measurements. While specific resolution figures can vary, TGCs generally achieve spatial resolution in the order of a few millimeters, balancing the need for speed and accuracy in

muon detection. Similar to RPCs, TGCs provide excellent temporal resolution, crucial for the ATLAS experiment's triggering system. This allows for the rapid identification and processing of muon events within the tight time constraints imposed by the LHC collision rate. TGCs work in conjunction with other types of detectors in the muon spectrometer, such as MDTs and CSCs, to provide a comprehensive muon detection and measurement system. Their ability to quickly and accurately identify muon tracks complements the high-precision tracking capabilities of these other detectors.

2.2.6 Trigger and Data Acquisition System

The Trigger and Data Acquisition System (TDAQ) [74] is designed to select potentially significant collision events from the vast number of particle interactions occurring each second. The high collision rate at the LHC makes it impractical to store all data, necessitating a real-time event filtering mechanism to handle and process the vast data volumes produced by particle collisions within the ATLAS detector.

With a brief bunch crossing interval of 24.95 ns (Table 2.1), the system requires distinct trigger levels to reduce the event rate for feasible data storage. During the Run-2 phase of the ATLAS experiment at the LHC, the ATLAS Trigger and Data Acquisition System (TDAQ) [74], depicted in Figure 2.15, was implemented as a two-level architecture, formed by the first-level trigger (Level-1) and the High-Level Trigger (HLT).

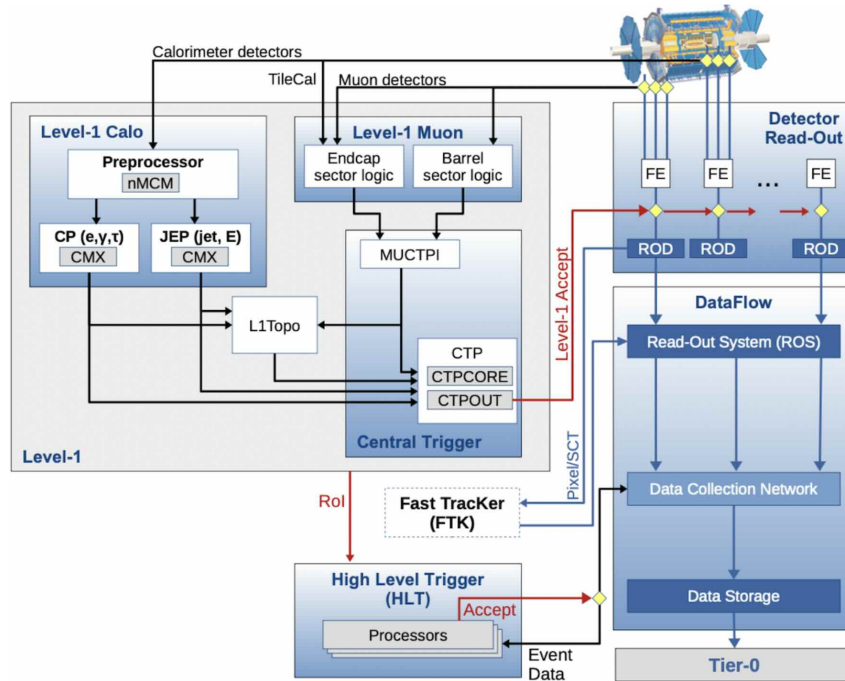


Fig. 2.15 Flow chart of the ATLAS TDAQ system showing the trigger components, detector read-out and data flow. Credits: [ATLAS](#)

2.2.6.1 Level-1 Trigger

The Level-1 (L1) trigger system is primarily hardware-based, designed to rapidly process detector data and make prompt decisions on whether to retain or discard an event. It reduces

the event rate from up to 40 MHz to approximately 100 kHz using custom electronics and swift algorithms. The L1 trigger utilizes preliminary data from detector subsystems, such as calorimeters and muon chambers, to identify potentially significant physics events, including high-energy jets, electrons, photons, muons, and missing transverse energy.

As shown in Figure 2.15, the L1 trigger comprises several subsystems: the L1 Calorimeter Trigger (L1Calo), L1 Muon Trigger (L1Muon), L1 Topological Trigger (L1Topo), and the Central Trigger Processor (CTP). The L1Calo analyzes energy patterns from the Electromagnetic and Hadronic Calorimeters to identify physics objects and detect missing transverse energy in real-time. The L1Muon uses inputs from the Resistive Plate Chambers and Thin Gap Chambers to perform preliminary identification and selection of muon events, evaluating their momenta and trajectories. The L1Topo, employing dual FPGA-based processors, conducts kinematic selections of events using data from the L1Calo and L1Muon systems.

The CTP coordinates and synchronizes the L1Calo, L1Muon, and L1Topo triggers, consolidating information to determine if an event should proceed to the High-Level Trigger (HLT) for further analysis. It also manages dead time, minimizing intervals after event selection during which the system cannot record subsequent events, thereby enhancing overall efficiency. The L1 trigger is characterized by its minimal latency, typically around 2.5 microseconds, crucial for keeping pace with the high collision rate of the LHC.

2.2.6.2 High Level Trigger

The Regions-of-Interest (RoIs) identified by the Level-1 trigger are passed to the High-Level Trigger (HLT), a sophisticated software-based system designed for rapid event kinematics reconstruction and application of specific selection criteria based on predefined trigger algorithms. The HLT is supported by a robust computing network that performs detailed analysis of preliminarily filtered events, utilizing data from all detector segments for complex reconstructions and selections.

Integrated with the ATLAS data acquisition system, the trigger mechanism ensures efficient and continuous data flow and archival. Events meeting HLT specifications are subsequently processed for offline reconstruction and analysis.

2.3 Upgrade and Data Acquisition in Run-3

After several years of intensive operational activities, the ATLAS Experiment embarked on its second maintenance phase, officially designated as *Long Shutdown 2* (LS2), spanning from 2018 to 2021. This period allowed critical upgrades and maintenance tasks on the experimental infrastructure. A multitude of sub-detectors within the ATLAS framework underwent enhancements, incorporating cutting-edge technologies to bolster their operational efficacy in anticipation of the higher collision energy and instantaneous luminosity anticipated in Run-3 [75]. In parallel, the Large Hadron Collider, along with its ancillary accelerator systems, received substantial upgrades. Following the conclusion of LS2, the LHC resumed operations, setting a new worldwide energy record with stable-beam collisions achieving 13.6 TeV. This achievement marked the beginning of a new data-taking phase, denoted as Run-3. As of the current date, data collection activities for Run-3 by the LHC and ATLAS have been ongoing for more than

two years (2022-2024). Subsequent sections provide a detailed account of the upgrades undertaken and the data acquisition processes in Run-3.

2.3.1 ATLAS Phase-I Upgrades for Run-3

The planned timetable for the LHC and HL-LHC projects is depicted in Figure 2.16. Throughout the duration of the LS2 phase, notable enhancements were implemented within the injector complex, most prominently the integration of a new linear accelerator (LINAC-4) [76]. This development aimed at augmenting the injection beam energy of the Proton Synchrotron Booster to facilitate a reduction in beam emittance. Additionally, novel cryogenic plants were established to delineate the cooling circuits for the superconducting radio frequency cavities distinct from those allocated for the superconducting magnets. The installation and commissioning of the ATLAS Phase-I Upgrade were pivotal events during LS2 as described in the following sections.



Fig. 2.16 Latest Time schedule of LHC/HL-LHC Plan (until February 2022) is shown. Until the thesis, ATLAS Phase-I Upgrade during LS2 was completed and the data-taking for Run-3 is ongoing. There the center-of-mass collision energy was increased to 13.6 TeV. The schedule of targeted integrated luminosity is 450 fb^{-1} during full Run-3. Credits: CERN

2.3.1.1 New Small Wheel Upgrades

The New Small Wheel Detectors (NSW) [77] represent an upgrade of the muon spectrometer in the end-cap regions. These detectors have been juxtaposed with the extensive 25-meter diameter *big wheel* detectors of ATLAS, positioned within the innermost layer of the forward muon spectrometer and the outer confines of the ATLAS experiment. Their primary function is to improve the robustness of muon tracking over the whole (HL-)LHC lifetime. This milestone was achieved following nearly a decade of meticulous planning, design, construction, and assembly efforts by the ATLAS collaboration, culminating in the realization of this advanced muon detector.

The NSW detectors incorporate two novel gaseous detector technologies: micro-megas (MM) and small-strip thin-gap chambers (sTGC). These technologies provide rapid and precise muon-tracking capabilities due to their small gap (5mm) and strip pitch (approximately 0.5mm), a feature critical for enhancing the spatial resolution offered by the NSW. The superior spatial resolution (100 μm) and angular resolution (approximately 1 mrad) of the NSW plays a crucial role in enabling the ATLAS trigger system to accurately ascertain whether a muon candidate has emanated from the interaction point, thereby significantly reducing the likelihood of recording data from extraneous background events.

2.3.1.2 Liquid Argon Calorimeter Upgrade

The Liquid Argon Calorimeter plays a key role within the ATLAS online event-selection framework. During LS2, new digital electronics for the LAr calorimeter was introduced to enhance the efficacy of trigger selection by offering improved resolution and greater granularity within the electromagnetic calorimeter trigger. These advancements in front-end electronics amplify the volume of information accessible at the trigger level by a factor of ten, thereby augmenting the system's proficiency in discriminating against jets while ensuring the efficient retention of electrons and photons.

Employing a novel, more refined granularity scheme called *Super Cells* [78], the calorimeter trigger is now fed with data from each layer of the calorimeter, enriching the detail and precision of the information gathered, while maintaining the functionality of the existing *legacy* trigger system. Furthermore, the calorimeter's original boards were revalidated during the Long Shut-down 2 period, ensuring a seamless continuation of operations amidst the upgrade process.

2.3.1.3 New Muon Chambers

The ATLAS experiment has been augmented with the addition of new muon chambers, comprising eight small-diameter Monitored Drift Tube (sMDT) modules and sixteen next-generation Resistive Plate Chambers [79]. These detectors have been specifically designed to endure increased particle fluxes and offer dependable standalone muon verification. The incorporation of these detectors into ATLAS significantly enhances the muon trigger coverage, a development that will prove to be crucial for the operational demands of the HL-LHC.

These novel muon chambers are distinguished by their compact design, representing an initial trial of the technology set to be employed in the forthcoming phase-2 upgrades for the HL-LHC. Notably, these installations introduce the first RPC chambers to the innermost layer of the muon spectrometer, in a sector referred to as BIS78, leading to more accurate momentum measurements for muons traversing these specific areas. Moreover, the newly installed sMDT chambers are characterized by their reduced tube diameter—15mm as opposed to the 30mm diameter of the conventional MDTs, thereby enhancing the rate capability by an order of magnitude. This improvement is essential for adapting to the highly demanding conditions anticipated in the HL-LHC era.

2.3.1.4 ATLAS Trigger Upgrades

The Trigger and Data Acquisition System has received enhancements in both its hardware and software components [80]. These upgrades enable the system to identify a broader array of collision events while keeping within the pre-established acceptance rate.

The aforementioned enhancements to the Liquid Argon calorimeter have augmented the granularity of data accessible to the trigger system. With this refined resolution, the system is equipped to more effectively filter out irrelevant background events. The calorimeter trigger has been modernized with the incorporation of large-scale Field-Programmable Gate Arrays, which can execute in real time more intricate algorithms for the identification of physics objects and to ascertain missing energy within the events with elevated precision.

Additionally, the New Small Wheel system and the BIS78 installations, previously discussed, span the transitional region between the barrel and end-cap sections of the ATLAS detector. This strategic placement enhances the trigger system's proficiency in accurately identifying muons and is anticipated to halve the rate of event selection.

In a significant overhaul, the software-based High-Level Trigger was entirely redeveloped to function within the multi-threaded software framework of the ATLAS experiment, AthenaMT. This redevelopment facilitates the execution of trigger algorithms and establishes a shared foundation between the trigger software and the offline software employed for reconstruction and physics analysis.

These advancements are poised to play a pivotal role during the LHC Run-3, a phase that will necessitate the allocation of substantial High-Level Trigger resources towards the execution of computationally demanding particle tracking tasks.

2.3.2 Performance and Data Acquisition Status

Figure 2.17(a) shows the total integrated luminosity of proton-proton collision in Run-3. The total delivered luminosity by LHC is around 175 fb^{-1} until 19 August 2024, while the total recorded luminosity by ATLAS is around 164 fb^{-1} . The pile-up distribution is shown in Figure 2.17(b). The value is 34 in the case of $\sqrt{s} = 13 \text{ TeV}$ during Run-2, while it increased to 52 at $\sqrt{s} = 13.6 \text{ TeV}$ during early Run-3.

By the end of Run-3, we expect the dataset available for analysis to expand threefold. Additionally, the increased collision energy will enhance the scope of our physics program, including an 11% boost in the production rate of Higgs boson pairs compared to Run-2. The enhancements to the ATLAS detector, its trigger system, software/computing frameworks, and analysis techniques will open new avenues for discovering phenomena such as feebly interacting or long-lived particles and allow for more precise tests of the Standard Model. Furthermore, ATLAS will broaden its investigation into less common processes, including Higgs boson decays into muon pairs, the generation of Higgs boson pairs, the production of triple gauge bosons, and the creation of quadruple top quarks.

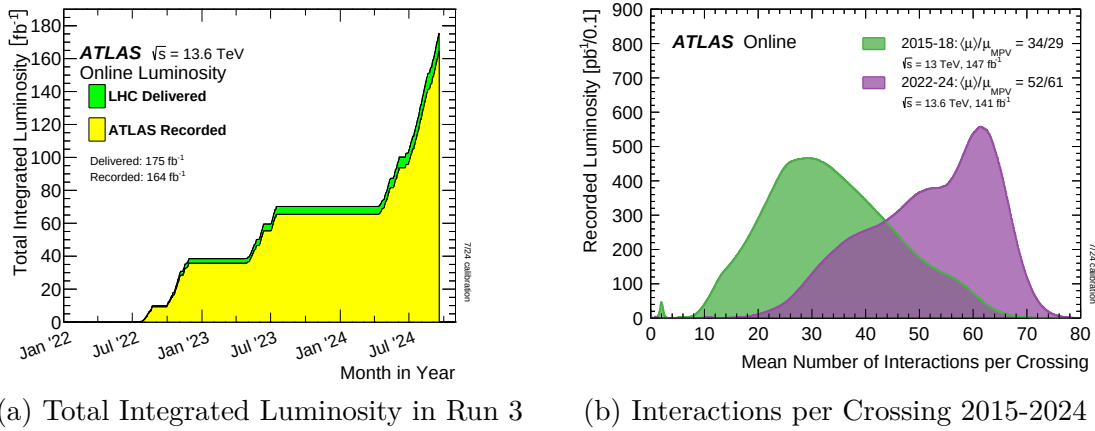


Fig. 2.17 (a) Total integrated luminosity in Run 3 at 13.6 TeV. Integrated luminosity versus time delivered to LHC (green) and recorded by ATLAS (yellow) during stable beams for pp collisions at $\sqrt{s} = 13.6$ TeV in LHC Run 3 (2022-2024). (b) Average number of interactions per crossing 2015-2024. The recorded luminosity versus the pile-up is shown, green for Run-2 and purple for early Run-3. Credits: ATLAS

CHAPTER 3

Detector Simulation and Object Reconstruction

The LHC accelerates protons in two opposite directions and collides them in the interaction point located at the center of the ATLAS detector. The particles produced in these collisions, or their hadronization and decay products, traverse the ATLAS detector and interact with the detector material. The charges or light generated by these interactions induce electric signals at the collecting electrodes of the various sub-detectors. These are filtered and recorded by the trigger and data acquisition system, and then reconstructed and analyzed off-line. The expected detector response to these particles is determined with a detailed simulation based on the Geant4 package [81], and further calibrated in data with control samples enriched in particles of a given species. Both simulated events and raw data undergo the same reconstruction algorithms.

Simulation in ATLAS uses sophisticated software models to predict particle interactions with the detector components, crucial for designing the detector and interpreting real data. Object reconstruction involves converting raw data from millions of sensor hits into meaningful information about particles created in collisions. This process includes identifying and reconstructing tracks and energy deposits, which can be attributed to various particles such as electrons, photons, and jets. These reconstructed objects are then used to study fundamental particles and forces, testing the Standard Model predictions and searching for new physics.

The architecture of the *ATHENA* framework [82], the primary software infrastructure of the ATLAS collaboration, is shown in Figure 3.1. It is designed based on the Gaudi framework [83], which supports numerous applications through base classes and common functionalities, as well as communication tools for various components. *ATHENA* includes simulation, reconstruction, and derivation tools, enabling extended physics analysis by looping over the input dataset from particle collisions.



Fig. 3.1

3.1 Monte Carlo Production

As illustrated in Figure 3.1, the standard full simulation chain in ATLAS consists of several steps, that can be grouped in three main parts: the generation of physical collision events, including the following decays of unstable particles and quark and gluon hadronization; the simulation of interactions between the final stable particles and detector materials; and the digitization of energy deposited in various regions of the detector. Each step produces a dedicated output data format, which serves as the input for the next step [84]. This simulation chain is based on the Monte Carlo method, a statistical technique used to simulate the random behavior of particles in the detector.

Both real collision data and simulation samples are processed by the same ATLAS trigger system, reconstruction, and derivation procedures. This ensures consistency and accuracy in the analysis. This section will describe the details of each step in the workflow.

3.1.1 Event Generation

Event generation is the first step of the simulation. Monte Carlo (MC) generators implement theoretical calculations of various elementary cross-sections and use them to generate, on a statistical basis, a list of particles produced in the collision and their energies and directions. Common generators include PYTHIA 8 [85], PowHeg [86], MadGraph [87], and Sherpa [88], which provide interfaces to the *ATHENA* framework. The generated events are stored temporarily in *EVNT* files.

During the generation process, *stable* particles with $c\tau > 10mm$ are recorded and propagated to interact with the detector before decaying. Particles with short lifetimes are decayed during the generation process without accounting for interactions with the detector, meaning their

interactions with materials and magnetic fields are ignored. Specific filters might be applied to events during generation to enhance some regions of phase space.

3.1.2 Detector Simulation

Events from the generation step are fed to a simulation of the detector response. In ATLAS, two primary simulation approaches are used to meet the statistical requirements of various physics analyses: *Full Simulation* and *Fast Simulation*.

The Full simulation is based on Geant4, and implements a detailed description of the geometry (size and materials) of the ATLAS detector. Geant4 is an open-source software package that provides fundamental physics models and particle transportation mechanisms to describe the propagation of generated particles from the pp collision into the material of the ATLAS detector. During the simulation, all possible decays and interactions with the detector material are considered. All energy deposits into the sensitive volumes of each sub-detector, along with their truth information regarding the creation or destruction of particles, are recorded in *HITS* files.

Due to the considerable CPU resources required for the fine-granularity calorimeter shower simulations, ATLAS has developed tools with parameterization-based and deep learning algorithms to replace the Geant4 simulation [89] with a Fast simulation. The fast-simulation used for the analysis of Run 2 data is called ATLFAST-II; an improved version, called ATLFAST-III, with more accurate parametrization, is being developed [90].

3.1.3 Hits Digitization

Upon completion of the detailed simulation using the Geant4 toolkit or ATLFAST, the energy deposits within the sensitive volumes of the detector are written into the *HITS* file. The digitization process converts these HITS, which emulate the electronic response of the detector, into actual data signals such as voltage levels or timing information at the pre-amplifier outputs. Additional truth and metadata information generated during digitization are recorded in Raw Data Objects (*RDO*) files. The digitization step also provides input for the hardware trigger.

In this context, the proton-proton collision of interest is considered the signal or hard-scattering process, while other proton-proton collisions are treated as background events, known as *pile-up*. The MC overlay [91] is designed to simulate the real data environment by adding pile-up events from additional minimum bias collisions to the signal events.

3.2 Object Reconstruction

The digitized signals are fed to the trigger system (in the case of real data) or to its simulated emulation (for simulated events), and the RAW data selected by the trigger system are stored at the main LHC computing center, the Tier-0 site at CERN, and backed up by the Tier-1 sites, large computing facilities located abroad and connected through the Worldwide LHC Computing Grid (WLCG). The following stages are the same for both simulated and actual particle collision data, and involve the reconstruction process. Figure 3.2 illustrates the nominal data flow of the reconstruction chain.

Before the physics streams, a calibration loop begins at the Tier-0 site. The data are used to update calibration constants and detector conditions in the condition database, addressing issues such as electronic noise, data corruption, disabled modules within sub-detectors, and the alignment of detector components. Once the calibration is completed, the data are transferred to the Tier-1 sites for further reprocessing. This procedure employs a uniform set of algorithms for both data types, except for those specifically addressing truth information. The reconstruction process generates Analysis Object Data (AOD) outputs, which provide a summary of the reconstructed event. These outputs are formatted in xAOD, a format compatible with both *ATHENA* and ROOT, facilitating further manipulation for user analysis.

In practical applications, xAODs are typically further processed to produce derived-xAODs (DAODs), or derivations, which are then utilized as input for physics analysis.

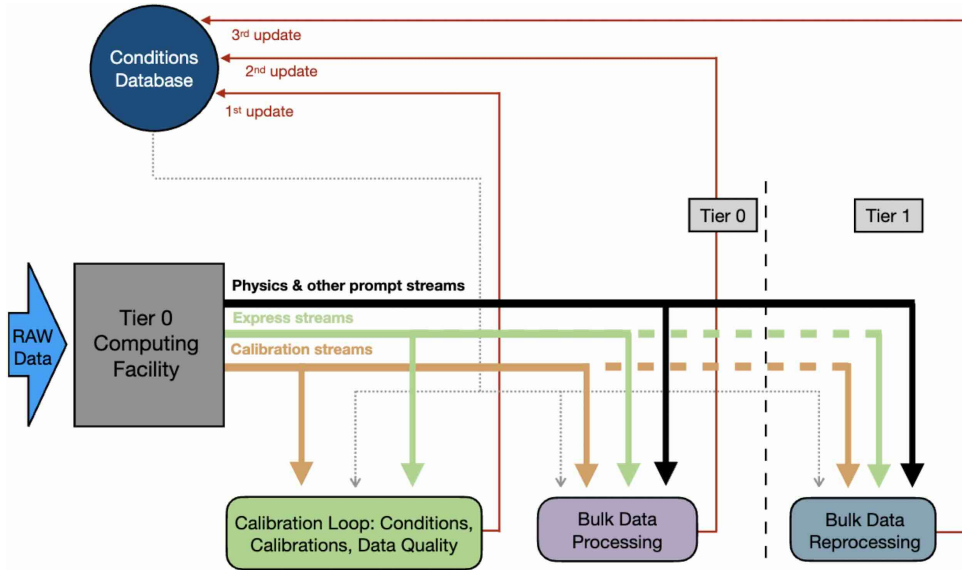


Fig. 3.2 Schematic flow chart of ATLAS data processing from the reconstruction to the data reprocessing stage.

The ATLAS detector primarily aims at measuring the momentum of charged particles through its tracking detectors (the inner detector and muon spectrometer) and the energy deposited by particles as they pass through its calorimeter systems (LAr and Tile calorimeters). Additional information such as detailed shower shapes in the calorimeters or track impact parameters are used for discrimination between different particle hypotheses. By integrating information from the various detector subsystems, the offline algorithms can reconstruct various physics objects, including charged particle tracks, primary vertices, calorimeter energy clusters, electrons, photons, muons, τ -leptons, jets, and event-level quantities such as E_T^{miss} . The following sections will describe the reconstruction of these objects in detail.

3.2.1 Photons

For the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis in Chapter 5, events with at least two photon candidates are required. This subsection will discuss the reconstruction, identification and isolation algorithms for photon candidates in the ATLAS experiment during the LHC Run-2.

3.2.1.1 Reconstruction and Calibration Algorithms

Photon objects are reconstructed and identified using the cluster information from the EM calorimeter and track information from the ID detector [92, 93]. First of all, dynamic, variable-sized topological clusters (topo-cluster) are formed from the cells of the EM and hadronic calorimeter. The EM energy of a cluster is determined by summing the energies of all the calorimeter cells within the cluster. Initial EM topo-clusters must require an EM energy exceeding 400 MeV and an EM-to-total energy ratio above 0.5 [94]. These EM topo-clusters are then further utilized to the photon reconstruction process.

Tracks are reconstructed in the ID detector and loosely matched to the fixed-sized clusters by using a sliding-window algorithm on EM calorimeter cells. In order to account for the energy loss from electron bremsstrahlung, the Gaussian Sum Filter (GSF) algorithm [95] is applied to refit the tracks to improve the accuracy of the track parameters. These tracks are then combined with the EM topo-clusters to identify the different photon objects.

Depending on the number of conversion vertex candidates in the ID matched to the EM cluster, the initial photon candidates is classified as either converted or unconverted candidates. A converted photon candidate is reconstructed from an EM topo-cluster that is matched to one or several conversion vertices. The conversion vertex candidates are built from the tracks in the ID detector. Two types of conversion vertices are considered: two-track vertices formed by opposite-charged tracks with invariant mass close to zero, and single-track vertices from single electron tracks without hits in the innermost layers of the detector. The tracks are further extrapolated to the second layer of the ECAL to perform the matching of the conversion vertices to the EM topo-cluster. Vice versa, an EM topo-cluster without any conversion vertex matched is considered as an unconverted photon candidate. The fraction of converted photons depends on the amount of material upstream of the ECAL and varies from 20% in the central region to 65% in the end-caps.

If an electron from a photon conversion undergoes bremsstrahlung radiation, typically occurring in the bending plane, it may be reconstructed as two separate clusters. To resolve this, nearby EM topo-clusters are merged into a final EM cluster, so-called supercluster. The process starts with the highest-energy cluster, merging nearby clusters within $\Delta\eta \times \Delta\phi = 0.075 \times 0.125$ unless already used. For converted photons, clusters within $\Delta\eta \times \Delta\phi = 0.125 \times 0.3$ are included if their best-matched track or conversion vertex matches the original. These final EM clusters, or superclusters, are retained as photon objects.

After the superclusters are built, the initial position corrections and energy calibrations are applied to them, and the track and conversion vertex matching procedures are repeated to construct the final photon objects. The energy calibration is performed for the uncalibrated objects using a multivariate (MVA) regression algorithm, based on boosted decision trees (BDT) to obtain the correction factors to correct for (1) the energy loss of the clusters in the inactive material before the calorimeter and (2) non-full longitudinal and lateral containment of the shower in the cluster. The various correction factors are applied to the converted and unconverted photon candidates [96]. Figure 3.3 shows the expected energy resolution $\sigma_{E_{calib}}/\sigma_{E_{gen}}$ of reconstructed photons in the simulation after the calibration, estimated from the interquartile range of the distribution of the energy ratio E_{calib}/E_{gen} .

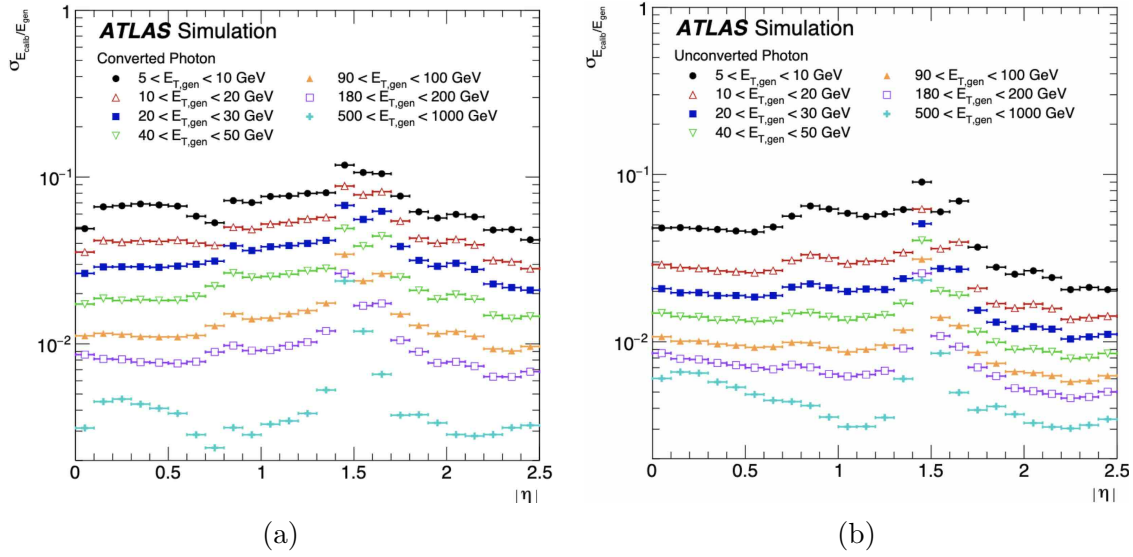


Fig. 3.3 Calibrated and reconstructed energy resolution $\sigma_{E_{calib}}/\sigma_{E_{gen}}$ as a function of $|\eta|$: (a) converted photons and (b) unconverted photons.

3.2.1.2 Identification and Isolation Algorithm

After the photon candidates are reconstructed and calibrated, the identification and isolation criteria are applied to select prompt, isolated photons and suppress backgrounds from hadronic jets. The photon identification algorithm is implemented by a cut-based method on the basis of some shower-shape discriminating variables [94]. Prompt photons typically generate narrower energy profiles in the electromagnetic calorimeter and exhibit reduced leakage into the hadronic calorimeter compared to background jets. To satisfy the identification criteria, photon candidates are thus required to deposit only a minimal fraction of their energy in the hadronic calorimeter, and their lateral shower shape must be consistent with that expected from a single electromagnetic shower.

Two reference selection criteria are employed: a loose criterion, which utilizes information solely from the second layer of the EM calorimeter and the hadronic calorimeter, primarily for purposes such as triggering and preselections, and a tight criterion, which incorporates additional information from the fine segmentation of the first layer of the EM calorimeter. The tight selection requirements are optimized separately for converted and unconverted photon candidates due to their different shower shape distributions, due for instance to the opposite-charge electron-positron tracks from a conversion opening up in the azimuthal plane, leading to wider showers along the ϕ direction.

The efficiency performance of tight photon identification is assessed in data using three distinct control samples [94], either enriched in inclusive photon production from QCD Compton scattering (*Matrix Method*), or in photons radiated from leptons in $Z \rightarrow l\bar{l}\gamma$ decays (*Radiative Z*), or in electrons from $Z \rightarrow e\bar{e}$ decays where the electron shower shapes are transformed to resemble photon shower shapes by means of a Smirnov algorithm (*Electron Extrapolation*). All these efficiency measurements require as preselections that the photon candidates are isolated from hadronic activity (as described later) and pass a looser identification working point.

To correct the MC simulation for efficiency differences with the data, efficiency scale factors are obtained by calculating the ratio between the data efficiency and MC efficiency as a function of conversion type and in bins of photon candidate transverse energy $E_T = E \sin \theta$ and η . The scale factors are then used to correct the simulation. The efficiencies of the photon identification with these three methods for unconverted and converted photon candidates are shown in Figure 3.4. The data-MC efficiency scale factors are also displayed for each measurement and the final combined scale factor is estimated by a weighted average of scale factors from individual measurements.

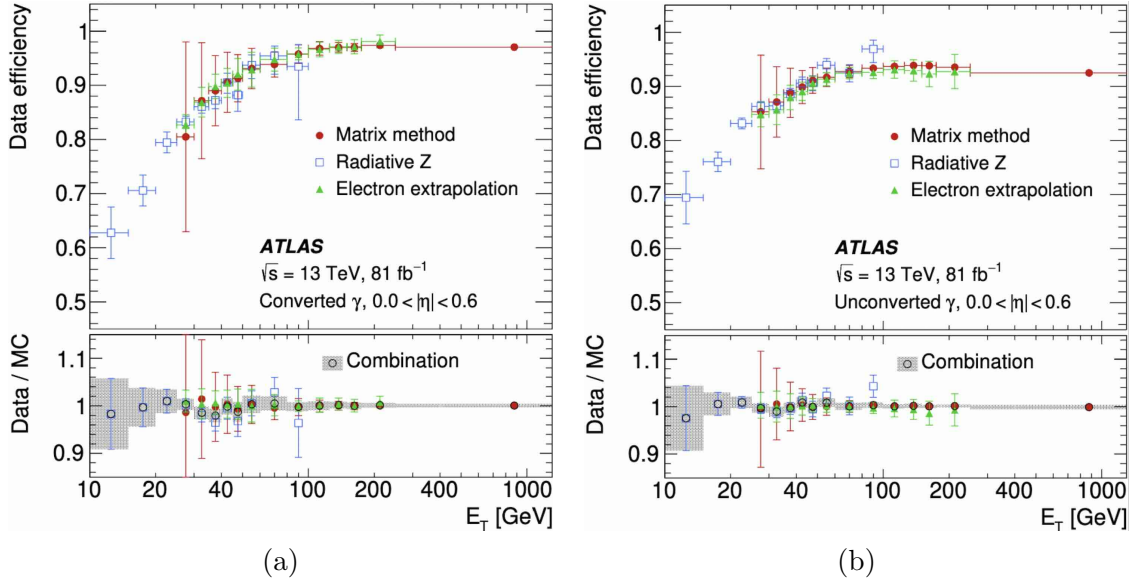


Fig. 3.4 Photon identification efficiency and the ratio of data-to-MC efficiencies with three efficiency methods for (a) converted photons and (b) unconverted photons as a function of E_T for $|\eta| < 0.6$. The combined scale factor is obtained using a weighted average of scale factors from individual measurements and the total uncertainty is shown in the band region.

To further reject some hadronic jet backgrounds, isolation criteria based on the tracks in the tracking detector and the energy deposits in the calorimeter are applied to photon candidates. The *calorimeter isolation* (E_T^{coneXX}) is calculated as the sum of the transverse energy of the positive-energy topological clusters within a cone ΔR around the photon candidate, corrected by subtracting the energy deposits from the photon itself (in the core of the cluster and leaking outside of the cluster but inside the isolation cone) and from pile-up:

$$E_T^{\text{coneXX}} = E_{T, \text{raw}}^{\text{isolXX}} - E_{T, \text{core}} - E_{T, \text{leakage}}(E_T, \eta, \Delta R) - E_{T, \text{pile-up}}(\eta, \Delta R) \quad (3.1)$$

where XX represents the cone size and $\Delta R = \text{XX}/100$ is the cone radius. The photon working points consider two cone sizes $\Delta R = 0.2$ and 0.4 . The *track isolation* (p_T^{coneXX}) is calculated by the sum of the transverse momenta of the tracks within a cone along the photon cluster direction, excluding the tracks matched to electrons or converted photons. The tracks must have $p_T > 1$ GeV and $|\eta| < 2.5$, more than seven silicon hits, at most one shared hits, at most

two silicon holes, at most one pixel hole [94], and the longitudinal impact parameter relative to the selected primary vertex must satisfy $|\Delta z_0| \sin \theta < 3$ mm. Three isolation requirements listed in Table 3.1 are defined using the above isolation variables.

Operation Point	Calorimeter Isolation	Track Isolation
Loose	$E_T^{\text{cone20}} < 0.065 \times E_T$	$p_T^{\text{cone20}} / E_T < 0.05$
Tight	$E_T^{\text{cone40}} < 0.022 \times E_T + 2.45 \text{ GeV}$	$p_T^{\text{cone20}} / E_T < 0.05$
TightCaloOnly	$E_T^{\text{cone40}} < 0.022 \times E_T + 2.45 \text{ GeV}$ at $p_T = 1 \text{ TeV}$	-

Tab. 3.1 The definition of photon isolation working points.

The calorimeter isolation efficiency is measured and illustrated in Figure 3.5. The differences between data and MC simulation are also displayed. As for the identification algorithms, the efficiency of the isolation algorithms is calibrated with data control samples and data/MC efficiency scale factors are extracted and used to correct the simulation.

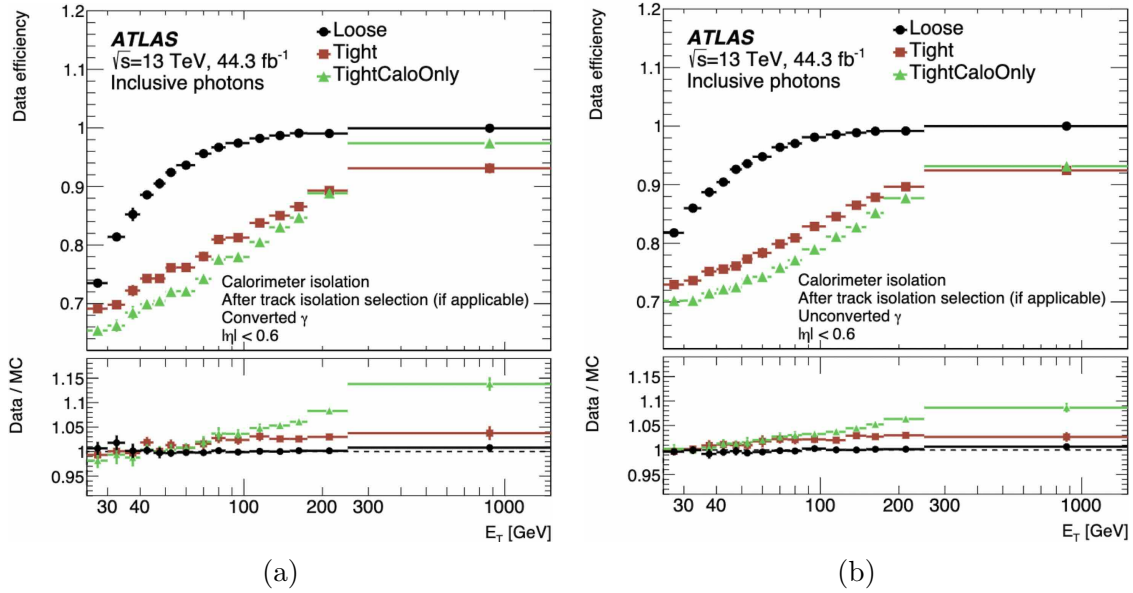


Fig. 3.5 Calorimeter isolation efficiency in data (top panel) and ratio of data-to-MC efficiencies (bottom panel) from inclusive photon samples for (a) converted photons and (b) unconverted photons as a function of E_T for $|\eta| < 0.6$.

The performance of the tight photon identification algorithm in the tight menu during Run-2 exhibits a notable degradation in efficiency at high levels of pile-up, as demonstrated in Figure 3.6. This dependence on pile-up is anticipated to become more pronounced during Run-3 and at the HL-LHC, where the average number of pileup interactions per bunch crossing is expected to increase to approximately 80 and 200 [97], respectively. In response to this challenge, a novel set of photon identification criteria has been developed, incorporating μ -dependent selection requirements to mitigate the adverse effects of pile-up on photon identification efficiency. The optimization of these identification algorithms has been performed using simulated samples of prompt and background photons, which will be described in Chapter 4.

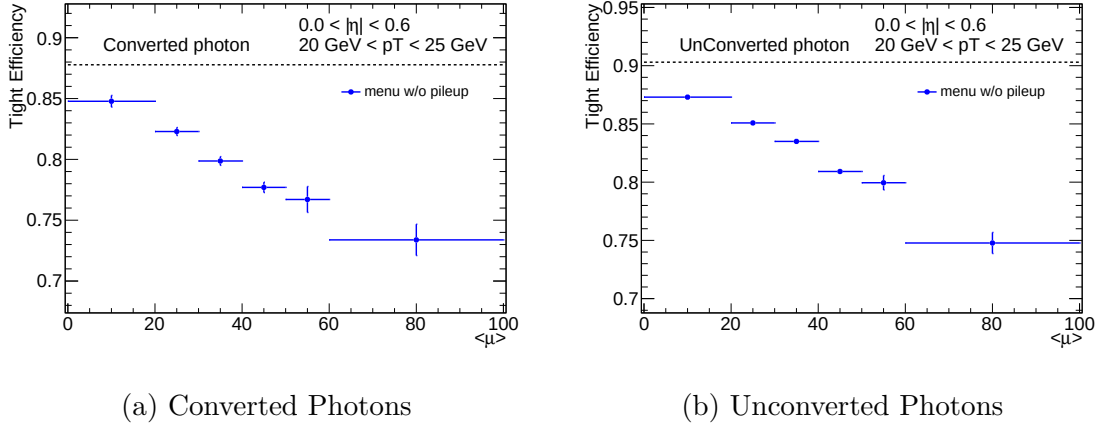


Fig. 3.6 Dependence on pile-up of photon identification efficiency of the Run-2 criteria at $|\eta| < 0.6$ using prompt photons with $20 \text{ GeV} < p_T < 25 \text{ GeV}$: (a) converted photons and (b) unconverted photons.

3.2.2 Electrons

The interaction of electrons with the detector material is governed by electromagnetic forces. In ATLAS, the inner detector and the electromagnetic calorimeter systems provide samplings of the electron trajectory and energy. The procedures for the reconstruction and calibration of electrons are similar to those for photons [94, 96].

Electron candidates are reconstructed using a topological cell clustering algorithm. The raw cluster energy is then calibrated using a multivariate regression method based on a BDT trained on simulated event samples of prompt electrons, with additional data-to-simulation correction factors determined from pure control samples of electrons from the decays of narrow resonances (Z , J/ψ) to electron pairs. The identification of electron candidates involves matching reconstructed tracks and interaction vertices to the cluster, ensuring that each candidate is associated with a single ID track originating from the primary vertex.

A likelihood method is used for electron identification, incorporating criteria such as shower shape, track-cluster matching, and amount of transition radiation produced in the TRT. The identification efficiency increases from 70% at $E_T = 20 \text{ GeV}$ to 90% as a function of transverse energy. Figure 3.7 illustrates the electron reconstruction and identification process in ATLAS.

Non prompt electrons, such as those from semi-leptonic decays of heavy-flavour quarks in jets, are further suppressed by means of an isolation requirement relying on information from both the tracking and calorimeter systems, as detailed in Section 3.2.1.2.

In the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis presented in Chapter 5, events containing isolated electron candidates are vetoed to suppress background from e.g. Higgs boson decays to two photons produced in association with top quark pairs.

3.2.3 Muons

Muons have a clean experimental signature due to their relatively long lifetime and low interaction cross-section with matter, enabling them to traverse the entire ATLAS detector. High-energy muons are produced in many processes of interests and allow relatively easy triggering for

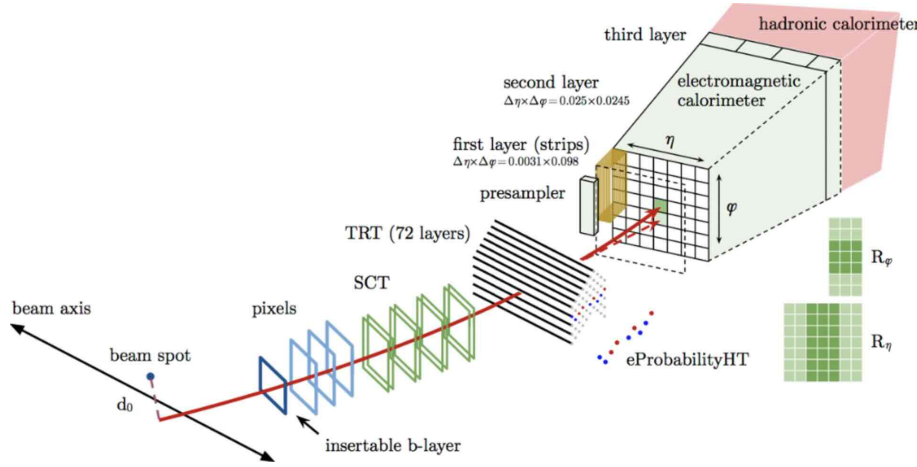


Fig. 3.7 Schematic picture of an electron passing through the ATLAS detector. The solid red line represents the track of the electron while the dashed red line indicates q photon from bremsstrahlung. Credits: [ATLAS](#)

those processes, and their (fast) reconstruction is thus pivotal procedure in high-energy collider experiments. Detection and reconstruction of muons in ATLAS are achieved by combining the information from the inner detector and the muon spectrometer, as elaborated in Section 2.2.5. The magnetic fields from the central solenoids and the air-core toroids are essential for bending the muon tracks and measuring their momenta in the two respective subsystems. Muons are independently reconstructed in both the inner detector and the muon spectrometer, and the resulting track collections are subsequently combined to form the final muon tracks used in physics analyses [98]. Four types of muon candidates are identified:

- Combined Muons (CB): tracks independently reconstructed in the ID and MS are matched to each other and subjected to a common refit to yield a new track replacing the two initial ones.
- Segment-Tagged Muons (ST): ID tracks are matched to local track segments in the MS.
- Calorimeter-Tagged Muons (CT): ID tracks are matched to energy deposits in the calorimeter compatible with a minimum-ionizing particle. CT muons are defined for the region $|\eta| < 0.1$ and the momentum range $15 < p_T < 100$ GeV, to recover the inefficiency of CB and ID due to a gap near $|\eta| \approx 0$ for routing the services to and from the detector.
- Extrapolated Muons (ME): reconstructed using only the MS tracks with a loose requirement on their origin from the interaction point.

The efficiency of muon reconstruction is measured using the tag-and-probe method with $J/\psi \rightarrow \mu^+ \mu^-$ and $Z \rightarrow \mu^+ \mu^-$ decays [98]. Within the full acceptance region, the reconstruction efficiency of muons is stable and approaches 99%.

To exclude muons from semi-leptonic decays within jets, a muon isolation criterion is employed. The isolation algorithms evaluate the activity surrounding the muon track, within a cone of given radius, by summing the transverse energy of all particles within this cone, excluding the muon itself. A muon is considered isolated if this sum is below a certain threshold.

A calibration of the muon momentum scale is essential to correct for systematic errors in

detector measurements. This involves adjusting the measured energy and momentum of muons to compensate for known biases and inaccuracies in the detector response. The calibration procedures use data from well-understood processes, such as Z boson decays. The distributions of quantities such as the di-muon invariant mass are calculated for data and for simulation with varying sizes of scale and resolution corrections, and the best values of the corrections are those leading to the best agreement between data and simulation [99].

In the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis presented in Chapter 5, events containing isolated muon candidates are vetoed to suppress background from e.g. Higgs boson decays to two photons produced in association with top quark pairs.

3.2.4 Jets

Jets, which are tightly collimated streams of particles, result from the hadronization of quarks and gluons (collectively called *partons*), due to the property of QCD interactions denoted “color confinement”. The ATLAS detector uses an advanced system of tracking detectors, calorimeters, and muon spectrometers to detect and analyze these jets with high precision.

Jets play a crucial role in investigating the Standard Model and exploring new physics, as signal processes such as top quark production, Higgs boson decays, and decays of supersymmetric particles most often lead to production of jets. Accurate jet reconstruction is thus vital for understanding particle interaction dynamics and testing theoretical predictions at the unprecedented energy levels achieved by the LHC.

The ATLAS detector employs sophisticated algorithms to reconstruct jets by clustering calorimeter energy deposits and correlating them with tracks from the inner detector. This approach ensures the precise measurement of their kinematic properties. The following section provides an overview of the reconstruction methods, jet energy scale calibration (JES), and jet flavour tagging algorithms used in ATLAS.

3.2.4.1 Jet Reconstruction Algorithm

As illustrated in Figure 3.8, partons produced from the elementary collision among proton constituents in the interaction point hadronise into hadrons, that deposit energy in the calorimeters and possibly tracks in the inner detector depending on their charge. Nearby calorimeter energy deposits and/or charged particle tracks are grouped together by a clustering algorithm into a single object that serves as a proxy for a parton. Several algorithms can be applied to reconstruct jets combining those information from calorimeter deposits and tracks. In the simulation, similar algorithms can be used to cluster truth-level hadrons or partons to define particle-level or parton-level kinematic observables. Lots of partons are produced in each event so a large number of jets can be reconstructed in a single event.

The clustering algorithms that are available have distinct criteria for constructing jets from calorimeter clusters and tracks, each offering specific advantages and limitations. An algorithm needs to consider the jets size and the Infra-Red and Collinear (IRC) safety requirements. Jet size controls the angular extent of the jet and determines how broad or narrow the reconstructed jets will be. A larger jet size includes more particles, potentially capturing more of the energy from the original parton but also including more background noise. Conversely, a smaller jet size is more precise but might miss some of the energy from the parton. Infra-red safety refers to an

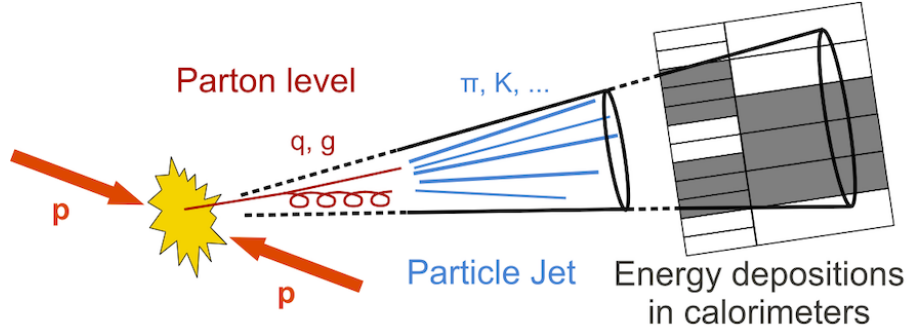


Fig. 3.8 Schematic view illustrating the formation of jets in the ATLAS detector. The partons are generated near the IP of the beam and through the hadronization process to the particle level jets and the energies of the hadronized particles deposits in the calorimeters. Credits: [ATLAS](#)

algorithm's insensitivity to the emission of low-energy (infra-red) particles, indicating that the final reconstructed jet remains unchanged when a soft (low-energy) gluon is added to the event. However, the collinear safety pertains to an algorithm's robustness against the splitting of particles into collinear pairs, where the particles travel in nearly identical directions. An algorithm is considered collinear safe if the "splitting" of a particle into two collinear particles does not modify the final jet configuration. Figure 3.9 provides a comparative analysis of jets produced by four common various clustering algorithms including k_t [100], Cambridge/Aachen [101], SIS-Cone [102], and anti- k_t [103]. In the ATLAS detector, the anti- k_t algorithm implemented in the FASTJET 3.2.2 [104] software package is considered as the default clustering algorithm of finding jets.

The jet clustering is either performed using as inputs "EM topo-clusters", i.e. topological clusters of calorimeter cells calibrated at the electromagnetic energy scale, or "PFlow" candidates, i.e. modified topo-clusters arising from a particle-flow algorithm [106] that also considers information from the tracker: if a charged track points to the cluster, the energies of the cells along the particle trajectory are replaced by the momentum of the track, which in general is determined with better accuracy from the inner detector. A third input set consists of LCW (local cluster weighting) topo-clusters, i.e. clusters where cell momenta have been reweighted based on the calculated probability of the cluster to be due to an electromagnetic or hadronic energy deposit, with weights that attempt to account for non-compensating calorimeter response, signal loss due to clustering thresholds, and energy losses in inactive material.

Two kinds of jets are reconstructed in ATLAS: small- R jets with $R = 0.4$ for partons using PFlow or EM topo-clusters and large- R jets with $R = 1.0$ for massive particles with hadronic decays using LCW topo-clusters. The jets at the reconstructed and uncalibrated levels are required to have $p_T > 7$ GeV and $|\eta| < 4.5$ [107]. Jets overlapping with isolated electrons within $\Delta R < 0.2$ and photons within $\Delta R < 0.4$ are removed in the jet reconstruction. By default small- R jets are reconstructed with the anti- k_t algorithm with $R = 0.4$ from PFlow candidates in ATLAS Run-2 data analyses. The jet energy scale calibration is applied to the reconstructed jets to correct the energy scale and resolution of the jets, which is described in the next section. Furthermore, a ghost matching algorithm [108] is used to associate the reconstructed jets with

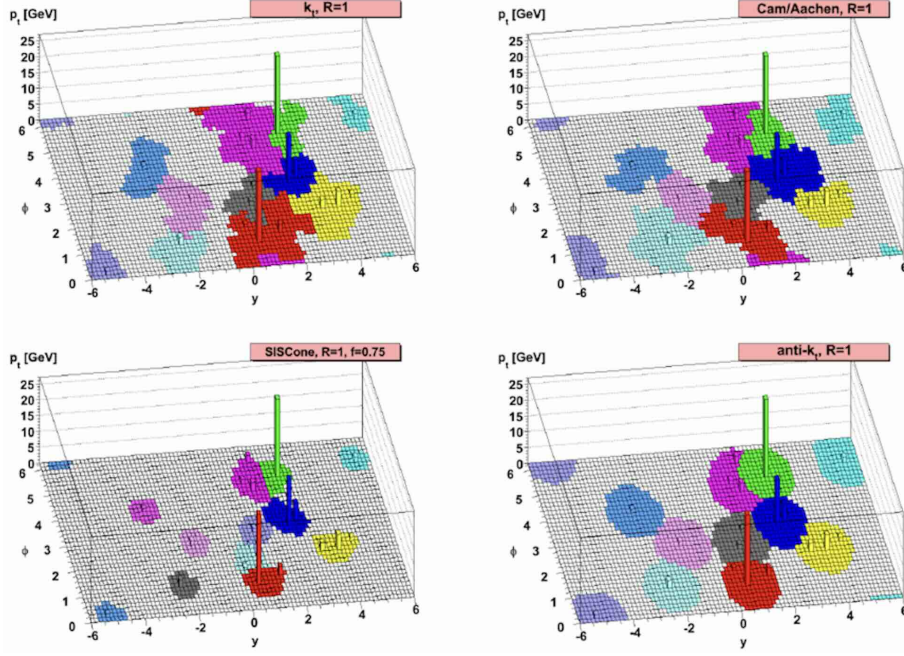


Fig. 3.9 Illustration of various jet clustering algorithms: k_t , Cam/Aachen, SISCone, and Anti- k_t [105].

truth particles in a way that minimizes biases in JES calibration and improves the resolution.

3.2.4.2 Jet Energy Scale Calibration

Jets require a calibration procedure to correct for detector non-uniformities, ensure accurate energy scales, mitigate pile-up and noise effects, improve energy resolution, meet the stringent requirements of physics analyses, reduce systematic uncertainties, enable meaningful comparisons with simulations, and achieve accurate event reconstruction. Without proper calibration, the measurements would be less precise and reliable, potentially leading to incorrect or inconclusive scientific results.

The full calibration chain in Figure 3.10 contains many sequential steps and all the procedures correct the four momentum of the jets, scaling the energy, momentum and mass of jets [107]. The calibration begins with reconstructed jets applying jet finding algorithms to tracking and/or calorimeter inputs. The following step is to correct jets for pile-up effects based on p_T density and jet area. Residual pile-up dependencies are then removed using the average number of interactions per bunch crossing (μ) and the number of primary vertices (N_{PV}), after which an absolute MC-based calibration adjusts the jets four-momentum to match the particle-level energy scale and derive the jet energy scale calibration factor defined as an inverse of the energy response. A global sequential calibration (GSC) reduces flavour dependence and energy leakage utilizing calorimeter, track, and muon-segment variable. In the last step, a residual *in situ* calibration determined from various control samples, such as jets recoiling against well calibrated photons and Z boson in photon+jet and Z +jet events, is applied to data to correct for discrepancies between data and simulations, ensuring accurate jet energy measurements.

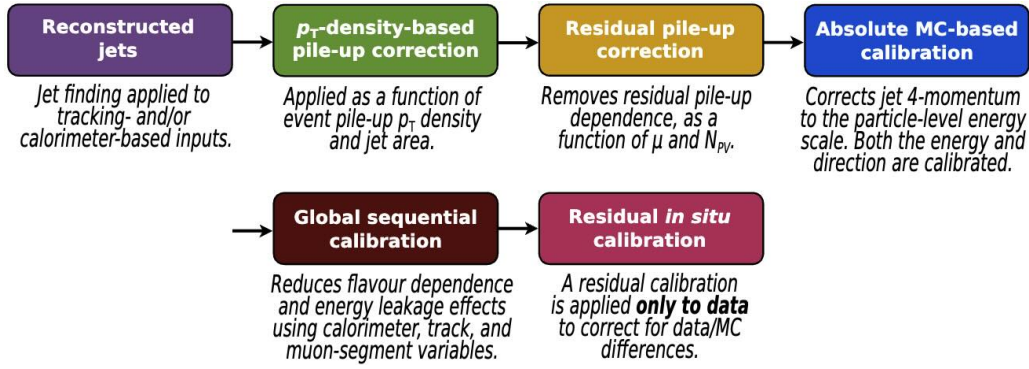


Fig. 3.10 Procedures of the energy scale calibration of reconstructed jets in ATLAS and the four-momentum of jets is fed into the calibration chain [107].

3.2.4.3 Jet Flavour Tagging Algorithm

As jets are produced from the hadronization of quarks and gluons, they can be classified based on the flavour of the initial parton. The identification of jets originating from b -quarks, c -quarks, and light-flavour quarks (u , d , s) or gluons is crucial for many physics analyses, including the search for the Higgs boson, top quark, and new physics. A b -jet tagging algorithm is used to identify jets originating from b -quarks, which have a relatively long lifetime and decay into b -hadrons that travel a measurable distance before decaying.

Figure 3.11 displays the structure of the b -jet tagger, known as *DL1*, and its enhanced versions *DL1r* and *DL1mu* [109], all relying on a deep-learning neural network (DNN) structure. The flavour tagging algorithm uses as input the features calculated both by low-level algorithms and high-level algorithms. The low-level algorithms utilize the directly reconstructed objects such as tracks and inner detector hits to construct low-level taggers such as IPxD [110], SV1 [111], Jet-Fitter [112], RNNIP [113] in Figure 3.11, while the high-level taggers integrate the outputs from the low-level taggers to more efficiently identify the flavor of jets and achieve better background rejection. The final decision of the flavour tagger is to calculate the likelihood of the jet being produced by the hadronization of a b -quark, a c -quark, or a light quark or gluon. The working point (WP) of the tagger is defined by the average efficiency of b -jet identification for b jets in $t\bar{t}$ events, and four working points are available in physics analysis: 60%, 70%, 77%, and 85%, corresponding to increasingly higher efficiency, looser selection and worse background rejection.

In the thesis, the b -jet identification is performed using the *DL1r* algorithm with a nominal average efficiency of 77% for b -jets and a rejection factor of 192 (6) for light-quark/gluon (c -quark) jets. The algorithm combines the kinematic features of b -hadron decays like the IP of the tracks and the displaced vertex in the ID as well as employs the variable built by recurrent neural network (RNNIP) to take the spatial and kinematic correlations between tracks inside the same b -hadron. *DL1r* returns three probabilities for b -jet (p_b), c -jet (p_c), and light-flavour jet (p_u), which are used to define the combined final discriminant:

$$D_{DL1r} = \log \frac{p_b}{f_c \cdot p_c + (1 - f_c) \cdot p_u}, \quad (3.2)$$

where f_c is a weighting factor between 0 and 1 that can be tuned to improve the background

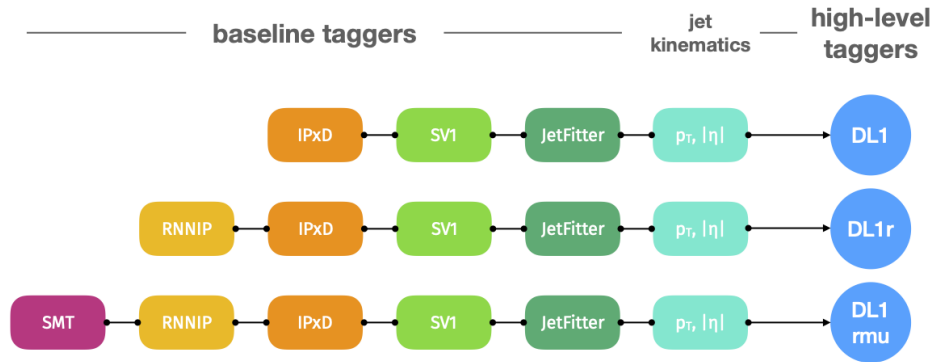


Fig. 3.11 The structure of b -jet tagger based on the deep-learning neural network. Three successively enhanced taggers are displayed: DL1, DL1r, and DL1mu. Credits: ATLAS

rejection for c -jets or light-flavour jets. To achieve a more fine-grained classification of the jet flavour, a pseudo-continuous b -tagging algorithm (PCBT) assigns a continuous score to each jet that meets the criteria for a given working point (WP) but fails to meet the next tighter threshold. The PCBT scores range from two to five, corresponding to jets passing the 85%, 77%, 70%, or 60% WP, respectively, while jets failing all WPs are assigned a score of one [114]. The tagging performance of several algorithms are compared from b -jet efficiency and background rejection factor, as illustrated in Figure 3.12. *DL1r* shows excellent performance in terms of background rejection vs b -jet efficiency. With the recent development of new deep-learning algorithm, the performance of state-of-the-art b -jet taggers in ATLAS like GN2v00 [115] have significantly improved, which will be crucial for future precision measurement and new physics searches in final states containing b -quarks.

3.2.4.4 Jets Vertex Tagging

The Jet Vertex Tagging (JVT) [116] is an essential tool for discriminating between jets originating from the primary proton-proton collision vertex and those resulting from pile-up interactions, which are additional collisions occurring in the same bunch crossing. The JVT algorithm leverages the transverse momentum of a jet and the sum of the squared transverse momenta of tracks associated to it. A key variable, the Jet Vertex Fraction (JVF), which represents the fraction of the jet p_T contributed by tracks from the primary vertex, is used to assign a likelihood score to each jet. Typically, a JVT score threshold of 0.59 is applied, which effectively rejects over 90% of pile-up jets while retaining more than 92% of jets from the primary vertex in central regions ($|\eta| < 2.4$).

The forward Jet Vertex Tagging (fJVT) [117] extends this pile-up mitigation capability to the forward region of the detector ($2.5 < |\eta| < 4.5$), where the track density is insufficient for traditional track-based methods. The fJVT algorithm utilizes calorimetric information, such as jet energy density and kinematic variables, to achieve similar levels of pile-up suppression. By incorporating both JVT and fJVT, ATLAS ensures comprehensive and uniform jet purity across the entire detector, crucial for precision measurements and searches for new physics in

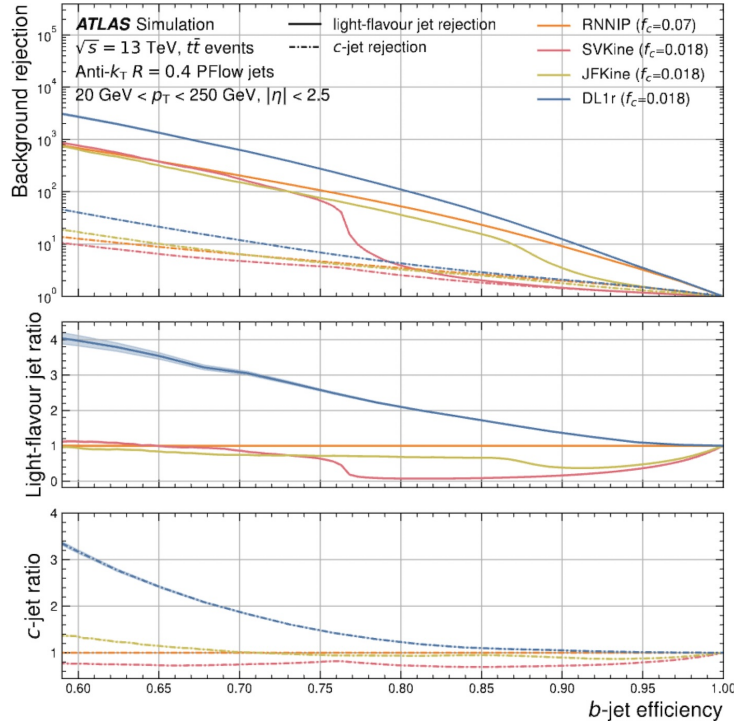


Fig. 3.12 Rejection factor of *light*-jet and *c*-jet as a function of *b*-jet efficiency for *DL1r* as well as for various low-level *b*-taggers [114].

high-pile-up environments. These sophisticated tagging techniques enable ATLAS to maintain high jet purity, critical for the accurate reconstruction of events and the extraction of significant physics results.

3.2.5 Tau Leptons

Tau leptons have a short lifetime and decay close to the interaction point. They are thus reconstructed indirectly from their decay products: missing transverse momentum from the neutrinos (described in the next section), electrons or muons in the case of leptonic decays, or jets in the case of hadronic decays. The jets are reconstructed with algorithms similar to those described in the previous section, with small radius, and additional requirements based on the number and total charge of tracks matched to the jet. Isolation criteria can be applied to the jet to suppress non-prompt tau-lepton candidates.

3.2.6 Missing Transverse Momentum

Apart from the detectable particles previously discussed, feebly interacting particles cannot be directly observed by the detector. However, these *invisible* particles can be inferred through the imbalance (called MET, or E_T^{miss}) of transverse momentum in the event that produced them, as shown in Figure 3.13. MET is a critical parameter for identifying events where not all particles are detected, often indicating the presence of neutrinos or other non-interacting particles like dark matter candidates.

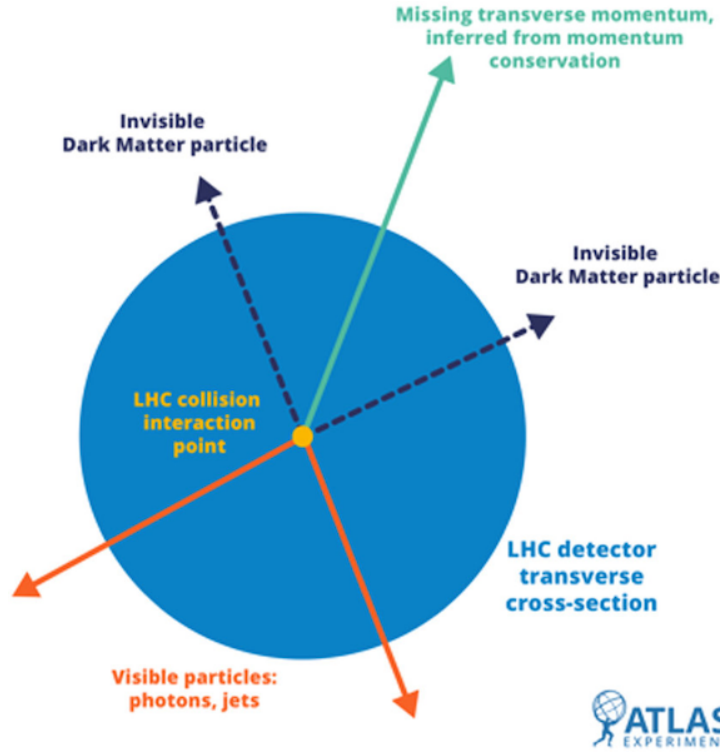


Fig. 3.13 Schematic diagram showing the missing transverse momentum in an event. The MET is calculated as the negative vector sum of the transverse momentum of all the reconstructed objects in the event. Credits: [ATLAS](#)

In a collision, the incoming particles are expected to have no net transverse momentum. Due to the conservation of momentum in absence of invisible particles in the final state carrying significant momentum, the total transverse momentum of all reconstructed particles in the final state should be zero. Reconstructed MET involves summing the transverse components of momentum of all reconstructed and calibrated high- p_T objects in the event. In particular, the missing transverse momentum E_T^{miss} is defined as the negative vector sum of the transverse momentum of all reconstructed objects [118]. The expression of MET and its components are written by:

$$E_T^{\text{miss}} = \sqrt{(E_x^{\text{miss}})^2 + (E_y^{\text{miss}})^2} \quad (3.3)$$

$$E_{x(y)}^{\text{miss}} = -E_{x(y)}^{\text{jets}} - E_{x(y)}^e - E_{x(y)}^\gamma - E_{x(y)}^{\tau\text{-had}} - E_{x(y)}^\mu - E_{x(y)}^{ST} \quad (3.4)$$

where $E_{x(y)}^{\text{jets}}, E_{x(y)}^e, E_{x(y)}^\gamma, E_{x(y)}^{\tau\text{-had}}, E_{x(y)}^\mu$ represent the sum of $x(y)$ component of the transverse momentum of all jets, electrons, photons, hadronic decaying τ leptons, and muons in an event, respectively. The term $E_{x(y)}^{ST}$ represents the soft term associated with low- p_T deposits not used to reconstruct the previous objects. Several algorithms have been proposed to reconstruct the soft term, aiming to reduce pile-up dependence. The default one in ATLAS physics analysis, named *Track-based Soft Term (TST)*, relying on ID tracks only, without considering the contribution neutral particles. An alternative method is called *Calorimeter-based Soft Term (CST)*, and

considers low-energy deposits in the topo-clusters of the calorimeter in addition to the tracks of the TST. The TST is computed as the sum of the transverse momenta of all ID tracks from the hard-scatter vertex that pass reconstruction quality and kinematic selections, and are not associated with any previously reconstructed objects. To avoid double-counting of the same objects, the overlap removal procedure is applied to the reconstructed objects before calculating the MET.

3.2.7 Primary Vertex

Besides particle candidates, a crucial aspect of the reconstruction of the primary vertex (PV) of the event, where the hard proton-proton collision of interest took place [119]. The primary vertex candidates of the event are identified from groups of tracks originating from a common point. Among those candidates, the primary vertex is selected as described in the following.

The reconstruction of ID tracks involves clustering hits from the pixel and SCT detectors to form space-points, followed by seeding and track finding using a combinatorial Kalman filter [120]. The process includes iterative pattern recognition, ambiguity solving with track scoring, and the use of neural networks to identify and assign merged clusters. High-resolution track fitting refines the track parameters, and quality cuts ensure the selection of accurate tracks. The performance of the reconstruction algorithms is validated using both simulated and real collision data to ensure robustness in dense environments [121].

Vertices with at least two associated tracks are considered PV candidates. Most analyses in ATLAS adopt the “hardest vertex”, i.e. the reconstructed primary vertex with the largest sum of squared tracks transverse momenta ($\sum p_T^2$), as the hard-scattering vertex candidate [122]. This method can be inaccurate for events producing only photons as high-momentum particles, such as a Higgs boson produced by gluon fusion and decaying to a photon pair, due to the absence of energetic tracks in the detector. However, precisely identifying the diphoton production vertex is essential for accurately measuring the diphoton invariant mass, $m_{\gamma\gamma} = \sqrt{2E_1E_2(1 - \cos\alpha)}$, where E_1 and E_2 are the energies of the leading and sub-leading photons, respectively, and α is the opening angle between them, since the direction of photon candidates is calculated from the position of the energy clusters in the electromagnetic calorimeter and the primary vertex. For this reason, in order to improve the quality of the primary vertex identification for the diphoton system, an Artificial Neural Network (ANN) [119] was developed using information from all reconstructed vertices, including primary vertex and track data. Additionally, directional information of the two photons, recorded by the inner detector in the case of converted photons, and the electromagnetic calorimeter longitudinal layers, is utilized.

In simulations of gluon-gluon fusion events, this neural-network algorithm achieves a 79% success rate in identifying a diphoton vertex within 0.3 mm of the actual production vertex [119]. The efficiency varies from 84% to 97% for other Higgs production modes, improving further when charged leptons or jet activity are present. The performance of the algorithm is validated using $Z \rightarrow e^+e^-$ events in both experimental data and simulations, where electron candidates are treated as photon candidates. The agreement between the observed data and the simulation results is very good.

In the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis, the PV identification efficiency of the ANN is 97% (94%) while that of the hardest-vertex algorithm is 94% (90%) for the vertices with longitudinal distance

to truth vertex less than $100 \mu\text{m}$ in simulated ggF (VBF) $HH \rightarrow b\bar{b}\gamma\gamma$ events. The ANN algorithm is also more robust against pile-up. The contribution to the mass resolution of the diphoton system from the photon direction is reduced; however, the dominant effect arises from the uncertainty in the photon energies and therefore the effect on the diphoton mass resolution overall is negligible.

CHAPTER 4

Mitigation of the Pile-up Dependence of the Photon Identification Algorithm

The algorithms used by ATLAS for the reconstruction and identification of photons are introduced in Section 3.2.1. Three different sets of cut-based criteria, denoted as loose, medium, and tight, are used to identify prompt photons with increasing purity and decreasing efficiency, by applying p_T and η -dependent requirements to lateral and longitudinal shower shape variables [94]. Most ATLAS analyses relying on photons in the final state require tight photon candidates. Due to its stringent selection requirements on the shower shape variables, the tight identification efficiency is rather sensitive to pile-up in the harsh environment of the LHC, getting lower with the increase of pile-up, as more energy is deposited in the topo-cluster used to reconstruct the photon candidate and to calculate the shower shapes. Two distinct methods can be targeted to mitigate the pile-up dependence of the photon identification: developing new variables that discriminate between signal and background, or re-optimizing the criteria on the variables already considered before. The work performed during my thesis and presented in this chapter focused on the re-optimization method and is described in more detail in Ref. [123].

4.1 Introduction and Challenges

The reconstruction and identification of prompt photons is essential at the LHC, where they are widely produced from the proton-proton collisions. Primary contributions to prompt photon production come from the non-resonant production of photon+jets and the continuum production of diphoton pairs, corresponding to the Feynman diagrams illustrated in Figure 4.1(a). Prompt photons can also be produced by Higgs boson decays, radiative decays of W and Z bosons, and other electroweak processes. In addition to these “direct” processes, parton fragmentation into a hard photon and another soft collinear parton can also lead to the production

of prompt photons, as shown in Figure 4.1(b).

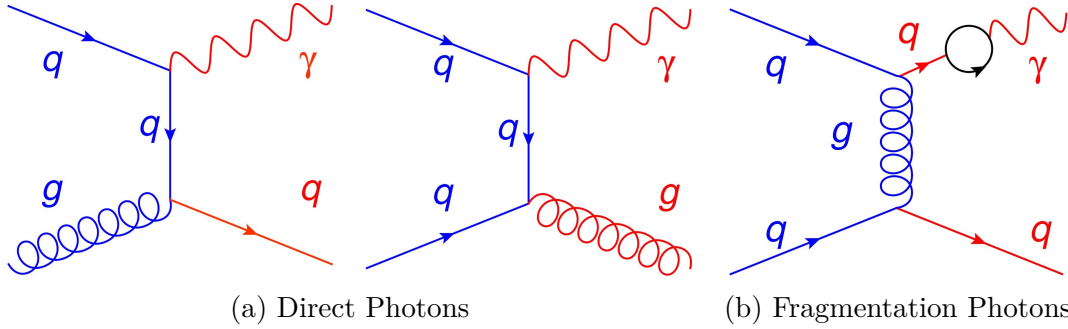


Fig. 4.1 Feynman diagrams for the main production processes of prompt photons at the LHC: (a) direct photons and (b) fragmentation photons.

The dominant backgrounds to prompt photon candidates are non-prompt photons, mainly collimated photon pairs from the decays of neutral mesons (typically π^0 and η) inside jets. They are produced in QCD processes with large cross sections compared to those of the processes producing prompt photons, and photon identification algorithms with large rejection factors for these background candidates are thus needed.

The photon tight identification algorithm used by ATLAS is dedicated to distinguishing prompt photons with good efficiency while rejecting the majority of the non-prompt photons, leading to high purity with only modest inefficiency, two essential factors for the study of the Higgs boson and of other rare processes in signatures with photons in the final state. The tight identification algorithm uses a set of stringent requirements on nine shower shape variables illustrated in Figure 4.2. In addition, loose and medium identification algorithms are designed to achieve higher efficiency but worse fake rejection. They are essential for triggering purposes and for defining the control regions used to estimate backgrounds from non-prompt photons. These algorithms use looser criteria than the tight algorithm, on subsets of the nine shower shape variables considered by the latter. As described in the previous section 3.2.1.1, since converted and unconverted photons show distinctive shower shape distributions in the calorimeter, different selections are applied by the photon identification algorithms to these two types of photon candidates.

Since the shower shapes depend on the transverse momentum energy of the photon candidates, p_T -dependent requirements are applied by the tight photon identification algorithm used in Run-2 ATLAS analyses [124]. The shower shapes are also affected by pile-up, since the larger is the number μ of pp collisions taking place in the same bunch crossing and the larger is the energy deposited in the cluster and the wider are the shower shape distributions. Given the significantly larger pile-up expected in Run-3 compared to Run-2, the photon identification criteria used in Run-2 are expected to be highly inefficient, and a new set of thresholds providing a better trade-off between efficiency and background rejection at high μ by means of μ -dependent requirements has been studied, as described in the following sections.

4.1.1 Definition of the Shower Shape Variables

Photon identification in ATLAS relies on ten shower-shape variables computed from the energy reconstructed in the cells of the photon candidate's topo-clusters. The definitions of the variables are illustrated in Figure 4.2.

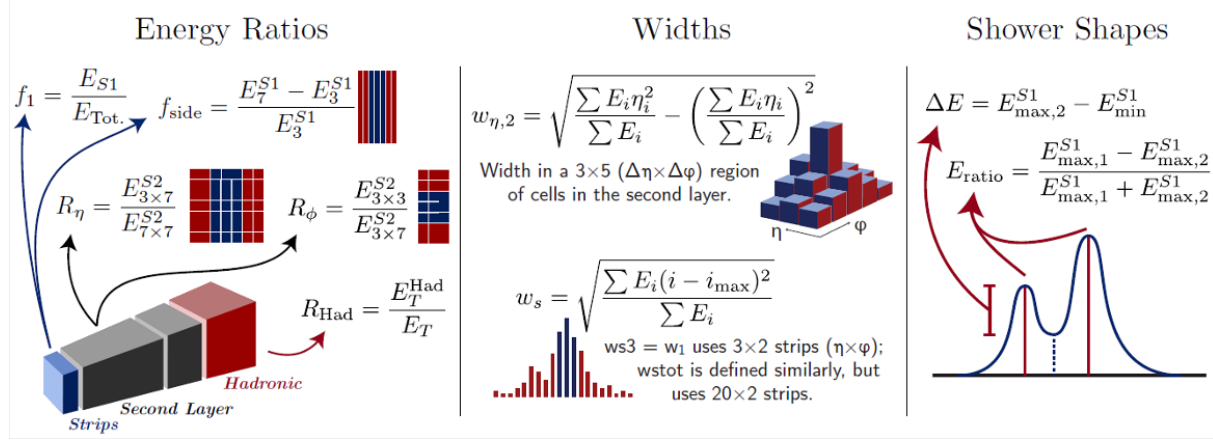


Fig. 4.2 Illustration of the discriminating variables used for photon identification. Some variables related to strips and cells are defined as energy ratios, while others describe the width and shape of the shower energy distribution. [125].

The acceptance regions for the photon identification are $|\eta| < 1.37$ or $1.52 \leq |\eta| < 2.37$, excluding the transition regions between the barrel and endcap sections of the EM calorimeter. Six variables are calculated from the energies in the cells of the first layer of the EM calorimeter, finely segmented along the η direction:

- **f_1** : the ratio of the energy deposited in the strip layer and the total energy of the cluster. This variable is used to select candidates with enough energy in the strip layer, such that the following variables can be computed in a reliable way.
- **f_{side}** : the energy fraction outside the core of three central strips, within a total of seven strips around the strip with highest energy in layer 1. Prompt photons on average show smaller values of f_{side} than background ones due to their narrower shower.
- **$w_{\eta 1}$** (also called **w_{s3}**): lateral shower width in the strips, $\sqrt{\frac{\sum E_i (i - i_{max})^2}{\sum E_i}}$ where i runs over all strips in a window of $\Delta\eta \approx 0.0625$ and i_{max} is the index of the highest-energy strip, calculated from a window of $\eta \times \phi = 3 \times 2$ strips around the strip with the highest energy deposit. Prompt photons are usually characterized by narrower showers and thus smaller values of $w_{\eta 1}$ than background ones.
- **w_{tot1}** : total lateral width, calculated similarly to $w_{\eta 1}$ but using a window $\eta \times \phi = 20 \times 2$ strips centered around the cell with the highest energy deposit in layer 2.
- **ΔE** : the difference in energy between the strip with the second highest local maximum and the strip with the minimum energy value located between the maximum and second maxima; 0 if no second minimum is found. Electromagnetic showers from prompt photons have usually a single maximum (and thus ΔE close to zero) while decays of neutral mesons

generate showers with two maxima that are sufficiently separated at low p_T , with larger ΔE .

- E_{ratio} : the ratio of the difference and the sum of the maximum and secondary maximum energy deposits in the strips, which quantifies the energy deposition. For prompt photons the second maximum, if any, arises from local fluctuations in the tail of the shower, resulting in a value of E_{ratio} close to one, while for background photons the two maxima correspond to the two showers from the photons from the neutral meson decay and are largely decorrelated, leading to a flatter distribution of E_{ratio} .

Three shower shape variables are calculated from the energies of the cells in the second layer of the EM calorimeter:

- $w_{\eta 2}$: lateral width of the shower, $\sqrt{\frac{\sum E_i \eta_i^2}{\sum E_i} - \left(\frac{\sum E_i \eta_i}{\sum E_i}\right)^2}$, where E_i is the energy and η_i is the pseudorapidity of i th cell and the sum is calculated with a window of $\eta \times \phi = 3 \times 5$ cells centered around the most energetic cell in layer 2.
- R_η : the ratio of the total energy of cells within a $\eta \times \phi = 3 \times 7$ window to the total energy of cells in a 7×7 window, both centered around the most energetic cell in layer 2.
- R_ϕ : the ratio of the total energy of cells within a $\eta \times \phi = 3 \times 3$ window to the total energy of cells in a 3×7 window, both centered around the most energetic cell in layer 2.

Prompt photons are expected to have smaller $w_{\eta 2}$ and R_η , R_ϕ closer to one than for background photons due to their narrower showers. The distribution of R_ϕ is larger for converted photons than unconverted ones because the electron and positron from the conversion are bent in opposite directions by the solenoidal magnetic field.

Two shower shape variables are related to the fraction of energy deposited in the hadronic calorimeter:

- R_{had} : the ratio of E_T in the hadronic calorimeter along $\eta \times \phi = 0.24 \times 0.24$ to E_T of the EM cluster.. Considering the depth of the hadronic layer with more than 20 times radiation length X_0 , prompt photons will deposit less energy in the hadronic layer than background ones and some negative values are allowed from the fluctuations.
- R_{had1} : similar to the previous variable, but only the first layer of the hadronic calorimeter is used.

The variable R_{had} is utilized over the range $0.8 < |\eta| < 1.37$, while R_{had1} is used for photon candidates with $|\eta| < 0.8$ or $1.52 < |\eta| < 2.37$.

The variables computed from the energies of the cells in the second layer of the EM calorimeter and the energy in the hadronic calorimeter are used by the loose identification algorithm, while all variables are considered in the tight one.

4.1.2 Challenges from pile-up

Due to the large number of protons in the same bunch and the large inelastic proton–proton cross-section, additional inelastic pp collisions can occur in the same bunch crossing as the hard-scattering process. As displayed in Figure 2.3, the average number of pileup collisions per bunch crossing $\langle \mu \rangle$ was approximately 34 during Run-2. In Run-3 there can be as many as 80 pileup event, as shown in Figure 2.17(b), and an average pileup value increasing each year (currently 52 in the first half of 2024). Such a large number of additional interactions, depositing energy in

the calorimeter, could significantly impact the reconstruction of the photon shower shapes and the efficiency of the photon identification algorithms.

Figure 3.6 illustrates the dependence of the efficiency of the tight identification algorithm on pileup as predicted by the simulation, indicating that higher pileup greatly reduces the efficiency for prompt photons. The tight efficiency for converted (unconverted) photons is expected to decrease from around 85% (87%) to 73% (75%) as μ increases from 0–20 to 60–100. Therefore, optimizing the shower shape requirements is essential to mitigate the μ -dependence of photon identification.

4.1.3 Monte Carlo Samples

The optimization of the photon identification algorithm is performed using simulated event samples of prompt and background photons. The MC samples were generated using the ATLAS simulation infrastructure, following the procedures outlined in Chapter 3. PYTHIA 8 was used to generate γ +jet events and QCD dijet events from which direct and fragmentation prompt photons (signal candidates) and neutral mesons decaying to photon pairs (background candidates) were produced. Samples were sliced by the p_T of the leading photon candidate and merged to cover a wide p_T range. Ntuples containing kinematic, shower-shape, and truth-level information were produced and used for the following studies. The samples are re-weighted to account for the cross sections of the generated processes and the filter efficiency, and to match the expected Run-3 pileup distribution.

4.2 Optimization Procedure

In the simulated event samples, reconstructed photon candidates are classified in separate samples based on their pseudorapidity ($|\eta|$), transverse momentum (p_T), pile-up (μ), and conversion types. They are separated into signal and background photons whether they are close in angle (ΔR) or not to a generated prompt photon. The tight criteria are then optimized separately in regions of pseudorapidity, transverse momentum and pile-up (μ) using the Toolkit for Multivariate Analysis (TMVA) [126]. The detailed procedures for event selection, categorization, and optimization are described in the following sections.

4.2.1 Event Selection and Categorization

Before performing the optimization, the following basic selections are applied to choose the photon candidates for the training:

- truth matching: signal (background) photons are required (not) to be matched to true prompt photons.
- kinematics: photon candidates are required to have $p_T > 20$ GeV and $|\eta| < 2.37$, excluding the transition region between the EM barrel and endcap sections ($1.37 < |\eta| < 1.52$).
- loose identification: all the photon candidates used in the optimization are required to pass the loose photon identification criteria, so that the optimized criteria for the tight photon identification algorithm used in offline analysis will be tighter than the loose ones applied at trigger level.

- isolation requirements: in offline analyses prompt photons are usually requested to pass both identification and isolation criteria to maximize the rejection of non-prompt candidates. A photon isolation requirement is applied ($E_T^{\text{iso, topocone40}} < 4$ GeV), so that the following optimization of the shower shape criteria maximizes the separation between signal and background based solely on shower shape information.
- event cleaning: photons are required to have sufficient energy deposited in the first layer of the accordion calorimeter so that the shower shape variables based on it are properly calculated (at least 0.5% of energy of the cluster deposited in the first layer of the electromagnetic calorimeter: $f_1 > 0.005$, $w_{\text{tots1}} > -10$ and $w_{\eta1} > -100$).

The photon candidates after the preselections are further divided into separate categories for the optimization procedure:

- first of all, due to their different shower shapes, particularly because of the opening azimuth angle of e^+e^- pairs from converted photons in the solenoid field leading to different cluster widths along ϕ , converted and unconverted photon candidates are studied separately;
- second, the optimization is performed separately in seven pseudorapidity regions, corresponding to regions of the detector with different quantity of the material upstream or different granularity of the readout cells;
- third, similarly to the Run-2 photon identification algorithm, the criteria are determined in bins of photon p_T , to account for the fact that the shower shapes get narrower at higher transverse momentum, and also that pile-up contributions are reduced at high p_T , as shown in Figure 4.3. The p_T bins that have been considered are the following (in units of GeV): 20-25, 25-30, 30-35, 35-40, 40-45, 45-50, 50-60, 60-80, > 80 , for a total of nine p_T regions.
- finally, the candidates are classified in six separate categories according to the level of pile-up, and the optimization is performed separately in each of them.

Figure 4.4-4.6 display the tight efficiency across different $|\eta|$, p_T , and μ bins, with the impact of pile-up quantified by the slope of a linear fit. Larger slopes reflect a stronger dependence of efficiency on μ . In specific $|\eta|$ and μ regions, the effect of pile-up on high- p_T photons is minimal, resulting in only slight efficiency reductions at higher p_T . Consequently, the optimization of photon identification criteria is focused on p_T regions below 60 GeV. The final categories for photon identification optimization are summarized in Table 4.1.

Optimization Categories for $ \eta $, p_T , μ							
$ \eta $	0-0.6	0.6-0.8	0.8-1.15	1.15-1.37	1.52-1.81	1.81-2.01	2.01-2.37
p_T [GeV]	UnConverted	$20 < p_T < 60$, 7 bins			$20 < p_T$, 9 bins		
	Converted	$20 < p_T$, 9bins	$20 < p_T < 60$, 7 bins		$20 < p_T$, 9 bins		
μ	0-20	20-30	30-40	40-50	50-60	60-100	

Tab. 4.1 Categories used for the optimization of the μ -dependent tight photon identification criteria defined by $|\eta|$, p_T , and μ .

4.2.2 Optimization of the Shower Shape Requirements with TMVA

The photon tight identification algorithm consists of orthogonal selections applied to nine shower shape variables. To account for the correlations between these discriminating variables

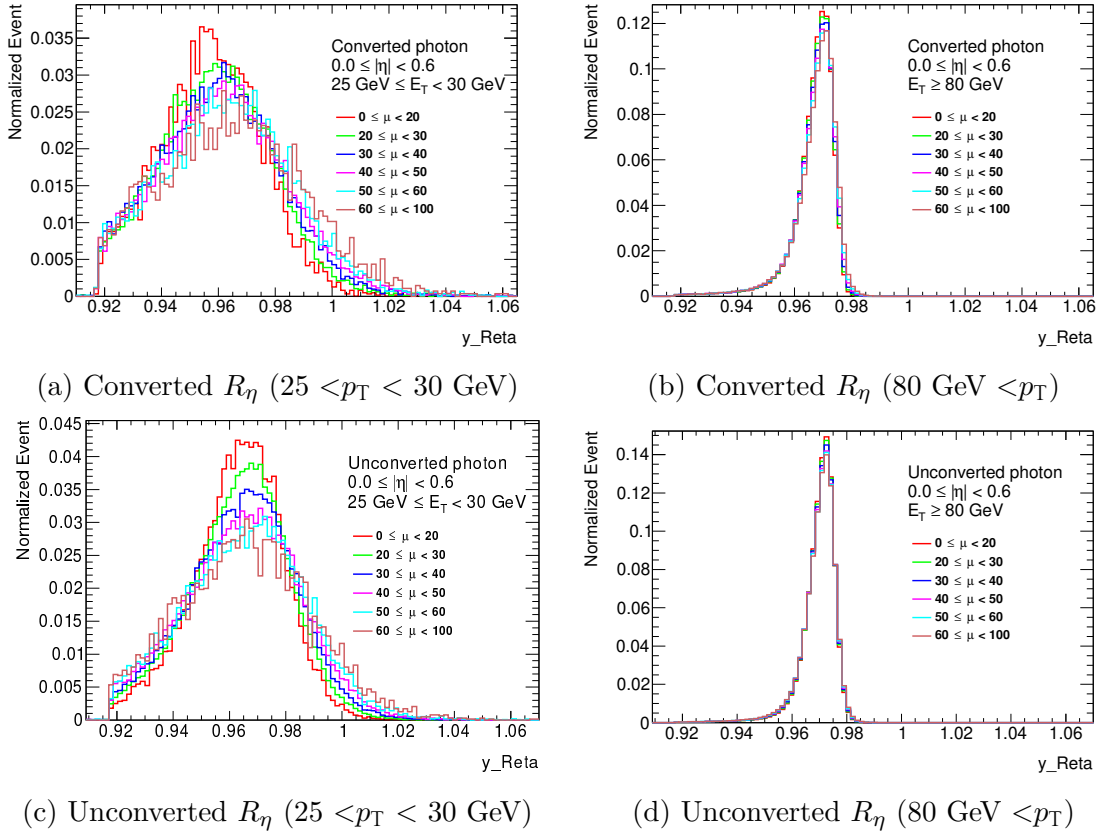
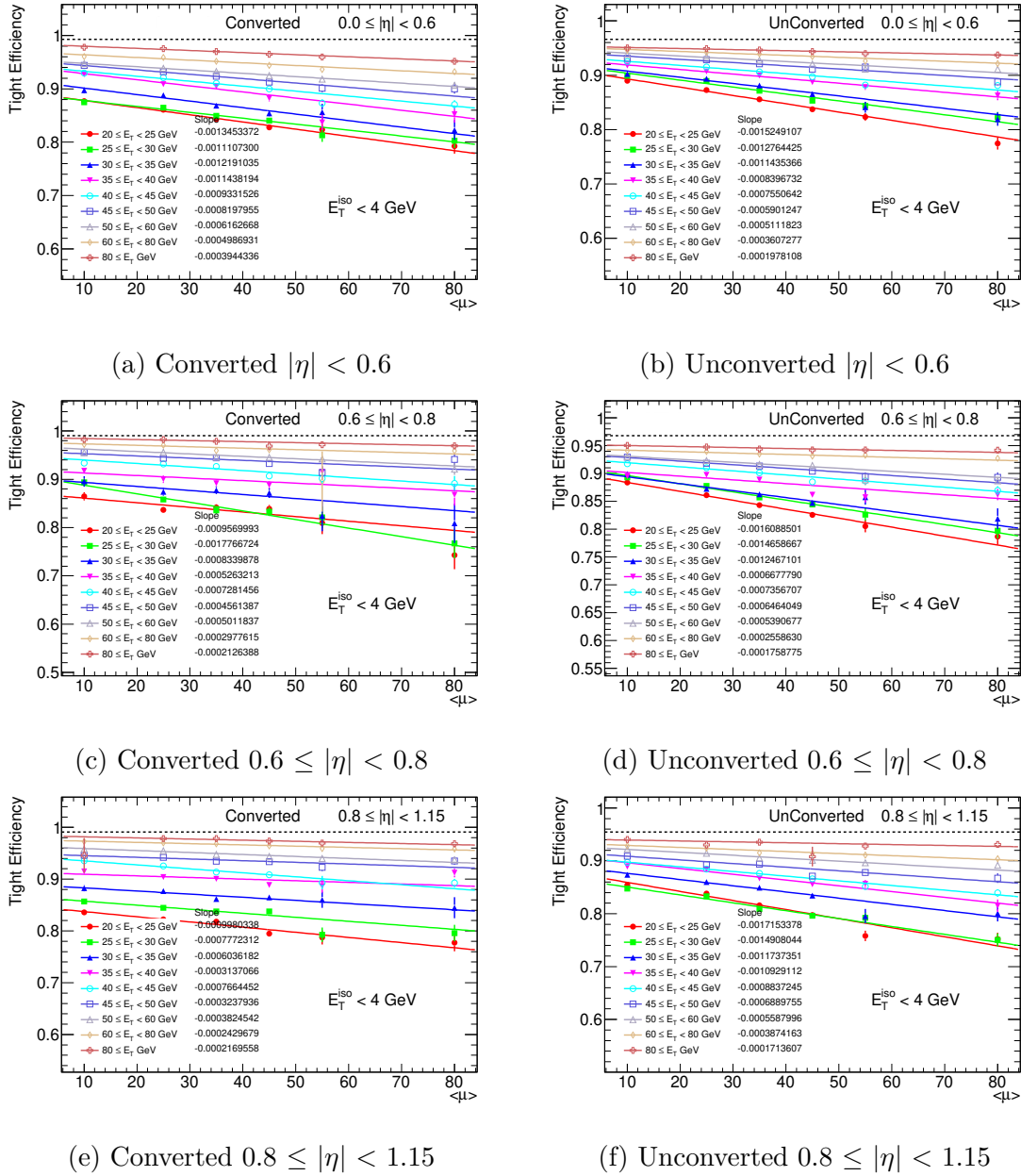


Fig. 4.3 Distributions of the variable R_η for various μ bins in the pseudorapidity region $|\eta| < 0.6$: (a) and (b) converted photons with $25 < p_T < 30$ GeV, $80 \text{ GeV} < p_T$, respectively; (c) and (d), unconverted photons in the same p_T ranges.

(DVs), the optimization of the photon identification criteria is performed in the multidimensional space of the requirements on all the variables using TMVA. The optimized selections are determined by first finding with TMVA the set of criteria that maximize background rejection for a given signal efficiency, for values of the signal efficiency varying between 0 and 100%. The final criteria are then determined by choosing a given the selections corresponding to a working point characterized by a given signal efficiency and background rejection.

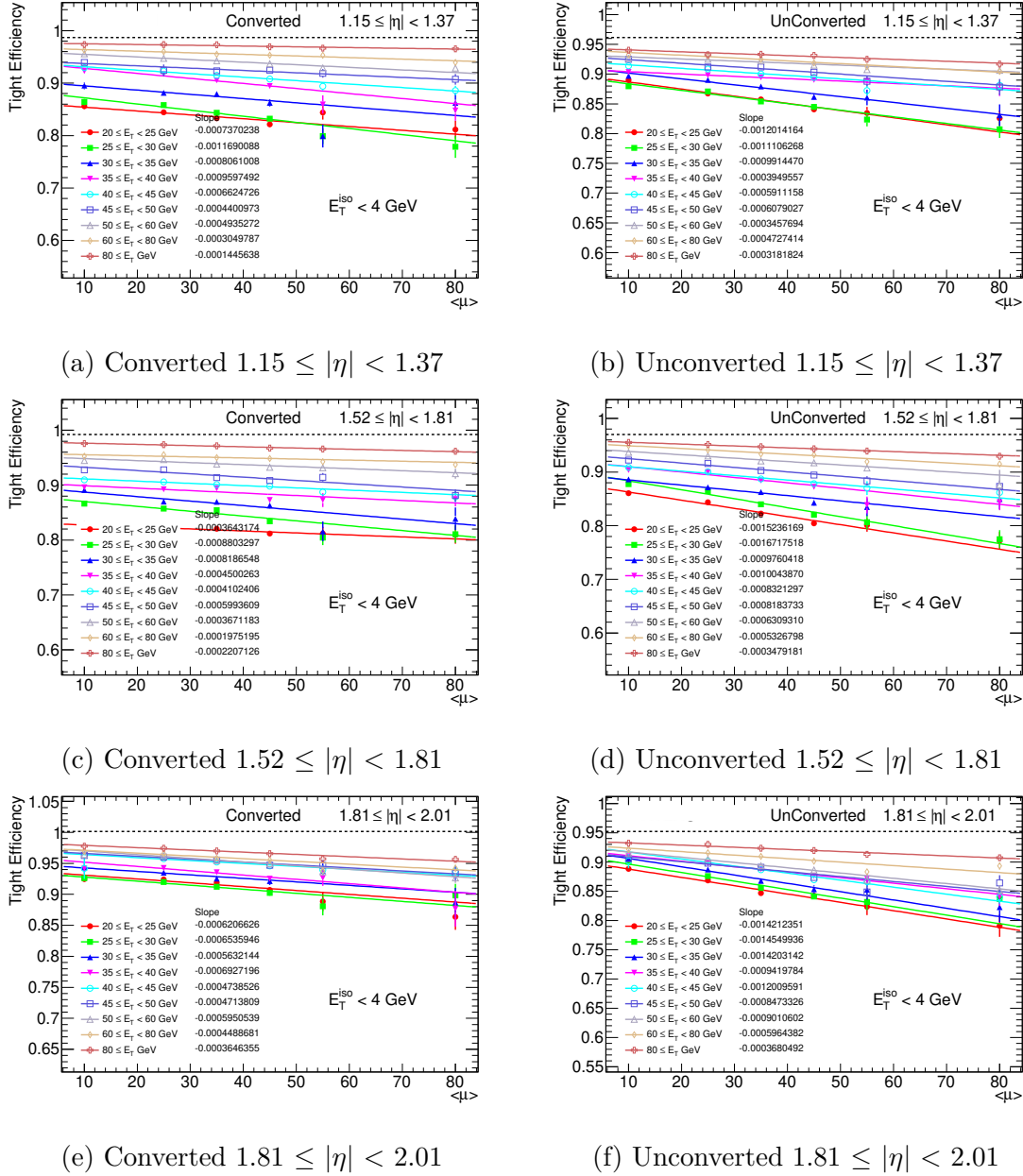
For each $|\eta|$, p_T , and μ region, separately for converted and unconverted photon candidates, an optimization is performed with TMVA, passing as input to the training the values of the nine shower shape variables for signal and background photon candidates in each region. The distributions of the shower shape variables in $|\eta| < 0.6$ and $20 < p_T < 25$ GeV are shown in Figure 4.7-4.8 and Figure 4.9-4.10, respectively for converted and unconverted photons. Once the training is completed, the optimal criteria on the shower shape variables are found by requiring a signal efficiency similar to that of the Run-2 criteria. The primary training parameters of TMVA are shown in Table 4.2. The parameters *CutRangeMin* and *CutRangeMax* determine the range of possible cut values for each shower shape. For variables used in the medium photon trigger, the parameters are configured to exceed the thresholds applied at trigger level. For variables not employed in the medium triggers, the parameters are adjusted to values that correspond to

**Fig. 4.4**

Tight efficiency of converted (left) and unconverted (right) photons versus various μ bins in each pseudorapidity region ($|\eta| < 0.6$, $0.6 \leq |\eta| < 0.8$, $0.8 \leq |\eta| < 1.15$) for various p_T bins, shown by different colors. Photon isolation was applied and a simple linear fit was performed to evaluate the decline of the efficiency by the slope to determine p_T ranges for which the optimization is performed.

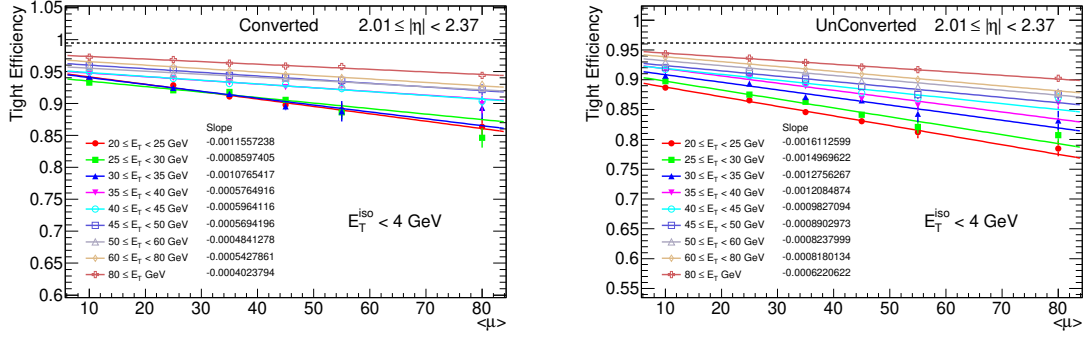
more than 99% of the distribution range of discriminant variables.

Table 4.3 displays the signal/background separation power of each shower shape variable in low pile-up region ($\mu < 20$) and high pile-up region ($50 < \mu < 60$) for converted and unconverted photon candidates at $|\eta| < 0.6$ and $20 < p_T < 25$ GeV. These variables exhibit similar separation

**Fig. 4.5**

Tight efficiency of converted (left) and unconverted (right) photons versus various μ bins in each pseudorapidity region ($1.15 \leq |\eta| < 1.37$, $1.52 \leq |\eta| < 1.81$, $1.81 \leq |\eta| < 2.01$) for various p_T bins shown by different colors. Photon isolation was applied and a simple linear fit was performed to evaluate the decline of the efficiency by the slope to determine p_T ranges for which the optimization is performed.

power at the low and high pile-up scenarios, with E_{ratio} being the most discriminating variable.

(a) Converted $2.01 \leq |\eta| < 2.37$ (b) UnConverted $2.01 \leq |\eta| < 2.37$ **Fig. 4.6**

Tight efficiency of converted (left) and unconverted (right) photons versus various μ bins in $2.01 \leq |\eta| < 2.37$ for various p_T bins shown by different colors. Photon isolation was applied and a simple linear fit was performed to evaluate the decline of the efficiency by the slope to determine p_T ranges for which the optimization is performed.

FitMethod	EffMethod	VarProp	PopSize	Steps	Cycles
GA	EffSel	FSmart	500	20	6

Tab. 4.2

Primary parameters for the optimization of TMVA.

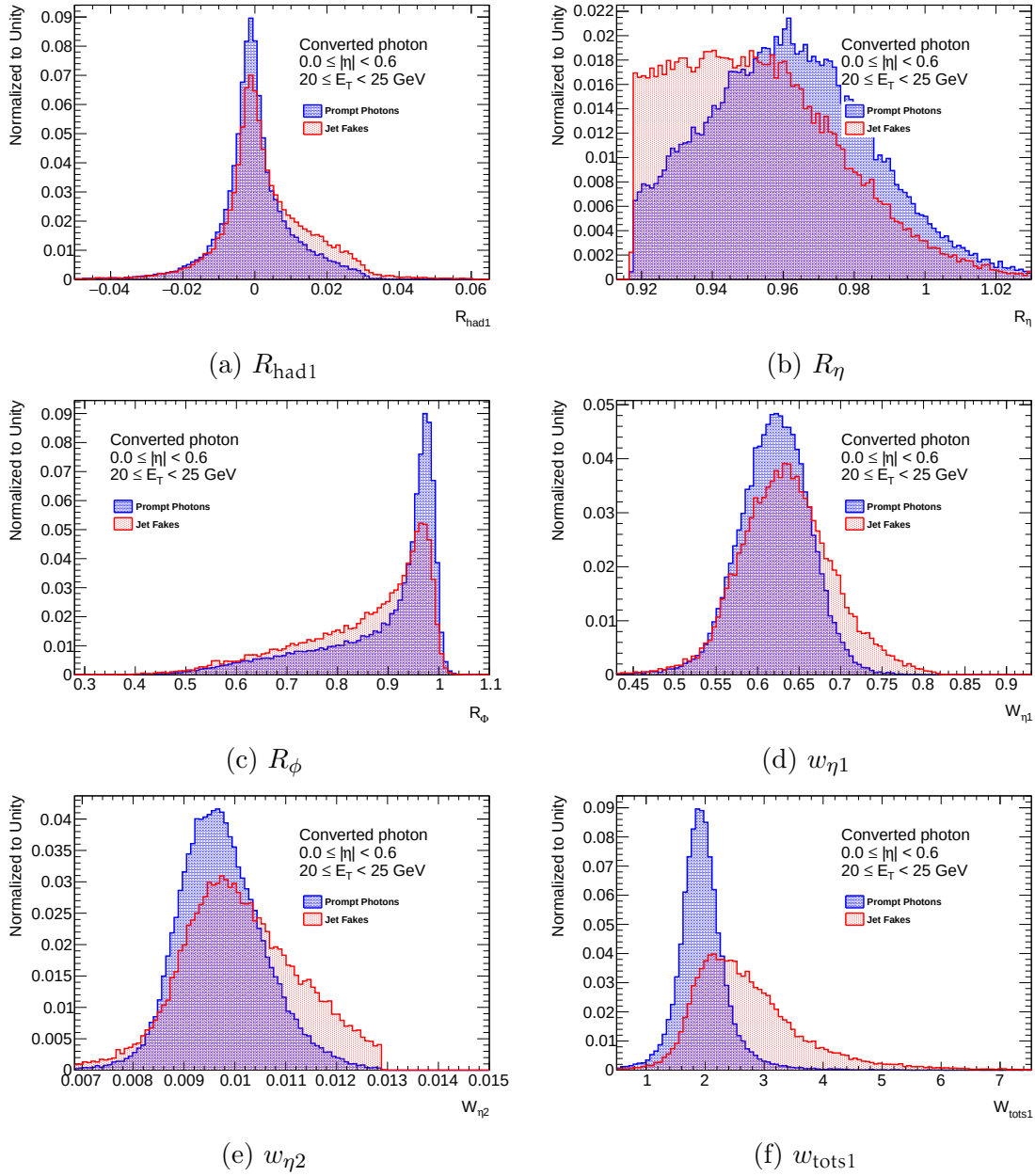
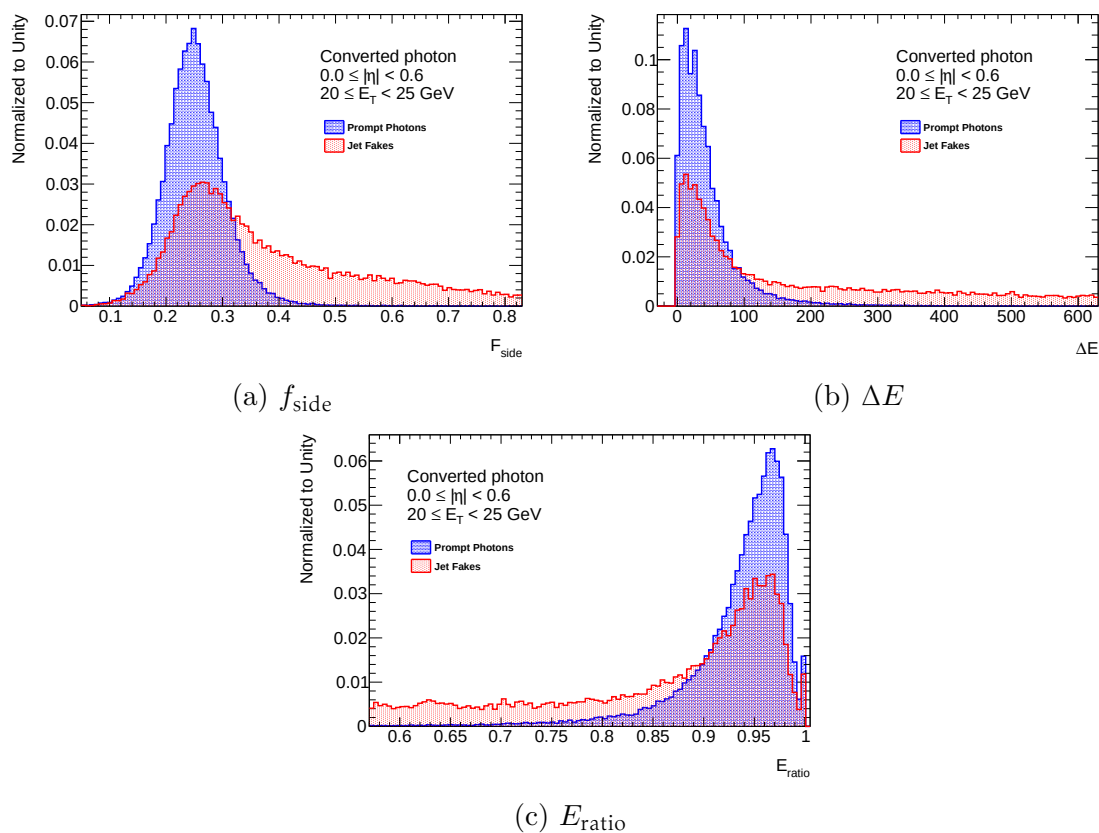


Fig. 4.7 Distributions of shower shape variables for converted prompt photons and fake photons in the pseudorapidity range $|\eta| < 0.6$ and with $20 < p_T < 25$ GeV. No photon isolation requirement is applied.

**Fig. 4.8**

Distributions of shower shape variables for converted prompt photons and fake photons in the pseudorapidity range $|\eta| < 0.6$ and with $20 < p_T < 25 \text{ GeV}$. No photon isolation requirement is applied.

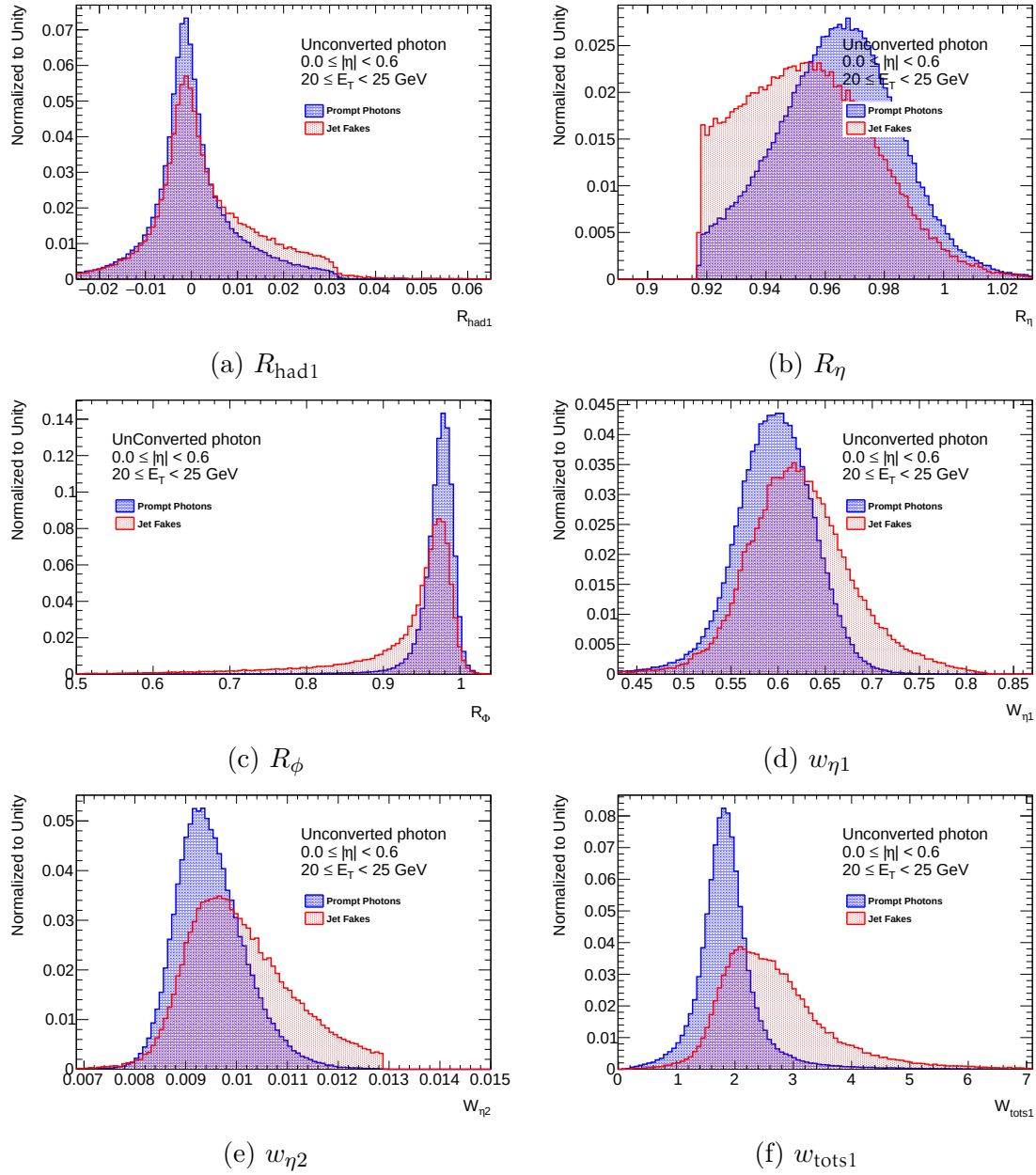
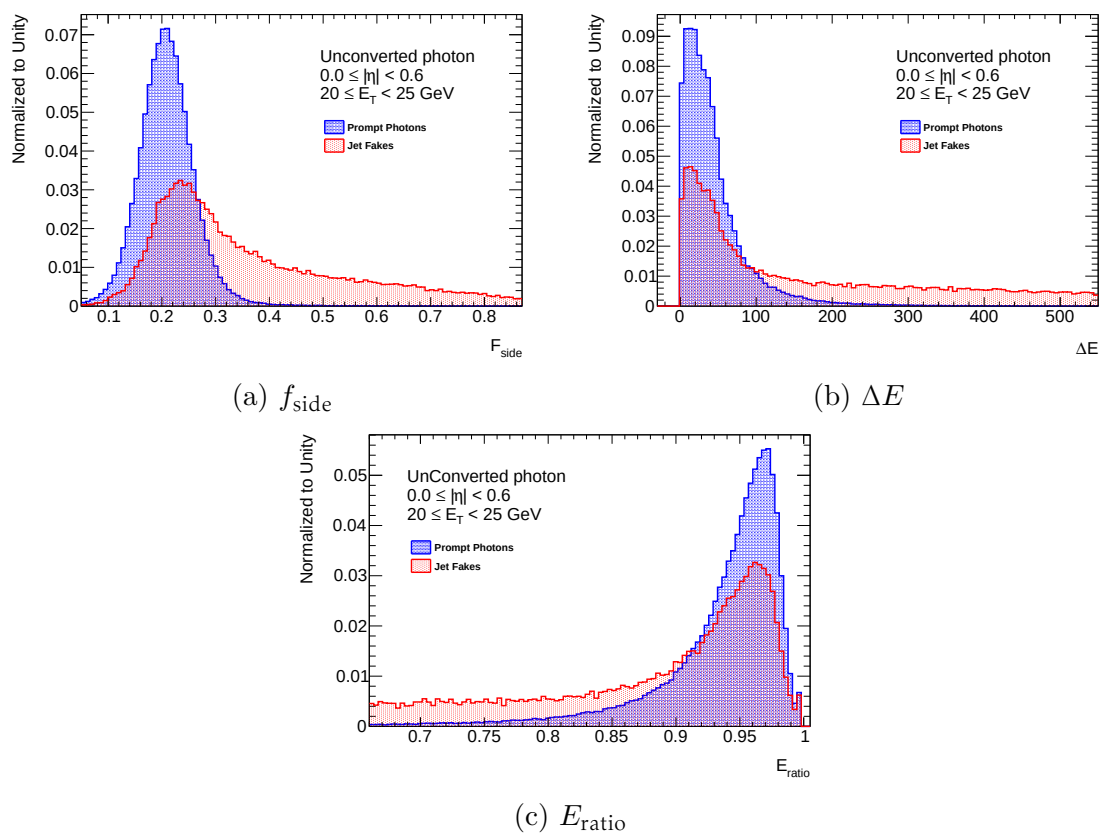


Fig. 4.9 Distributions of shower shape variables for unconverted prompt photons and fake photons in the pseudorapidity range $|\eta| < 0.6$ and with $20 < p_T < 25$ GeV. No photon isolation requirement is applied.

**Fig. 4.10**

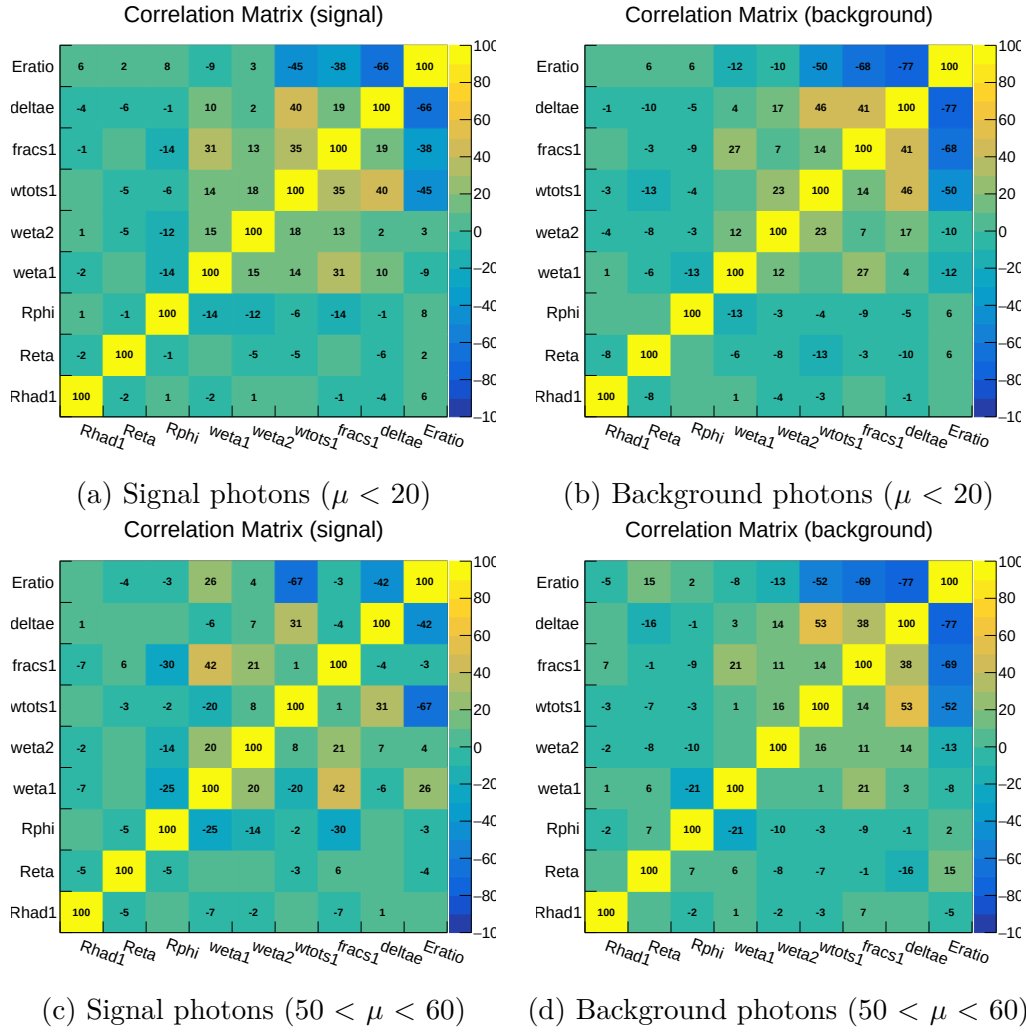
Distributions of shower shape variables for unconverted prompt photons and fake photons in the pseudorapidity range $|\eta| < 0.6$ and with $20 < p_T < 25$ GeV. No photon isolation requirement is applied.

pile-up regions	UnConverted Photons			Converted Photons		
	Rank	Variable	Separation	Rank	Variable	Separation
Low pile-up: $0 < \mu < 20$	1	E_{ratio}	3.934e-01	1	E_{ratio}	4.330e-01
	2	ΔE	3.550e-01	2	ΔE	3.426e-01
	3	f_{side}	3.350e-01	3	w_{tots1}	3.388e-01
	4	w_{tots1}	3.229e-01	4	f_{side}	2.949e-01
	5	R_{ϕ}	1.415e-01	5	$w_{\eta 2}$	7.143e-02
	6	$w_{\eta 2}$	1.233e-01	6	$w_{\eta 1}$	5.320e-02
	7	$w_{\eta 1}$	1.017e-01	7	R_{η}	4.370e-02
	8	R_{η}	7.788e-02	8	R_{had1}	3.898e-02
	9	R_{had1}	2.095e-02	9	R_{ϕ}	3.700e-02
High pile-up: $50 < \mu < 60$	1	E_{ratio}	3.470e-01	1	E_{ratio}	3.375e-01
	2	f_{side}	2.847e-01	2	ΔE	2.728e-01
	3	ΔE	2.806e-01	3	f_{side}	2.500e-01
	4	w_{tots1}	2.321e-01	4	w_{tots1}	2.309e-01
	5	R_{ϕ}	9.435e-02	5	$w_{\eta 1}$	8.951e-02
	6	$w_{\eta 1}$	8.942e-02	6	$w_{\eta 2}$	7.258e-02
	7	$w_{\eta 2}$	8.568e-02	7	R_{ϕ}	6.443e-02
	8	R_{η}	2.832e-02	8	R_{had1}	4.073e-02
	9	R_{had1}	1.891e-02	9	R_{η}	3.155e-02

Tab. 4.3 Rankings of the separation power of the shower shape variables for converted and unconverted photons with $|\eta| < 0.6$ and $20 < p_{\text{T}} < 25$ GeV at low ($\mu < 20$) and high ($50 < \mu < 60$) pile-up.

Figure 4.11 and Figure 4.12 present the correlation matrices for shower shape variables associated with signal and background converted or unconverted photon candidates with $|\eta| < 0.6$ and $20 < p_{\text{T}} < 25$ GeV, for either low ($\mu < 20$) and high ($50 < \mu < 60$) pile-up scenarios. They indicate that the correlations among these variables are generally small, and all of them are thus helpful in discriminating between signal and background. The correlations in the high pile-up region are similar to those for low pile-up.

The optimization returns, for each possible value of the signal efficiency between 0 and 100%, in steps of 1%, a set of requirements on the DVs that minimizes the background efficiency. The receiver operating characteristic (ROC) curves showing the signal and background efficiency of the optimized criteria for the converted and unconverted photons are shown in Figures 4.13.

**Fig. 4.11**

Discriminating variables correlation matrix for signal (left) and background (right) converted photon candidates with $|\eta| < 0.6$ and $20 < p_T < 25$ GeV, for low ($\mu < 20$: top) and high ($50 < \mu < 60$: bottom) pile-up.

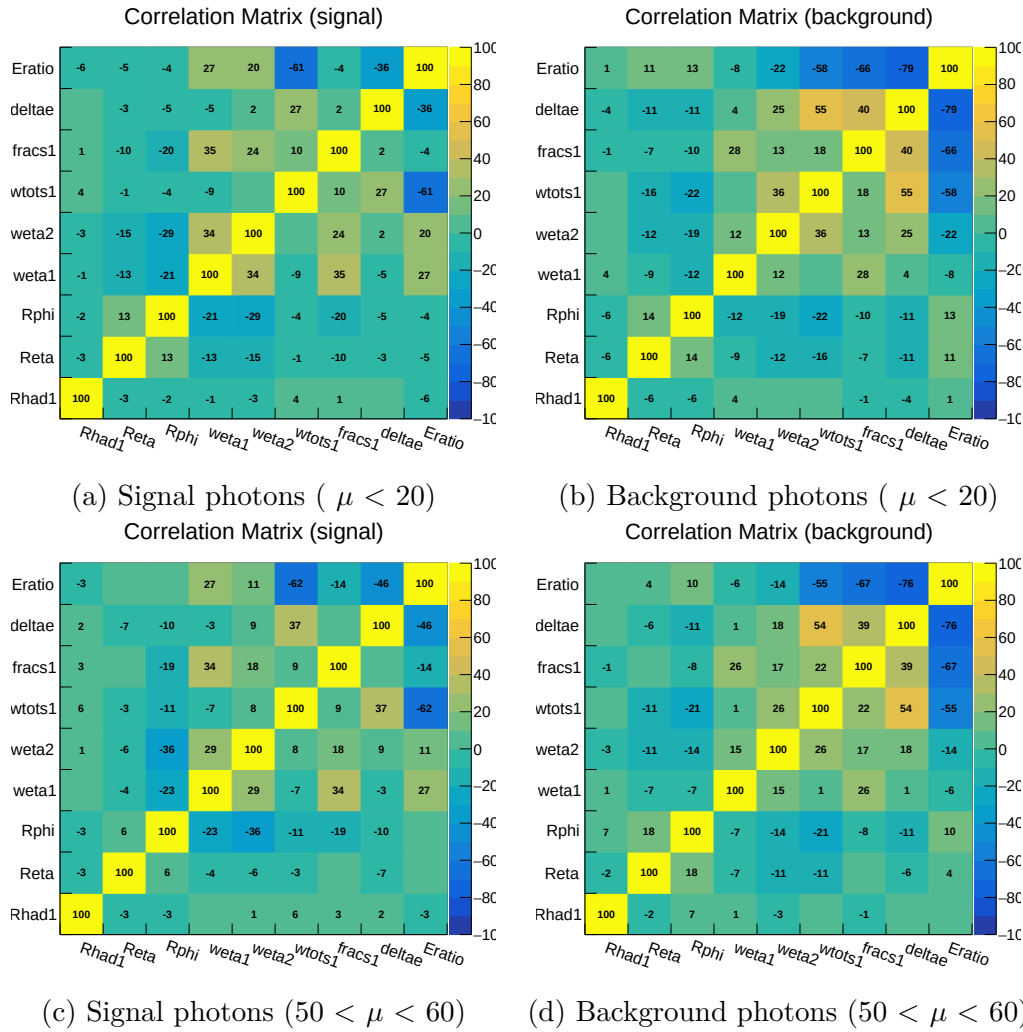


Fig. 4.12

Discriminating variables correlation matrix for signal (left) and background (right) unconverted photon candidates with $|\eta| < 0.6$ and $20 < p_T < 25$ GeV, for low ($\mu < 20$: top) and high ($50 < \mu < 60$: bottom) pile-up.

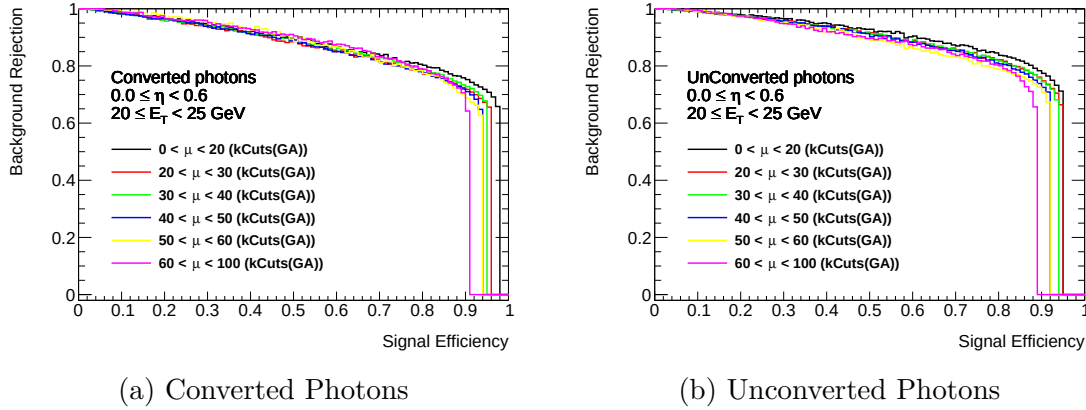


Fig. 4.13 ROC curves showing background efficiency versus signal efficiency in various μ bins for photon candidates with $|\eta| < 0.6$ and $20 < p_T < 25$ GeV, respectively for (a) converted and (b) unconverted photons.

4.2.3 Definition of the New Criteria

The requirements of the reoptimized tight identification algorithm are chosen in order to yield a signal efficiency similar to that of the Run-2 p_T -dependent algorithm at $\mu \approx 30$. The requirements on some variables fluctuate quite significantly among neighboring μ bins due to the large number of shower shapes on which the optimization is performed, their correlations (that can lead to a tighter cut on one variable and a looser one on a different variable in one μ bin, and vice versa in another bin), and the limited amount of candidates in the signal and background training samples. To limit such fluctuations, an additional procedure is applied to smooth the values of the cuts while maintaining a similar signal efficiency. The algorithm *isotonic regression* [127] is used to ensure the monotonic dependence of the cuts with pileup. After deriving the set of cuts in each region, the tight efficiency and background rejection are evaluated.

4.2.3.1 Converted Photons

The working points for converted photons in all regions are shown in Table 4.4. These values indicate that the signal efficiency is consistent across all μ bins within each $|\eta|$ and p_T region, ensuring high efficiency even at high pileup levels. The cut values at the given working points are illustrated with red (green) solid lines after (before) smoothing in Figure 4.14-4.15 for photon candidates with $|\eta| < 0.6$ and $20 < p_T < 25$ GeV. The cut values for the first category in the reoptimized, μ -dependent identification criteria for converted photons are listed in Table 4.5. More results for other regions are available in an internal ATLAS note, written to document the full procedure and results in detail [123].

4.2.3.2 Unconverted Photons

The working points for unconverted photons in all regions are shown in Table 4.6, demonstrating that the signal efficiency is consistent across all μ bins within each $|\eta|$ and p_T region. The set of cut values at the given working points are depicted with red (green) solid lines after (before) smoothing in Figure 4.16-4.17 for photon candidates with $|\eta| < 0.6$ and $20 < p_T < 25$

p_T [GeV]	20-25	25-30	30-35	35-40	40-45	45-50	50-60	60-80	80<
$0 < \eta < 0.6$	86%	88%	90%	91%	92%	93%	94%	95%	95%
$0.6 \leq \eta < 0.8$	84%	88%	90%	91%	92%	93%	94%	-	-
$0.8 \leq \eta < 1.15$	83%	87%	89%	91%	92%	93%	94%	-	-
$1.15 \leq \eta < 1.37$	85%	88%	90%	91%	92%	93%	94%	-	-
$1.52 \leq \eta < 1.81$	86%	88%	90%	91%	92%	93%	94%	95%	95%
$1.81 \leq \eta < 2.01$	86%	88%	90%	91%	92%	93%	94%	95%	95%
$2.01 \leq \eta < 2.37$	86%	88%	90%	91%	92%	93%	94%	95%	95%

Tab. 4.4 Targeted working points for converted photon candidates in various $|\eta|$ and p_T regions. "-" represents that the regions are not optimized.

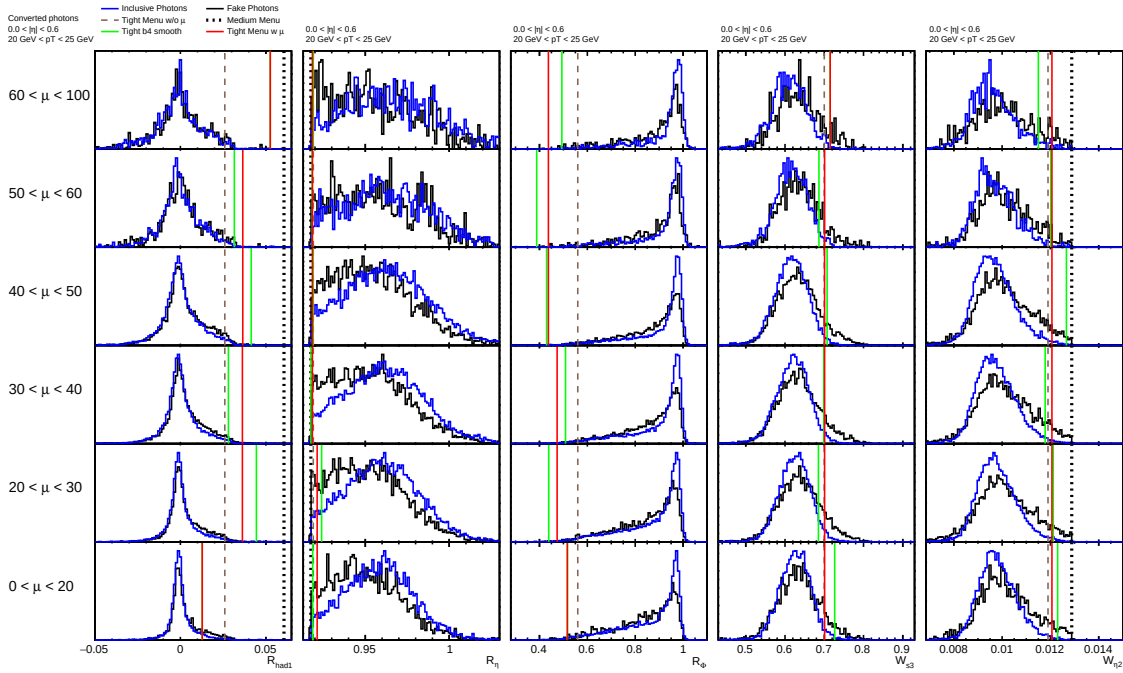


Fig. 4.14 Signal photon (blue) and background photon (black) shower shape distributions (R_{had1} , R_η , R_ϕ , w_{s3} , $w_{\eta2}$) in bins of μ for converted photon candidates with $|\eta| < 0.6$ and $20 \leq p_T < 25$ GeV. The cuts used by the Run-2 photon identification algorithm are indicated with brown dashed lines. The optimized, μ -dependent criteria are indicated with green solid line (before smoothing) and red solid line (after smoothing). The black dotted line represents the thresholds applied by the medium photon identification algorithm at trigger level in Run 2.

GeV. The cut values for the first category in the reoptimized, μ -dependent identification criteria for unconverted photons are listed in Table 4.7. Additional results for other regions are available in Ref. [123].

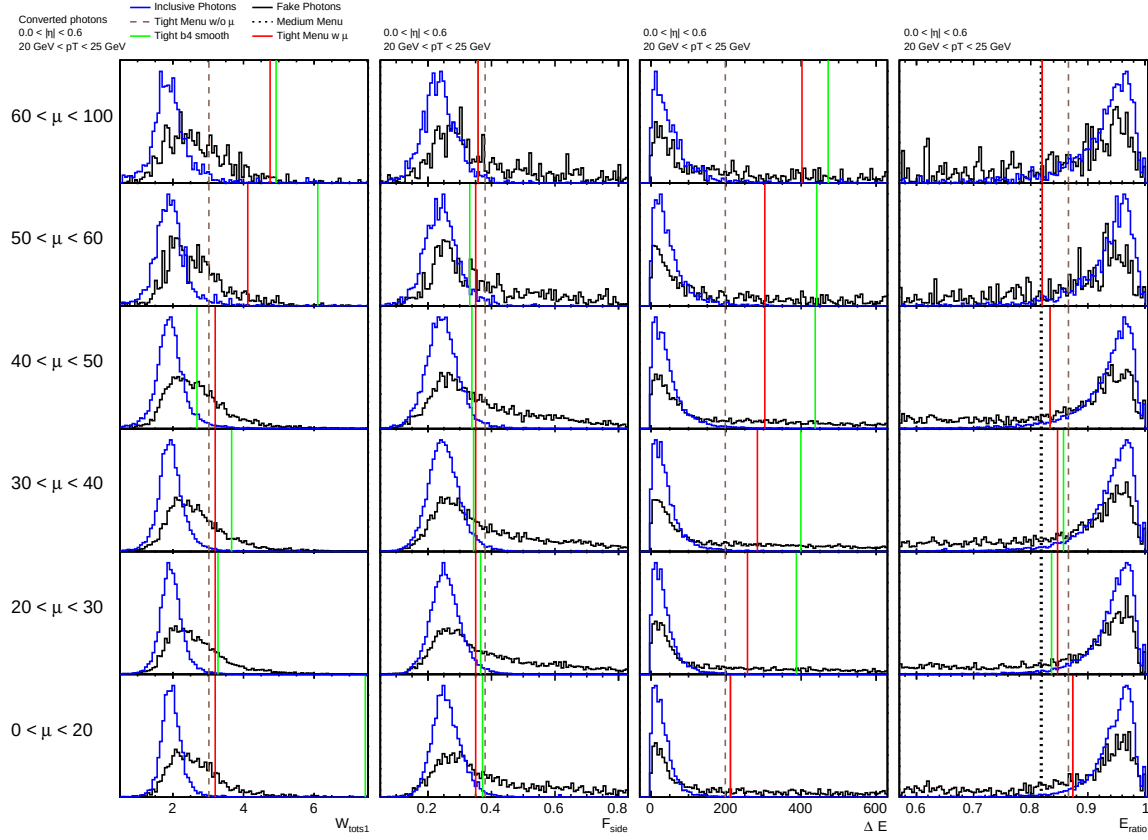


Fig. 4.15 Signal photon (blue) and background photon (black) shower shape distributions (w_{tots1} , f_{side} , ΔE , E_{ratio}) in bins of μ for converted photon candidates with $|\eta| < 0.6$ and $20 \leq p_T < 25$ GeV. The cuts used by the Run-2 photon identification algorithm are indicated with brown dashed lines. The optimized, μ -dependent criteria are indicated with green solid line (before smoothing) and red solid line (after smoothing). The black dotted line represents the thresholds applied by the medium photon identification algorithm at trigger level in Run 2.

4.3 Results and Conclusions

The dependence of the performance of the new criteria, obtained with the optimization procedure described in the previous section, on pile-up, in terms of prompt photon efficiency and background rejection, is studied and illustrated in the following sections. Additionally, the p_T -dependence of the criteria is investigated to ensure consistent performance across the p_T spectrum.

4.3.1 Dependence on pile-up

The signal efficiency and background rejection versus pile-up for various $|\eta|$ ranges and $20 < p_T < 25$ GeV are illustrated in Figure 4.18-4.20 and Figure 4.22-4.23 for converted and

μ	$R_{\text{had}} <$	$R_{\eta} >$	$R_{\phi} >$	$w_{\eta 1} <$	$w_{\eta 2} <$	$w_{\text{tots1}} <$	$f_{\text{side}} <$	$\Delta E <$	$E_{\text{ratio}} >$
$0 < \mu < 20$	0.012796	0.921303	0.516540	0.700814	0.012063	3.198798	0.350265	211.7	0.873562
$20 \leq \mu < 30$	0.036284	0.921303	0.473768	0.700814	0.012063	3.198798	0.350265	257.1	0.846904
$30 \leq \mu < 40$	0.036284	0.918470	0.473768	0.700814	0.012063	3.198798	0.350265	283.5	0.846904
$40 \leq \mu < 50$	0.036503	0.918470	0.437272	0.700814	0.012063	3.198798	0.350265	303.3	0.833876
$50 \leq \mu < 60$	0.036503	0.918470	0.437272	0.700814	0.012063	4.120450	0.350265	303.3	0.820089
$60 \leq \mu < 100$	0.052595	0.918470	0.437272	0.715145	0.012063	4.753150	0.357902	402.3	0.820033
<i>Run-2 criteria</i>	0.026	0.919	0.560	0.700	0.012	3.020	0.380	198.000	0.866

Tab. 4.5 Re-optimized tight identification criteria after smoothing, for converted photon candidates with $|\eta| < 0.6$ and $20 \leq p_T < 25$ GeV. For comparison, the last line shows the criteria used by the Run-2 algorithm, that do not depend on pile-up. "<" denotes less than the corresponding cut while ">" indicates greater.

p_T [GeV]	20-25	25-30	30-35	35-40	40-45	45-50	50-60	60-80	80<
$0 < \eta < 0.60$	89%	90%	90%	91%	92%	92%	92%	-	-
$0.60 \leq \eta < 0.80$	89%	90%	90%	91%	92%	92%	92%	-	-
$0.80 \leq \eta < 1.15$	86%	88%	90%	91%	92%	92%	92%	-	-
$1.15 \leq \eta < 1.37$	88%	90%	90%	91%	92%	92%	92%	92%	93%
$1.52 \leq \eta < 1.81$	89%	90%	90%	91%	92%	92%	92%	92%	93%
$1.81 \leq \eta < 2.01$	89%	90%	90%	91%	92%	92%	92%	92%	93%
$2.01 \leq \eta < 2.37$	89%	90%	90%	91%	92%	92%	92%	92%	93%

Tab. 4.6 Targeted working points for unconverted photon candidates in various $|\eta|$ and p_T regions. "-" represents that the regions are not optimized.

μ	$R_{\text{had1}} <$	$R_{\eta} >$	$R_{\phi} >$	$w_{\eta 1} <$	$w_{\eta 2} <$	$w_{\text{tots1}} <$	$f_{\text{side}} <$	$\Delta E <$	$E_{\text{ratio}} >$
$0 < \mu < 20$	0.044104	0.919492	0.908673	0.678361	0.011982	4.293525	0.292467	210.7	0.858532
$20 \leq \mu < 30$	0.049070	0.919492	0.908673	0.678361	0.011982	4.364575	0.320160	245.5	0.841555
$30 \leq \mu < 40$	0.049070	0.918068	0.908673	0.687227	0.011982	4.506675	0.320160	262.9	0.821566
$40 \leq \mu < 50$	0.050443	0.917838	0.901834	0.694193	0.011982	4.613250	0.320160	268.9	0.821566
$50 \leq \mu < 60$	0.050443	0.917678	0.781633	0.694193	0.011982	4.613250	0.329031	268.9	0.821566
$60 \leq \mu < 100$	0.050443	0.917605	0.598078	0.788337	0.012775	5.501375	0.503315	344.1	0.818613
<i>Run-2 criteria</i>	0.042	0.920	0.935	0.676	0.012	3.710	0.315	239.000	0.820

Tab. 4.7 Re-optimized tight identification criteria after smoothing, for unconverted photon candidates with $|\eta| < 0.6$ and $20 \leq p_T < 25$ GeV. For comparison, the last line shows the criteria used by the Run-2 algorithm, that do not depend on pile-up. "<" denotes less than the corresponding cut while ">" indicates greater.

unconverted photons, respectively. The performance are studied using photon candidates that pass isolation requirements.

In Figure 4.18-4.21, which depicts the performance for converted photons, the μ -dependent criteria maintain stable efficiency as pile-up increases and show a relative efficiency gain of 5-10% compared to the Run-2 criteria at high pile-up. However, this improvement in efficiency comes at the cost of reduced fake photon rejection under high pile-up conditions. Since the working

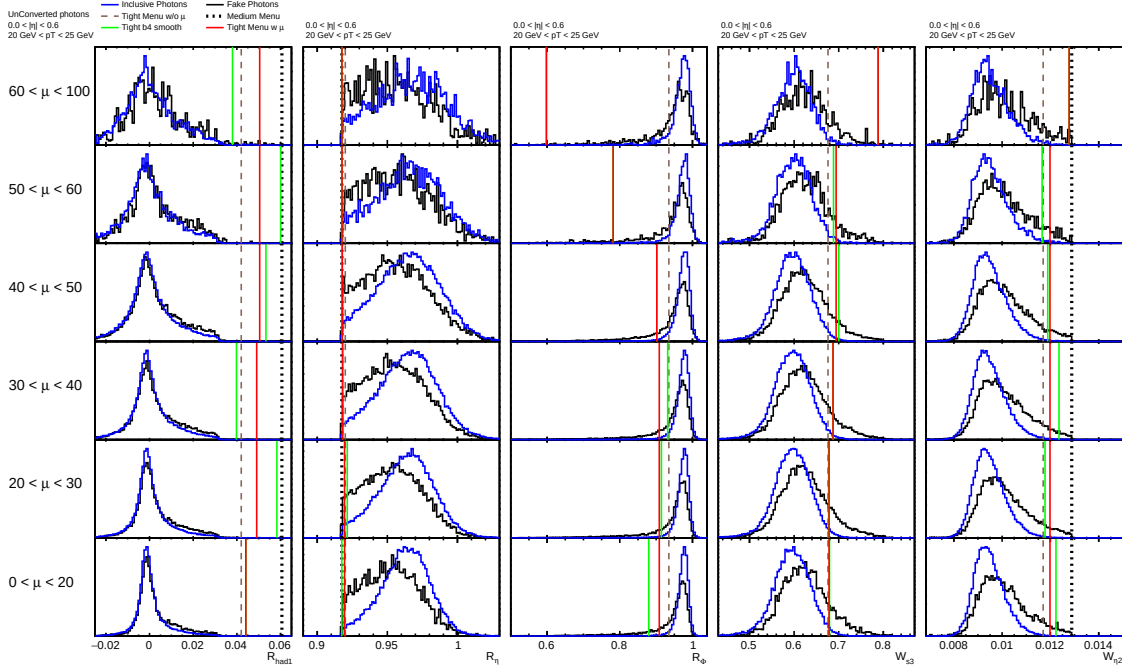


Fig. 4.16 Signal photon (blue) and background photon (black) shower shape distributions (R_{had1} , R_η , R_ϕ , w_{s3} , $w_{\eta2}$) in bins of μ for unconverted photon candidates with $|\eta| < 0.6$ and $20 \leq p_T < 25$ GeV. The cuts used by the Run-2 photon identification algorithm are indicated with brown dashed lines. The optimized, μ -dependent criteria are indicated with green solid line (before smoothing) and red solid line (after smoothing). The black dotted line represents the thresholds applied by the medium photon identification algorithm at trigger level in Run 2.

point for all μ bins is defined based on the efficiency of the Run-2 algorithm at $\mu \approx 30$, there is a significant efficiency decrease in the first μ interval (0–20) due to the stringent cuts on DVs; however, the fraction of events with such a low pile-up in Run-3 is negligible.

Figure 4.22–4.25 show the results for unconverted photons. The μ -dependent criteria demonstrate good stability in efficiency vs pile-up and perform significantly better than the Run-2 criteria at high pile-up in terms of prompt photon efficiency, although this also reduces the fake photon rejection at large pile-up.

In the highest pile-up bins, the prompt photon efficiency increases by 10–15%, while the background rejection worsens by 20–25%. This is still advantageous for instance for measuring Higgs boson decays to two photons, where the background is composed roughly for 70% by prompt diphoton and 30% by photon+jet candidates. A 10–15% increase in photon efficiency translates into 21–32% larger Higgs boson signal and prompt diphoton background yields, and combined with a rejection worse by 20–25% leads to a 32–44% increase in photon+jet background yield. Altogether, this yields an expected increase of 9–13% in sensitivity for Higgs boson decays to two photons. For searches of Higgs boson pairs to $b\bar{b}\gamma\gamma$, where most of the background comes from single Higgs boson production followed by $H \rightarrow \gamma\gamma$ decays and from diphoton continuum

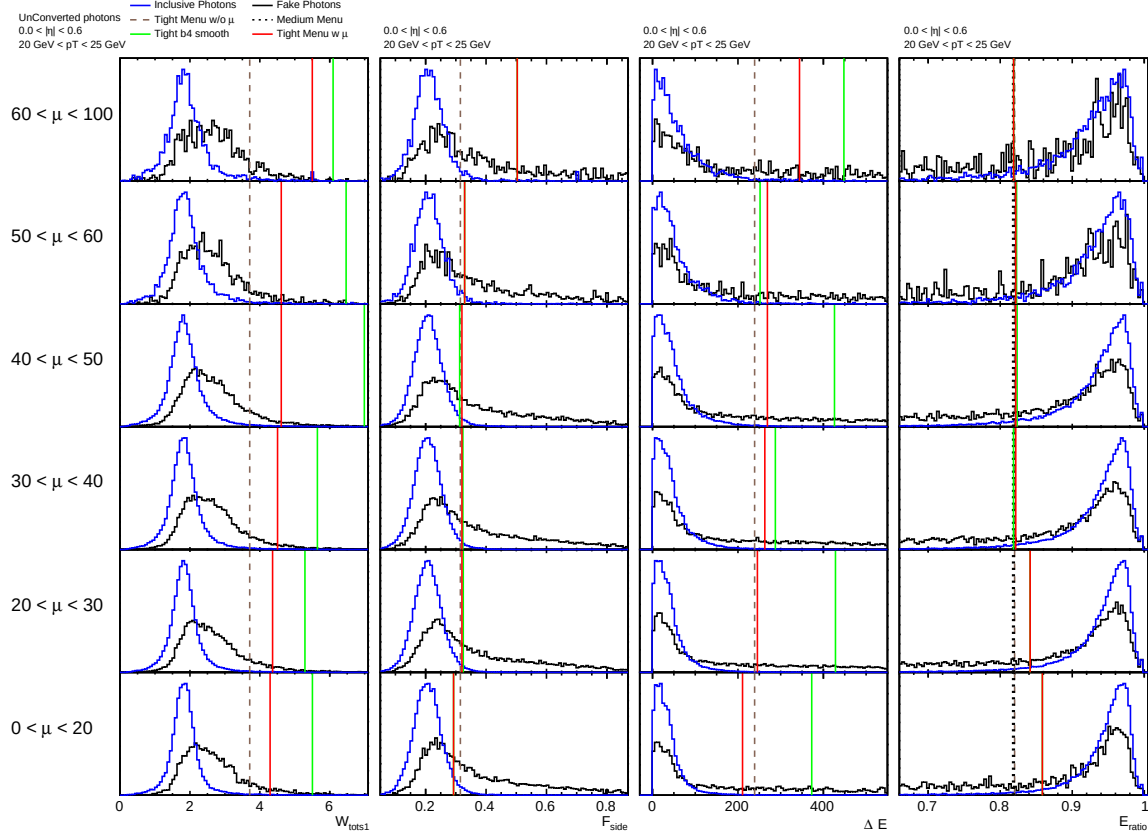


Fig. 4.17 Signal photon (blue) and background photon (black) shower shape distributions (w_{tots1} , f_{side} , ΔE , E_{ratio}) in bins of μ for unconverted photon candidates with $|\eta| < 0.6$ and $20 \leq p_T < 25$ GeV. The cuts used by the Run-2 photon identification algorithm are indicated with brown dashed lines. The optimized, μ -dependent criteria are indicated with green solid line (before smoothing) and red solid line (after smoothing). The black dotted line represents the thresholds applied by the medium photon identification algorithm at trigger level in Run 2.

production, a prompt photon efficiency increase by 10-15% would lead to a 10-15% increase in significance for the $HH \rightarrow b\bar{b}\gamma\gamma$ signal.

4.3.2 Dependence on p_T

The p_T -dependence of the performance of the new criteria and of the Run-2 ones for various pile-up bins at distinct $|\eta|$ regions are illustrated in Figure 4.26-4.29 for converted photons and Figure 4.30-4.33 for unconverted photons, respectively. Comparing the results in Figure 4.26 (a) and (d), the prompt photon efficiency of the new criteria at low transverse momentum and medium to high pileup is significantly improved compared to the Run-2 criteria. Similar results are observed in other $|\eta|$ regions. Additionally, in the low p_T regions, the efficiency of the μ -dependent criteria remains quite stable as pile-up increases. For unconverted photons in

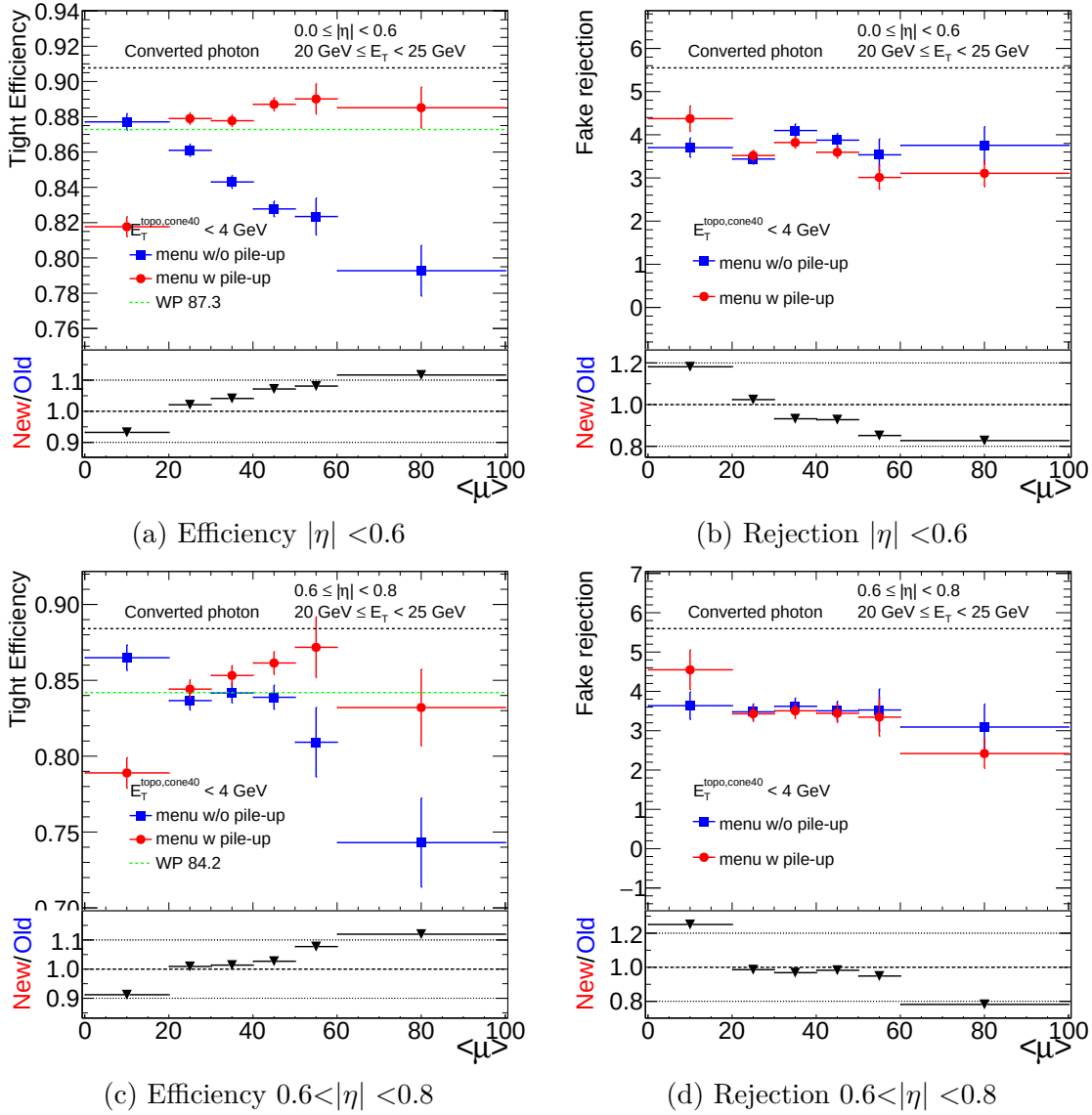


Fig. 4.18 Efficiency (a and c) and background rejection (b and d) for converted photons with $20 < p_T < 25$ GeV across different $|\eta|$ ranges ($|\eta| < 0.6$, $0.6 < |\eta| < 0.8$), comparing the reoptimized μ -dependent criteria (red) to the Run-2 requirements (blue) as a function of pile-up. The targeted working point is labeled by the horizontal dashed line (green). Photon *loose* identification criteria and *isolation* requirements are applied.

Figure 4.30 (a) and (d), the μ -dependent criteria perform much better than the Run-2 ones under high pile-up conditions. These observations lead to the conclusion that the new criteria are more efficient in low μ regions than the previous ones and more stable across all μ regions, with the efficiency trend vs p_T being consistent with that of the Run-2 algorithm for low pile-up.

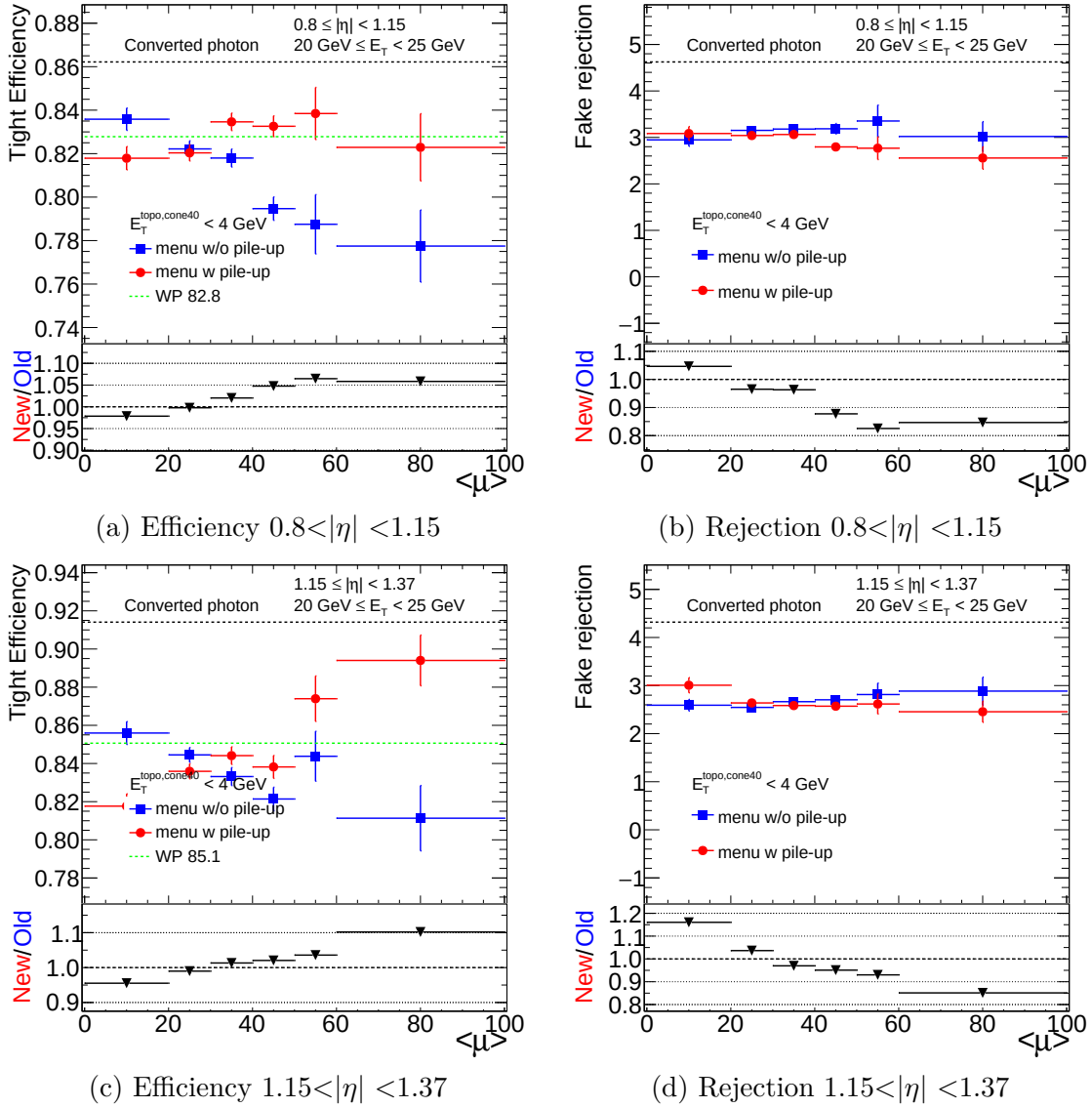


Fig. 4.19 Efficiency (a and c) and background rejection (b and d) for converted photons with $20 < p_T < 25$ GeV across different $|\eta|$ ranges ($0.8 < |\eta| < 1.15$, $1.15 < |\eta| < 1.37$), comparing the reoptimized μ -dependent criteria (red) to the Run-2 requirements (blue) as a function of pile-up. The targeted working point is labeled by the horizontal dashed line (green). Photon *loose* identification criteria and *isolation* requirements are applied.

4.3.3 Conclusions

Confronted with the more complex pile-up conditions in Run-3, the tight photon identification criteria used in Run-2 show a decline in prompt photon identification efficiency. μ -dependent selection requirements on nine discriminating shower shape variables are optimized with TMVA to mitigate the inefficiency of the Run-2 photon identification algorithm at high pile-up. The performance of the new criteria are evaluated in terms of prompt photon efficiency and back-

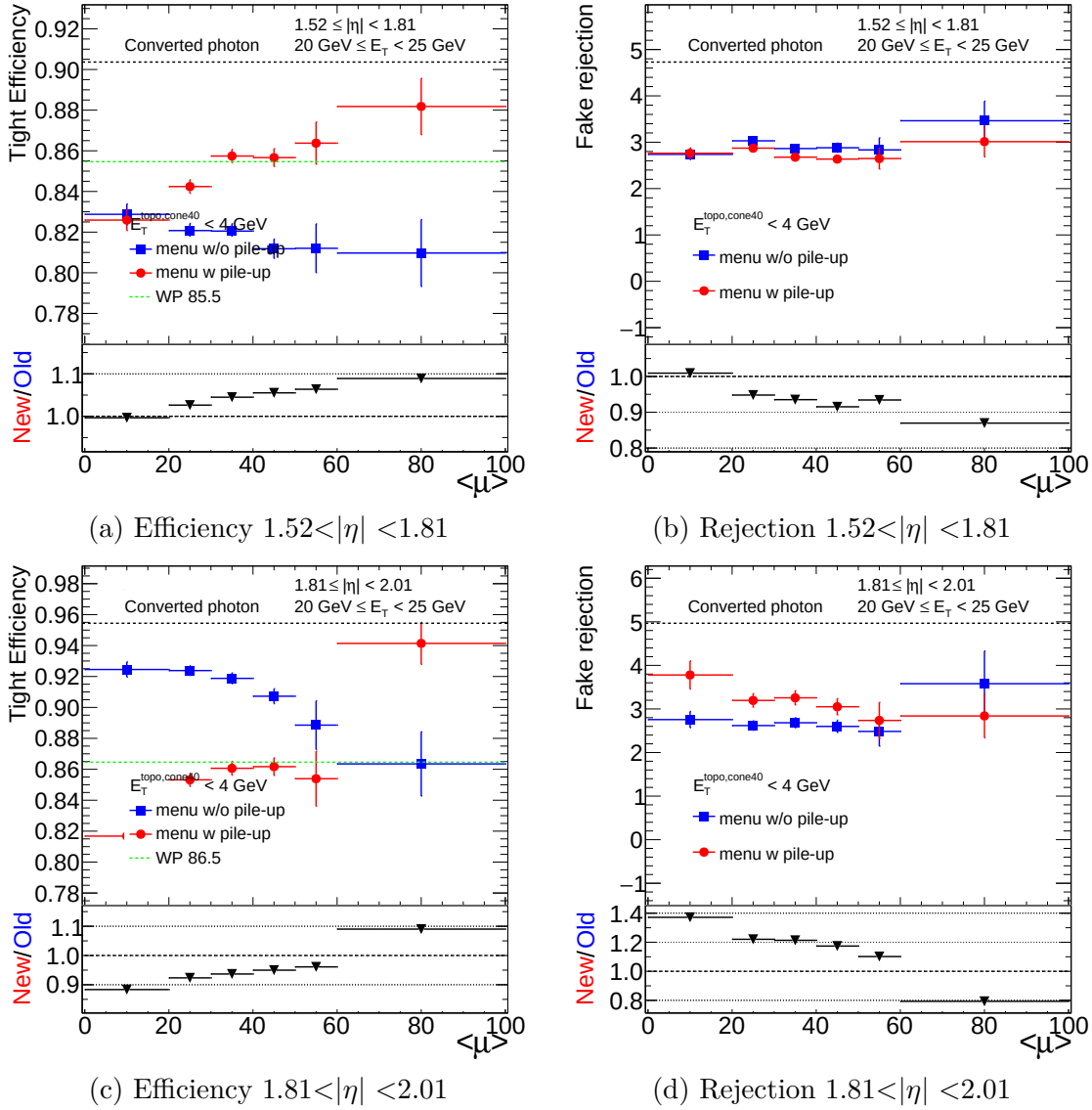


Fig. 4.20 Efficiency (a-c) and background rejection (d-f) for converted photons with $20 < p_T < 25$ GeV across different $|\eta|$ ranges ($1.52 < |\eta| < 1.81$, $1.81 < |\eta| < 2.01$), comparing the reoptimized μ -dependent criteria (red) to the Run-2 requirements (blue) as a function of pile-up. The targeted working point is labeled by the horizontal dashed line (green). Photon *loose* identification criteria and *isolation* requirements are applied.

ground rejection. The thresholds on the shower shape variables for the new photon identification algorithm proposed for Run-3 are chosen in order to yield similar efficiency to those of the Run-2 algorithm at modest pile-up ($\mu \approx 30$). The new requirements improve the performance of photon tight identification for both converted and unconverted photons, particularly under high pile-up conditions. The efficiency of the new selection criteria is also more stable across the full range of pile-up, although this improvement in performance comes at the cost of a reduced fake rejection

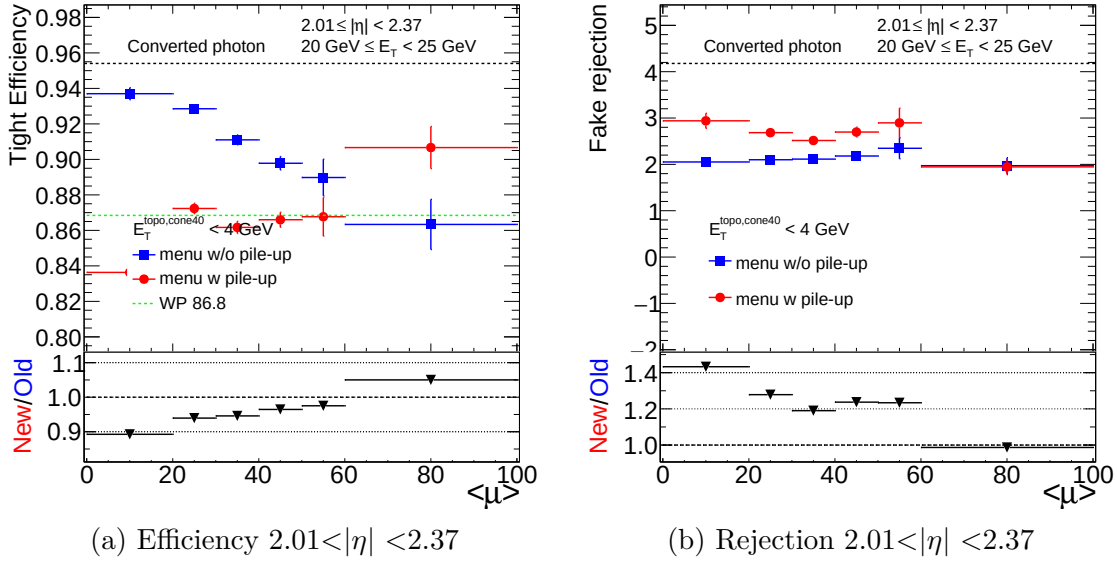
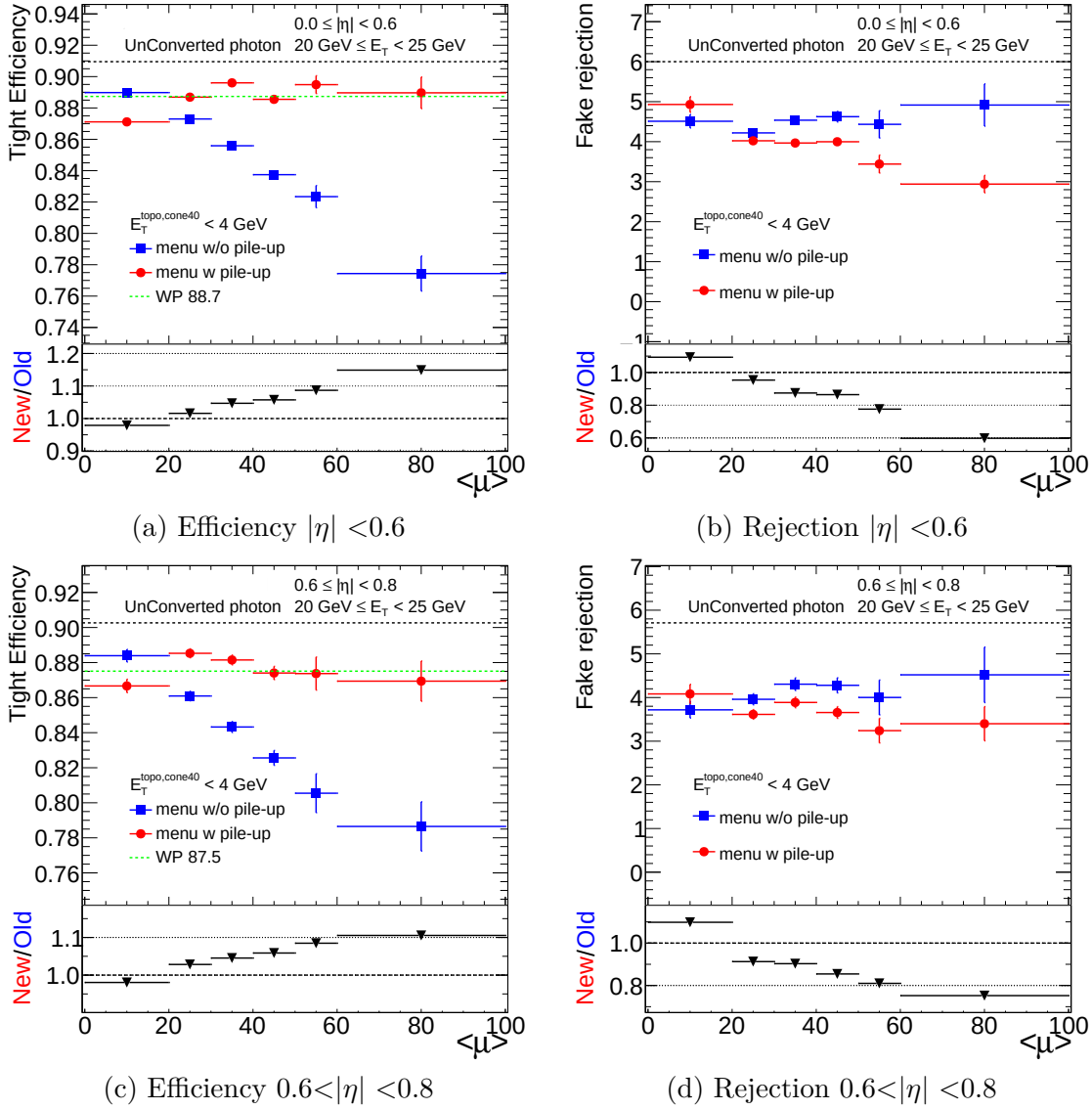
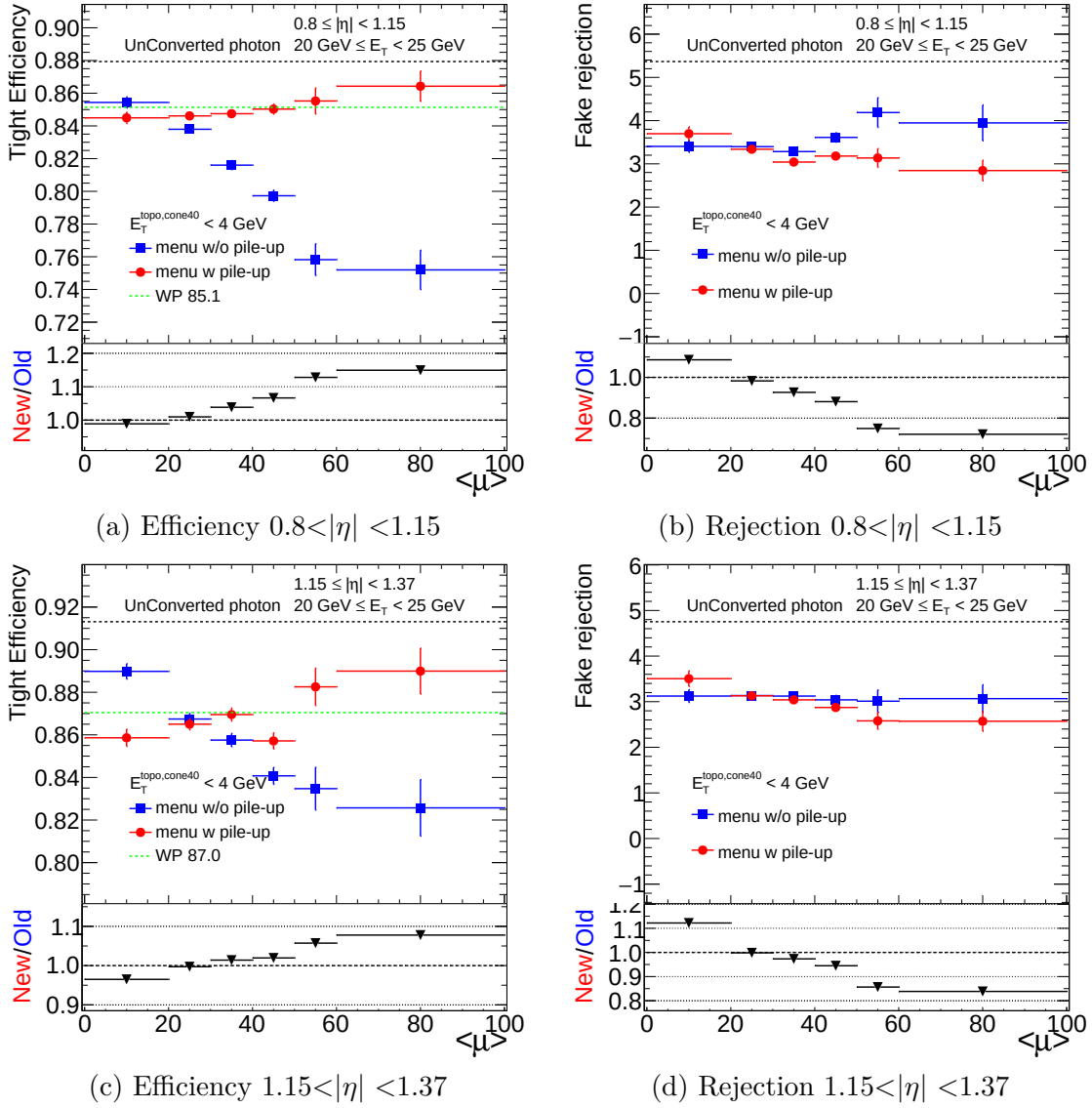


Fig. 4.21 Efficiency (a) and background rejection (b) for converted photons with $20 < p_T < 25 \text{ GeV}$ and $2.01 < |\eta| < 2.37$, comparing the reoptimized μ -dependent criteria (red) to the Run-2 requirements (blue) as a function of pile-up. The targeted working point is labeled by the horizontal dashed line (green). Photon *loose* identification criteria and *isolation* requirements are applied.

rate. Additionally, the p_T -dependence of the new proposed photon identification criteria has been checked and found to be consistent with that of the Run-2 menu at low pile-up, ensuring reliable performance across the p_T spectrum. Finally, the new photon identification algorithm was implemented into the ATHENA framework introduced in Chapter 3 for use in ATLAS offline analyses and further performance studies. Overall, the increase in prompt photon efficiency and the typical purity of (di)photon signals under study leads to an expected improvement in sensitivity close to 10-15% at high pile-up.

**Fig. 4.22**

Efficiency (a and c) and background rejection (b and d) for unconverted photons with $20 < p_T < 25$ GeV across different $|\eta|$ ranges ($|\eta| < 0.6$, $0.6 < |\eta| < 0.8$), comparing the reoptimized μ -dependent criteria (red) to the Run-2 requirements (blue) as a function of pile-up. The targeted working point is labeled by the horizontal dashed line (green). Photon *loose* identification criteria and *isolation* requirements are applied.

**Fig. 4.23**

Efficiency (a and c) and background rejection (b and d) for unconverted photons with $20 < p_T < 25$ GeV across different $|\eta|$ ranges ($0.8 < |\eta| < 1.15$, $1.15 < |\eta| < 1.37$), comparing the reoptimized μ -dependent criteria (red) to the Run-2 requirements (blue) as a function of pile-up. The targeted working point is labeled by the horizontal dashed line (green). Photon *loose* identification criteria and *isolation* requirements are applied.

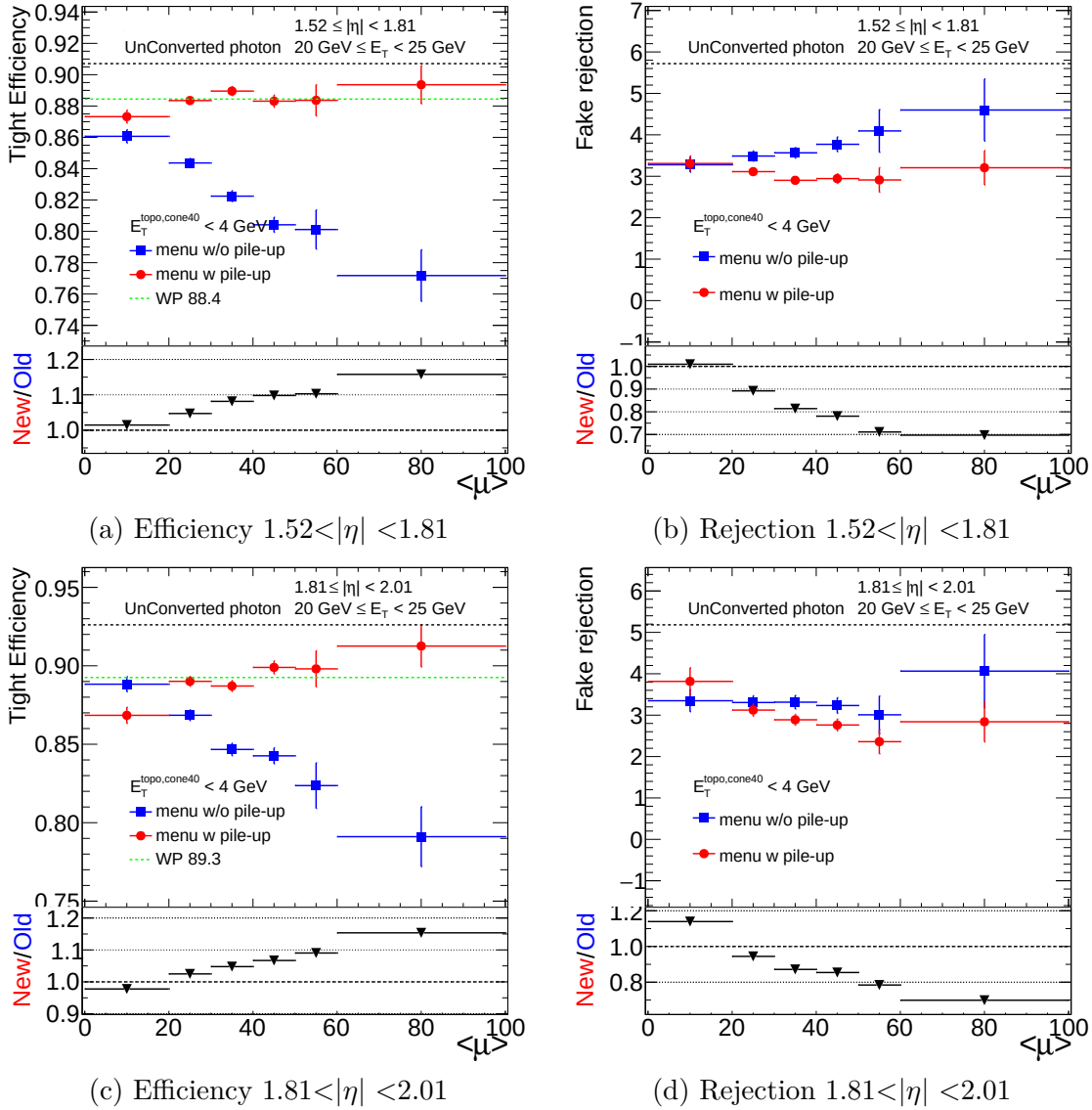


Fig. 4.24 Efficiency (a and c) and background rejection (b and d) for unconverted photons with $20 < p_T < 25$ GeV across different $|\eta|$ ranges ($1.52 < |\eta| < 1.81$, $1.81 < |\eta| < 2.01$), comparing the reoptimized μ -dependent criteria (red) to the Run-2 requirements (blue) as a function of pile-up. The targeted working point is labeled by the horizontal dashed line (green). Photon *loose* identification criteria and *isolation* requirements are applied.

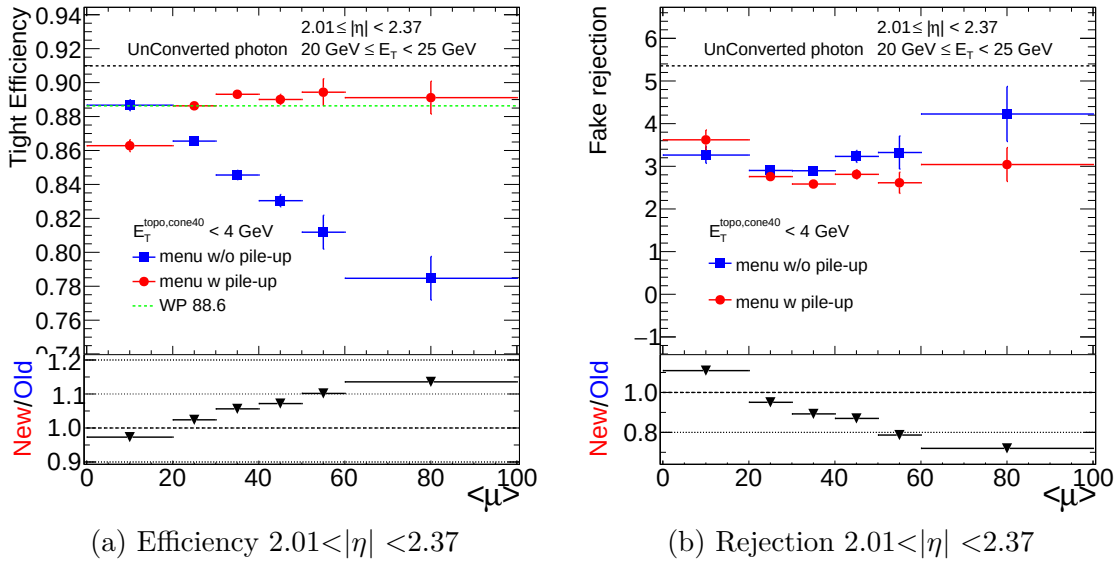
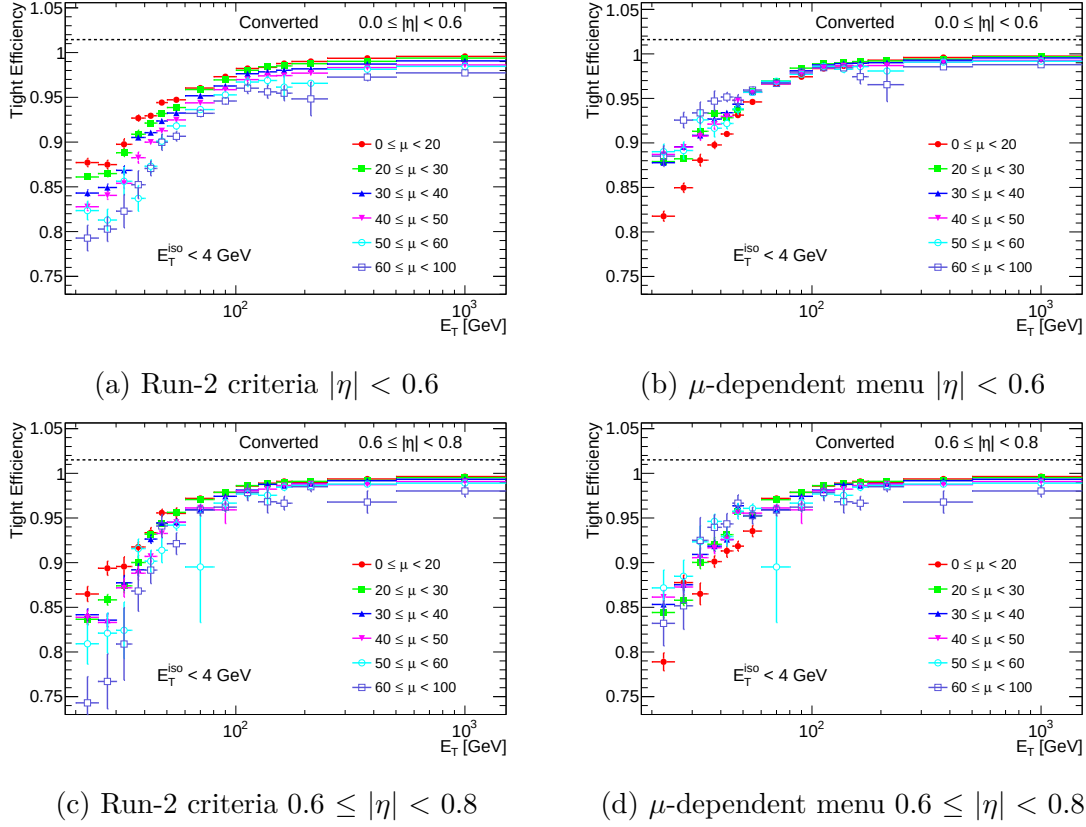


Fig. 4.25 Efficiency (a) and background rejection (b) for unconverted photons with $20 < p_T < 25 \text{ GeV}$ and $2.01 < |\eta| < 2.37$, comparing the reoptimized μ -dependent criteria (red) to the Run-2 requirements (blue) as a function of pile-up. The targeted working point is labeled by the horizontal dashed line (green). Photon *loose* identification criteria and *isolation* requirements are applied.

**Fig. 4.26**

The efficiency versus p_T in different μ bins for the Run-2 criteria (a and c) and the new μ -dependent requirements (b and d) in different $|\eta|$ regions ($|\eta| < 0.6$, $0.6 \leq |\eta| < 0.8$) for converted photons. Photon *loose* identification criteria and *isolation* requirements are applied.

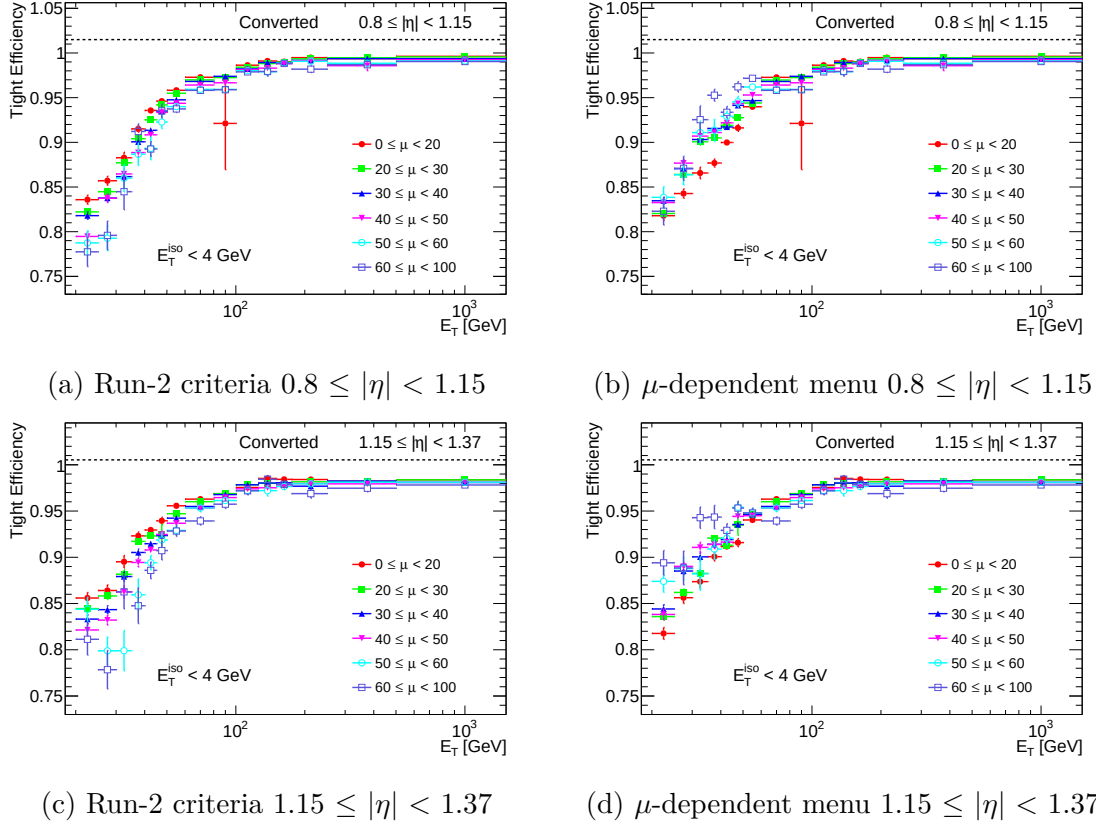
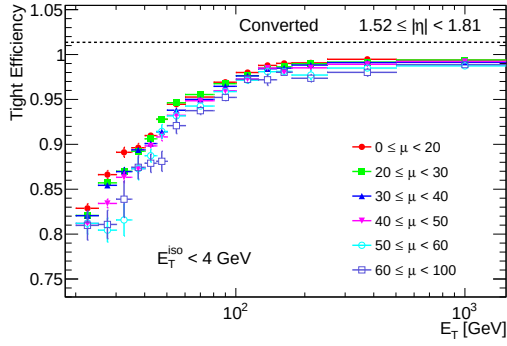
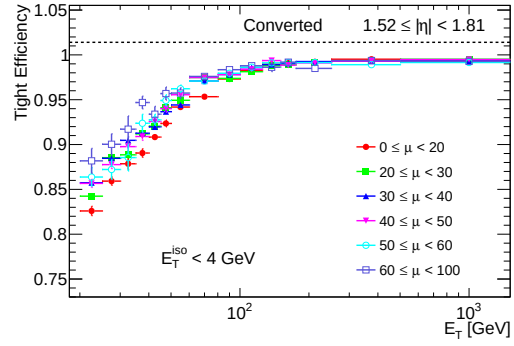
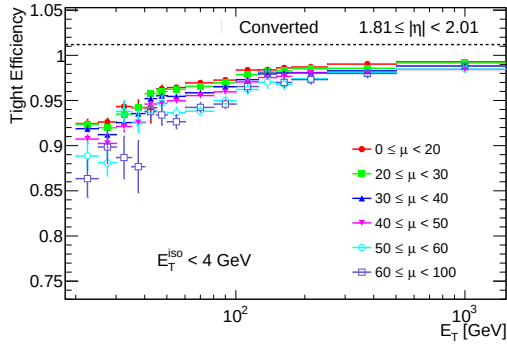
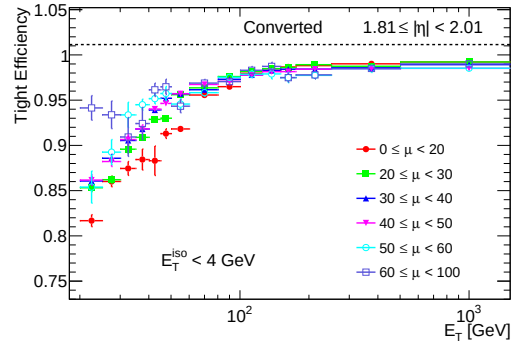
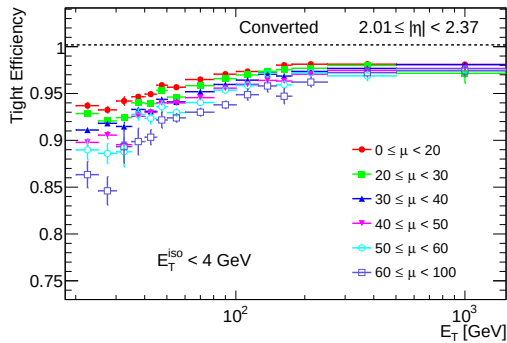
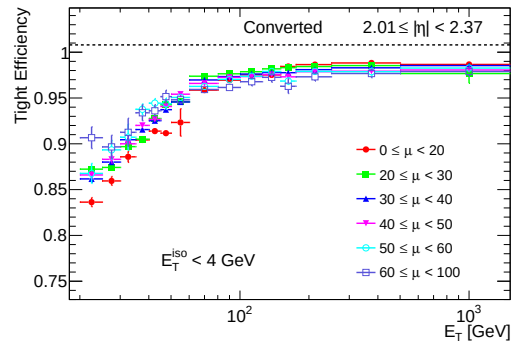


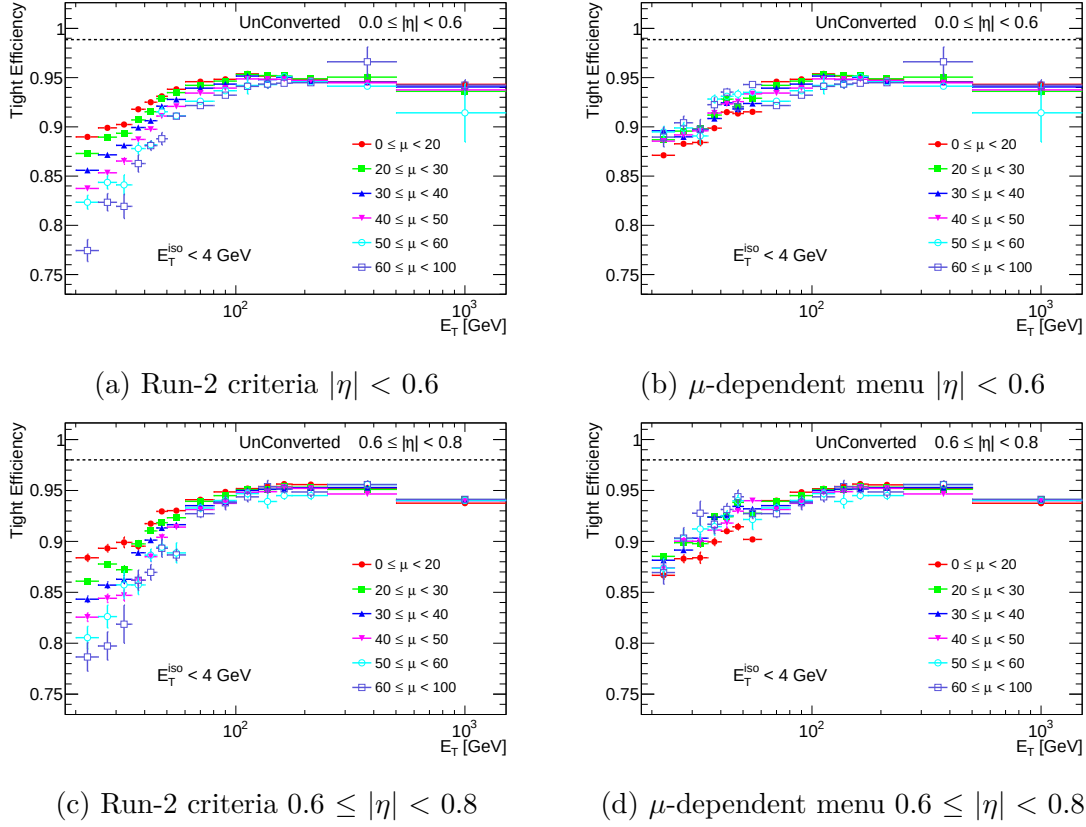
Fig. 4.27 The efficiency versus p_T in different μ bins for the Run-2 criteria (a and c) and the new μ -dependent requirements (b and d) in different $|\eta|$ regions ($0.8 \leq |\eta| < 1.15$, $1.15 \leq |\eta| < 1.37$) for converted photons. Photon *loose* identification criteria and *isolation* requirements are applied.

(a) Run-2 criteria $1.52 \leq |\eta| < 1.81$ (b) μ -dependent menu $1.52 \leq |\eta| < 1.81$ (d) Run-2 criteria $1.81 \leq |\eta| < 2.01$ (f) μ -dependent menu $1.81 \leq |\eta| < 2.01$ **Fig. 4.28**

The efficiency versus p_T in different μ bins for the Run-2 criteria (a and c) and the new μ -dependent requirements (b and d) in different $|\eta|$ regions ($1.52 \leq |\eta| < 1.81$, $1.81 \leq |\eta| < 2.01$) for converted photons. Photon *loose* identification criteria and *isolation* requirements are applied.

(a) Run-2 criteria $2.01 \leq |\eta| < 2.37$ (b) μ -dependent menu $2.01 \leq |\eta| < 2.37$ **Fig. 4.29**

The efficiency versus p_T in different μ bins for the Run-2 criteria (a) and the new μ -dependent requirements (b) in $2.01 \leq |\eta| < 2.37$ for converted photons. Photon *loose* identification criteria and *isolation* requirements are applied.

**Fig. 4.30**

Efficiency versus p_T for unconverted photons in different μ bins, displayed for the Run-2 criteria (a and c) and the new μ -dependent requirements (b and d) across various $|\eta|$ regions ($|\eta| < 0.6$, $0.6 \leq |\eta| < 0.8$). Photon *loose* identification criteria and *isolation* requirements are applied.

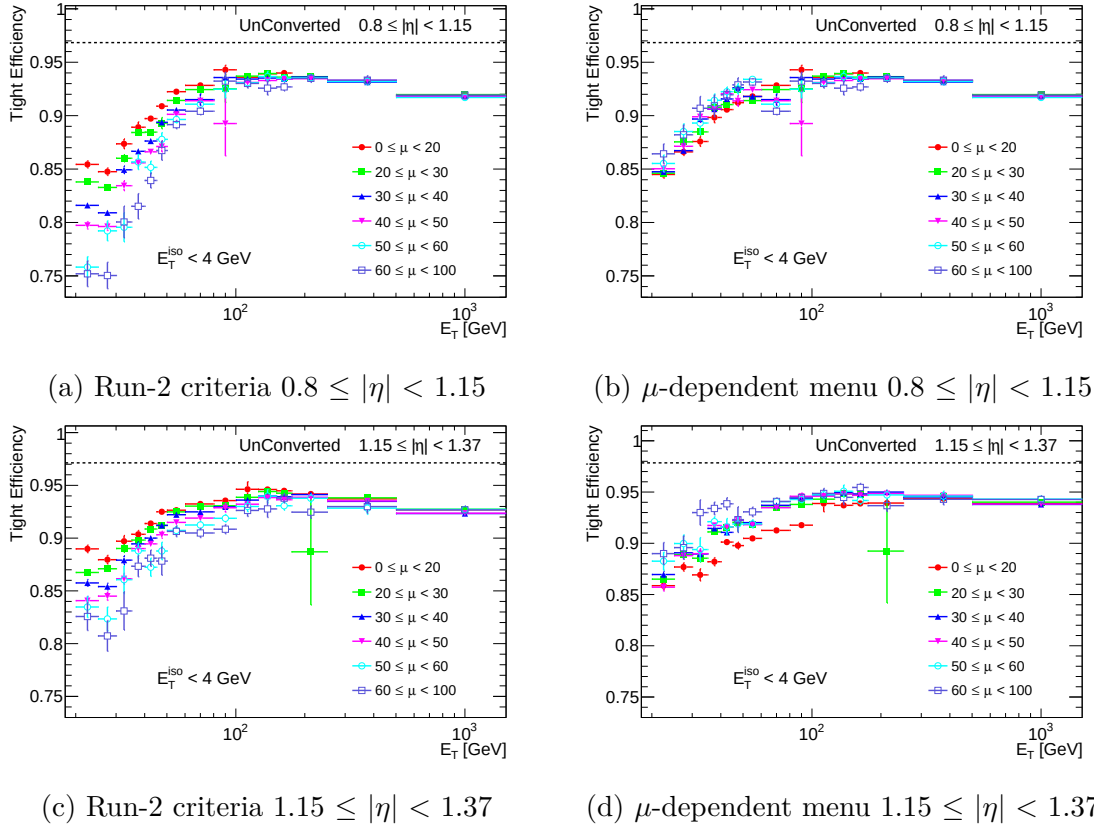


Fig. 4.31 Efficiency versus p_T for unconverted photons in different μ bins, displayed for the Run-2 criteria (a and c) and the new μ -dependent requirements (b and d) across various $|\eta|$ regions ($0.8 \leq |\eta| < 1.15$, $1.15 \leq |\eta| < 1.37$). Photon *loose* identification criteria and *isolation* requirements are applied.

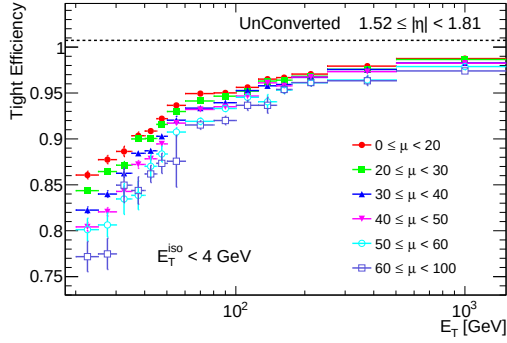
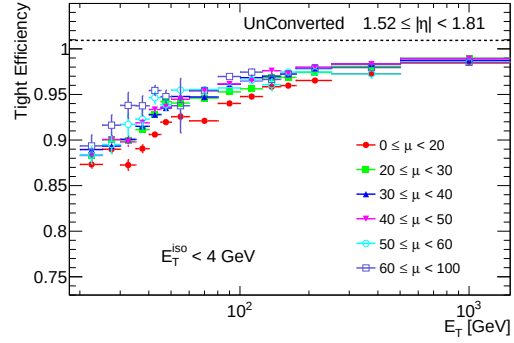
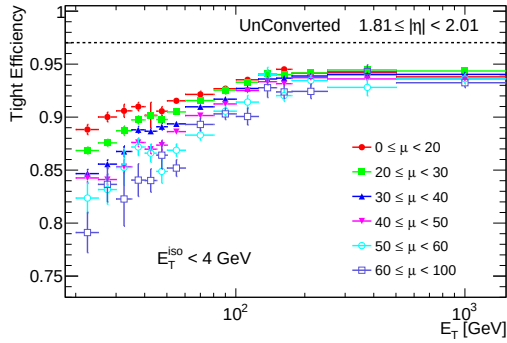
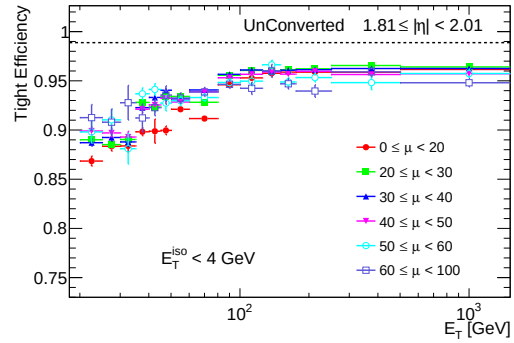
(a) Run-2 criteria $1.52 \leq |\eta| < 1.81$ (b) μ -dependent menu $1.52 \leq |\eta| < 1.81$ (c) Run-2 criteria $1.81 \leq |\eta| < 2.01$ (d) μ -dependent menu $1.81 \leq |\eta| < 2.01$

Fig. 4.32 Efficiency versus p_T for unconverted photons across different μ bins, for the Run-2 criteria (a and c) and the new μ -dependent requirements (b and d) within the $|\eta|$ regions ($1.52 \leq |\eta| < 1.81$, $1.81 \leq |\eta| < 2.01$). Photon *loose* identification criteria and *isolation* requirements are applied.

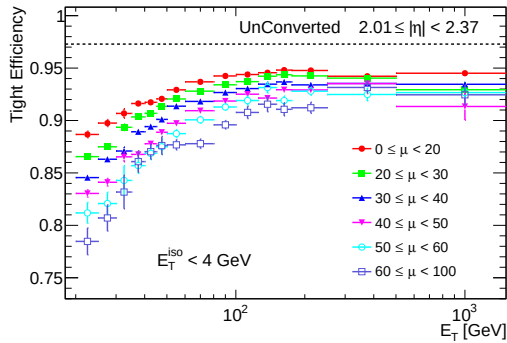
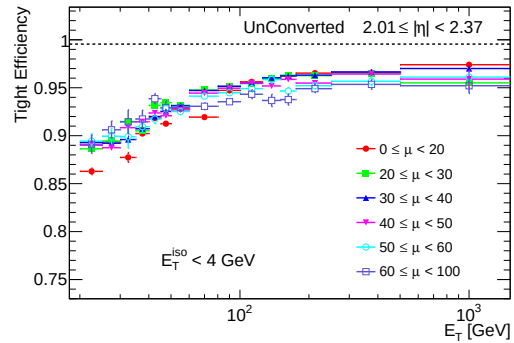
(a) Run-2 criteria $2.01 \leq |\eta| < 2.37$ (b) μ -dependent menu $2.01 \leq |\eta| < 2.37$

Fig. 4.33 Efficiency versus p_T for unconverted photons in the $|\eta|$ range $2.01 \leq |\eta| < 2.37$, for the Run-2 criteria (a) and the new μ -dependent requirements (b) across different μ bins. Photon *loose* identification criteria and *isolation* requirements are applied.

Search for Higgs Boson Pair Production in the $b\bar{b}\gamma\gamma$ Final State

The landmark discovery of the Higgs boson in 2012 [6, 7] has ignited a wave of research aimed at uncovering its intrinsic properties and couplings to other particles, with notable contributions from the ATLAS and CMS collaborations. A critical aspect of this research is the investigation of the Higgs boson self-coupling, which is essential for a deeper comprehension of the Higgs mechanism, particularly in the context of electroweak symmetry breaking. Precise measurements of Higgs boson self-coupling would offer valuable insights into the Higgs field potential, thereby advancing the precision tests of electroweak theory. One intriguing avenue of research is the direct probing of the Higgs boson self-coupling through the production of Higgs boson pairs (HH). As described in Section 1.3.1, the two dominant HH production modes in the Standard Model are gluon-gluon fusion (ggFHH) and vector boson fusion (VBFHH). Figure 1.16 shows the branching ratios of the decays of Higgs boson pairs in the Standard Model, among which the $b\bar{b}\gamma\gamma$ final state plays a prominent role due to large $H \rightarrow b\bar{b}$ branching ratio, the clean diphoton signature and low backgrounds. This chapter will present a comprehensive analysis of the $HH \rightarrow b\bar{b}\gamma\gamma$ channel, utilizing the entire ATLAS Run-2 dataset.

5.1 Motivation

Higgs boson pair production and decay have been described in Section 1.3.1, where the leading-order Feynman diagrams, cross-sections and branching ratios in pp collisions at $\sqrt{s} = 13$ TeV are discussed in detail. As illustrated in Figure 1.17, deviations in the Higgs coupling strengths from the SM values can result in an enhancement of the Higgs pair boson production cross-section. The HH production cross-section is influenced by the Higgs self-coupling λ , which is the product of the SM value λ_{SM} times a strength modified κ_λ . Even relatively small

variations of κ_λ from one could lead to a significant increase in the HH cross-section, with the sign of the coupling potentially quadrupling the rate [128]. Additionally, VBFHH production can be enhanced by anomalous values of the modifier κ_{2V} of the coupling of the interaction between a vector boson pair and a Higgs boson pair ($VVHH$).

The $HH \rightarrow b\bar{b}\gamma\gamma$ channel was firstly investigated in ATLAS in 2015 [129] and is still under active research. With increasingly larger data sets and more advanced analysis techniques, the results made great progress in the past few years, with 95% CL upper limits on the HH cross-section reduced from 2.2 pb with 20 fb⁻¹ of 8 TeV ATLAS data to 0.13 pb with 139 fb⁻¹ of 13 TeV ATLAS data [130].

This chapter presents the search for $HH \rightarrow b\bar{b}\gamma\gamma$ with the full ATLAS Run 2 data. The analysis focuses on the ggFHH and VBFHH production modes. It proceeds in the following way: after an initial reconstruction and event preselections, the events are classified in mutually orthogonal categories. Signal and background yields, from which cross-sections are determined, are estimated by a simultaneous fit to the diphoton invariant mass distribution in data in the reconstructed event categories.

The chapter is organized as follows. The data and MC samples, along with the parameterization methods used to generate signal samples with arbitrary values of the κ_λ and κ_{2V} coupling strength modifiers, are detailed in Section 5.2. Section 5.3 discusses the statistical methods used for the interpretation of the data in terms of HH cross-sections, κ_λ and κ_{2V} . The requirements applied at event reconstruction and preselections are depicted in Section 5.4. Two distinct event categorization strategies, a baseline and an alternative one, are respectively presented in Section 5.5 and Section 5.6. These two sections also cover the modeling of signal and background events and the expected results of the statistical interpretation of the events classified in these two alternative ways. The comparisons of the results for these two strategies are performed in Section 5.7. The choice of the continuum background model for the final fit to the data and the related systematic uncertainty is detailed in Section 5.8. The other sources of systematic uncertainties are addressed in Section 5.9. The results of the baseline analysis applied to the data are given in Section 5.10.

5.2 Data and Simulated Event Samples

The data and MC event samples used in this analysis are described in this section. The common procedures of MC event generation and simulation in ATLAS are presented in Section 3.1, while the details about the Higgs boson pair signal MC will be described in the following sections. In Section 1.3.1 it has been shown that the dominant Higgs boson pair production modes are mainly affected by four coupling modifiers, κ_λ , κ_t , κ_{2V} and κ_V . The analysis presented here mainly focuses on constraining κ_λ and κ_{2V} , while the other coupling modifiers, which are constrained by single-Higgs boson production measurements that are in excellent agreement with the Standard Model, are assumed to be equal to unity.

5.2.1 Data

The analysis uses pp collisions at $\sqrt{s} = 13$ TeV, collected with the ATLAS detector between 2015 and 2018 using single-photon and di-photon triggers. The details of data-taking

in Run-2 are presented in Section 2.1.2. Photon-specific triggers are designed to select events containing one or two high- p_T photons. Two diphoton triggers with loose or medium identification criteria are adopted. In 2015-2016, the trigger `HLT_g35_loose_g25_loose` detected events with at least two photons, with p_T thresholds of 25 GeV for the sub-leading photon and 35 GeV for the leading photon at HLT, passing loose photon identification criteria. This trigger was seeded by two energy deposits greater than 15 GeV at L1. In 2017-2018, the trigger `HLT_g35_medium_g25_medium_L12EM20VH` detected diphoton events with the same p_T thresholds at HLT, but required larger energy deposits, exceeding 20 GeV in the EM calorimeter at L1, with an additional hadronic core isolation (H) requirement. The two photon candidates had to pass medium photon identification criteria. Additionally, two single photon triggers were implemented: `HLT_g120_loose` in 2015 and `HLT_g140_loose` in 2016-2018. These triggers identified events with at least one loose photon, with p_T thresholds of more than 120 GeV and 140 GeV at HLT, respectively. Single photon triggers were considered to target potential boosted Higgs bosons with p_T greater than 650 GeV, which decay into a pair of closely collimated photons. These triggers are also useful in events where the leading photon has a significantly higher p_T than the sub-leading photon. However, the simulation of HH events indicated that only 0.1% of the signal is collected by single-photon triggers and not by di-photon triggers [130].

The aggregate integrated luminosity is 140 fb^{-1} after trigger and good data-quality requirements, with a relative uncertainty of 0.83%. After the online trigger selections, the events undergo further processing through offline selection, as detailed in Section 5.4.

5.2.2 Simulation: ggFHH Signal

As described in Section 1.3.1, the ggFHH production mode is induced at leading order by two Feynman diagrams whose amplitudes are affected by two coupling modifiers, κ_λ and κ_t , with a SM cross-section equal to 31.05 fb at $\sqrt{s} = 13 \text{ TeV}$ and $m_H = 125.0 \text{ GeV}$. The interference between the two diagrams results in the SM in a partial suppression of the total cross-section.

5.2.2.1 Generated ggFHH Samples

Signal events at generator level were produced at NLO using the matrix element calculated by `Powheg-Box-V2` and `Finite Top` [131, 132], which provide comprehensive NLO corrections and account for the finite mass of the top quark. The NLO corrections to Higgs pair production increase the cross-section by approximately 70-100%, depending on the choice of parameters such as the top quark mass approximation and the inclusion of higher-dimensional operators [133]. The `PDF4LHC15_nlo_30_pdfas` parton distribution function (PDF) set [134] was used for the matrix element calculation. The parton-level generated events were interfaced to `Pythia 8.244` in order to simulate parton showering, hadronization and underlying event. The systematic uncertainty stemming from the chosen event generator is assessed using alternative samples generated with `Herwig 7.1`. The `H7-UE-MMHT` tune was used for modeling underlying events, while the `H7-MMHT2014LO` tune was applied for simulating parton shower and hadronization processes. Two samples were generated for $\kappa_\lambda = 1$ and 10, respectively targeting the SM and BSM processes, as listed in Table 5.1. The cross-section for a given value of κ_λ was determined using next-to-next-to-leading order (NNLO) calculations. These calculations account for a finite top quark mass in real emission processes and apply an infinite top mass approximation for two-loop virtual corrections (FTApprox) [135], resulting in about a 20% increase compared to the

NLO result [136]. The relationship between the cross-section and κ_λ for any given value of the latter is described by a quadratic function, whose parameters are obtained by fitting the values predicted by the simulations for a few fixed values of κ_λ . This function is rescaled to match the SM total cross-section when $\kappa_\lambda = 1$ [135, 137].

ggFHH Signal Mode	Generator and Showering	PDF (ME)	PDF+Tuning (PS)	σ [fb]	Events
$\kappa_\lambda = 1$	POWHEG + PYTHIA8	PDFLHC	A14NNPDF23LO	31.05	1.518M
$\kappa_\lambda = 10$	POWHEG + PYTHIA8	PDFLHC	A14NNPDF23LO	672.53	0.719M

Tab. 5.1 Event generator and PDF set of the ggFHH signal samples at various κ_λ values. The cross-sections are given at $\sqrt{s} = 13$ TeV and $m_H = 125.0$ GeV.

5.2.2.2 κ_λ -reweighted ggFHH Samples

Due to limited computing resources, simulated ggFHH event samples for other values of κ_λ values were produced from the previous samples using a κ_λ -reweighting method [138]. This method assumes that ggFHH kinematics depends solely on m_{HH} in first approximation, and reweights the fully-simulated sample generated for $\kappa_\lambda = 1$ such that the true m_{HH} distribution matches the expected one. The reweighting method calculates the weight factor ($h_{m_{HH},i}^{\kappa_\lambda}/h_{m_{HH},i}^{\text{SM}}$) for each bin i of truth m_{HH} at a specific value of κ_λ . The expected m_{HH} distribution for any given value of κ_λ is obtained through a linear combination method applied to three different distributions as follows.

Summing the two amplitudes corresponding to the two ggFHH Feynman diagrams shown in Figure 1.14, the total amplitude for ggFHH production is:

$$\mathcal{A}_{\text{ggF}}(\kappa_\lambda, \kappa_t) = \kappa_t^2 \mathcal{A}_1 + \kappa_t \kappa_\lambda \mathcal{A}_2, \quad (5.1)$$

where A_i indicate the normalization coefficients of the two amplitudes. As a result, the cross-section of ggFHH can be parameterized as:

$$\begin{aligned} \sigma_{\text{ggF}}(\kappa_\lambda, \kappa_t) &\propto |\mathcal{A}_{\text{ggF}}(\kappa_t, \kappa_\lambda)|^2 \\ &\propto \kappa_t^4 \cdot |A_1|^2 + \kappa_t^3 \kappa_\lambda \cdot 2\Re(\mathcal{A}_1^* \mathcal{A}_2) + \kappa_t^2 \kappa_\lambda^2 \cdot |A_2|^2 \\ &\propto \kappa_t^2 (\kappa_t^2 \cdot |A_1|^2 + \kappa_t \kappa_\lambda \cdot 2\Re(\mathcal{A}_1^* \mathcal{A}_2) + \kappa_\lambda^2 \cdot |A_2|^2) \end{aligned} \quad (5.2)$$

Differentiating the cross-section as a function of the Higgs boson pair invariant mass yields:

$$\frac{d\sigma_{\text{ggF}}}{dm_{HH}}(\kappa_\lambda, \kappa_t) = \kappa_t^2 \left(\kappa_\lambda^2 \cdot a_1(m_{HH}) + \kappa_\lambda \kappa_t \cdot a_2(m_{HH}) + \kappa_t^2 \cdot a_3(m_{HH}) \right) \quad (5.3)$$

where the coefficients are $a_1 = |A_2|^2$, $a_2 = 2\Re(\mathcal{A}_1^* \mathcal{A}_2)$, $a_3 = |A_1|^2$. Setting κ_t to unity yields:

$$\frac{d\sigma_{\text{ggF}}}{dm_{HH}}(\kappa_\lambda) = \kappa_\lambda^2 \cdot a_1(m_{HH}) + \kappa_\lambda \cdot a_2(m_{HH}) + a_3(m_{HH}) \quad (5.4)$$

The coefficients $a_i(m_{HH})$ are determined by solving the following system of three differential equations using three ggFHH m_{HH} distributions of samples of events generated at particle level

for values of $\kappa_\lambda = 0, 1, 20$:

$$\begin{aligned}\frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(\kappa_\lambda = 0) &= a_3(m_{\text{HH}}) \\ \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(\kappa_\lambda = 1) &= a_3(m_{\text{HH}}) + a_2(m_{\text{HH}}) + a_1(m_{\text{HH}}) \\ \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(\kappa_\lambda = 20) &= a_3(m_{\text{HH}}) + 20a_2(m_{\text{HH}}) + 400a_1(m_{\text{HH}})\end{aligned}\quad (5.5)$$

The true m_{HH} distribution for any value of κ_λ can thus be obtained from the three distributions for $\kappa_\lambda = 0, 1, 20$ as:

$$\begin{aligned}\frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(\kappa_\lambda) &= \kappa_\lambda^2 \cdot \left[\frac{1}{20} \cdot \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(0) - \frac{1}{19} \cdot \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(1) + \frac{1}{380} \cdot \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(20) \right] \\ &\quad + \kappa_\lambda \cdot \left[-\frac{21}{20} \cdot \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(0) + \frac{20}{19} \cdot \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(1) - \frac{1}{380} \cdot \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(20) \right] \\ &\quad + \frac{d\sigma_{\text{ggF}}}{dm_{\text{HH}}}(0)\end{aligned}\quad (5.6)$$

Considering the observed allowed ranges with $-1.5 < \kappa_\lambda < 6.7$ from the previous analysis [130], ggFHH sample for $\kappa_\lambda = 6.5$ reweighted from the SM ggFHH sample is considered to optimize the event selection.

5.2.3 Simulation: VBFHH Signal

Section 1.3.1 shows that the signal VBFHH production mode is induced at leading order by three Feynman diagrams involving the coupling modifiers κ_λ , κ_{2V} and κ_V , yielding a total SM cross-section of 1.726 fb at $\sqrt{s} = 13$ TeV and $m_{\text{H}} = 125.0$ GeV.

5.2.3.1 Generated VBFHH Samples

The VBFHH signal samples were generated at leading order (LO) with `MadGraph5_aMC@NLO 2.6.0`. The `NNPDF3.0nlo` PDF set was used for the parton-level event generation, while parton showering, hadronization and underlying event simulation were handled by `PYTHIA 8.244` with the `A14 NNPDF23L0` tune. Several samples were produced with various values of the three coupling modifiers, as summarized in Table 5.2 and detailed in Table 5.3, and fully simulated. The simulations were normalized to next-to-next-to-next-to-leading order (N3LO) VBFHH cross-section calculations. Six of this samples are used as *basis* samples for the linear combination procedure, while the remaining ones are used as *test* samples to validate the procedure. The chosen basis for the VBFHH parametrization has been proven to effectively model the VBFHH kinematics over a wide parameter space, encompassing κ_λ , κ_{2V} , and κ_V values for BSM scenarios.

5.2.3.2 Parameterized VBFHH Samples with κ_λ and κ_{2V}

Unlike ggFHH production, where the kinematic properties of the events can be inferred from the m_{HH} distribution, VBFHH production is more complex due to the presence of two forward jets from the hadronization of valence quarks in the hard-scattering process. This complexity makes it challenging to find a single variable that fully describes the VBFHH kinematics.

Coupling Modifiers	Values													
κ_λ	1	1	1	1	1	1	0	2	10	1	1	1	0	-5
κ_{2V}	1	0	0.5	1.5	2	3	1	1	1	1	1	1	0	1
κ_V	1	1	1	1	1	1	1	1	1	0.5	0.5	1.5	1	0.5

Tab. 5.2 Values of the coupling modifiers for the generated VBFHH event samples. The samples with red colors are used as *basis* samples and the remaining ones are considered as *test* samples, as described in the following section.

VBFHH Signal Mode	Generator and Showering	PDF (ME)	PDF+Tuning (PS)	σ [fb]	Events
$\kappa_\lambda = 1, \kappa_{2V} = 1, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	1.726	0.4M
$\kappa_\lambda = 1, \kappa_{2V} = 0, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	27.206	0.399M
$\kappa_\lambda = 1, \kappa_{2V} = 0.5, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	9.683	0.2M
$\kappa_\lambda = 1, \kappa_{2V} = 1.5, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	3.364	0.2M
$\kappa_\lambda = 1, \kappa_{2V} = 2, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	14.583	0.199M
$\kappa_\lambda = 1, \kappa_{2V} = 3, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	65.676	0.199M
$\kappa_\lambda = 0, \kappa_{2V} = 1, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	4.637	0.2M
$\kappa_\lambda = 2, \kappa_{2V} = 1, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	1.565	0.198M
$\kappa_\lambda = 10, \kappa_{2V} = 1, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	98.587	0.198M
$\kappa_\lambda = 1, \kappa_{2V} = 1, \kappa_V = 0.5$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	11.014	0.2M
$\kappa_\lambda = 1, \kappa_{2V} = 1, \kappa_V = 1.5$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	66.407	0.2M
$\kappa_\lambda = 0, \kappa_{2V} = 0, \kappa_V = 1$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	37.153	0.2M
$\kappa_\lambda = -5, \kappa_{2V} = 1, \kappa_V = 0.5$	MADGRAPH + PYTHIA8 + EVTGEN	NNPDF	A14NNPDF23LO	6.495	0.2M

Tab. 5.3 Event generator and PDF set for VBFHH samples at various κ_λ , κ_{2V} and κ_V values. The cross-sections are given at $\sqrt{s} = 13$ TeV and $m_H = 125.0$ GeV.

Therefore, the reweighting method previously described is not suitable for this production mode. Instead, a linear combination method based on generated and fully simulated samples after the reconstruction and preselection is directly applied to produce the distribution of any variable for the specified κ_λ , κ_{2V} , and κ_V values. Figure 1.15 illustrates the three leading-order Feynman diagrams for VBFHH production. The total scattering amplitude at LO is expressed as:

$$\mathcal{A}_{\text{VBF}}(\kappa_\lambda, \kappa_{2V}, \kappa_V) = \kappa_\lambda \kappa_V \mathcal{A}_1 + \kappa_{2V} \mathcal{A}_2 + \kappa_V^2 \mathcal{A}_3 \quad (5.7)$$

where A_i represent the normalization coefficients of the diagrams. The VBFHH production cross-section is thus:

$$\begin{aligned} \sigma_{\text{VBF}}(\kappa_\lambda, \kappa_{2V}, \kappa_V) &\propto |\mathcal{A}_{\text{VBF}}(\kappa_\lambda, \kappa_{2V}, \kappa_V)|^2 \\ &\propto \kappa_\lambda^2 \kappa_V^2 \cdot |A_1|^2 + \kappa_{2V}^2 \cdot |A_2|^2 + \kappa_V^4 \cdot |A_3|^2 \\ &\quad + \kappa_\lambda \kappa_{2V} \kappa_V \cdot 2\Re(\mathcal{A}_1^* \mathcal{A}_2) + \kappa_\lambda \kappa_V^3 \cdot 2\Re(\mathcal{A}_1^* \mathcal{A}_3) + \kappa_{2V} \kappa_V^2 \cdot 2\Re(\mathcal{A}_2^* \mathcal{A}_3) \\ &\propto x_1 \cdot \kappa_\lambda^2 \kappa_V^2 + x_2 \cdot \kappa_{2V}^2 + x_3 \cdot \kappa_V^4 + x_4 \cdot \kappa_\lambda \kappa_V \kappa_{2V} + x_5 \cdot \kappa_\lambda \kappa_V^3 + x_6 \cdot \kappa_{2V} \kappa_V^2 \end{aligned} \quad (5.8)$$

where x_i are the coefficients of the quadratic equation, independent of the coupling modifiers.

A system of six equations can be obtained by applying the previous equation to the six *basis* samples in Table 5.2. Solving the system leads to expressions for the six coefficients in terms of the cross-sections of the six basis samples. Inserting these expressions in the previous equation

leads to the following expression for the VBFHH cross-section as a function of κ_λ , κ_{2V} , and κ_V for any value of these coupling modifiers:

$$\begin{aligned} \sigma_{\text{VBF}}(\kappa_\lambda, \kappa_{2V}, \kappa_V) = & \left(\kappa_{2V}^2 - \frac{373\kappa_{2V}\kappa_\lambda\kappa_V}{594} - \frac{1150\kappa_{2V}\kappa_V^2}{297} - \frac{\kappa_\lambda^2\kappa_V^2}{9} + \frac{1033\kappa_\lambda\kappa_V^3}{594} + \frac{853\kappa_V^4}{297} \right) \cdot \sigma_{\text{VBF}}(1, 1, 1) \\ & + \left(\frac{2\kappa_{2V}\kappa_\lambda\kappa_V}{3} - \frac{2\kappa_{2V}\kappa_V^2}{3} + \frac{\kappa_\lambda^2\kappa_V^2}{10} - \frac{53\kappa_\lambda\kappa_V^3}{30} + \frac{5\kappa_V^4}{3} \right) \cdot \sigma_{\text{VBF}}(0, 1, 1) \\ & + \left(\frac{\kappa_{2V}\kappa_\lambda\kappa_V}{27} - \frac{\kappa_{2V}\kappa_V^2}{27} + \frac{\kappa_\lambda^2\kappa_V^2}{90} - \frac{13\kappa_\lambda\kappa_V^3}{270} + \frac{\kappa_V^4}{27} \right) \cdot \sigma_{\text{VBF}}(10, 1, 1) \\ & + \left(-\frac{4\kappa_{2V}^2}{3} - \frac{4\kappa_{2V}\kappa_\lambda\kappa_V}{33} + \frac{60\kappa_{2V}\kappa_V^2}{11} + \frac{4\kappa_\lambda\kappa_V^3}{33} - \frac{136\kappa_V^4}{33} \right) \cdot \sigma_{\text{VBF}}(1, 1.5, 1) \\ & + \left(\frac{\kappa_{2V}^2}{3} + \frac{5\kappa_{2V}\kappa_\lambda\kappa_V}{66} - \frac{10\kappa_{2V}\kappa_V^2}{11} - \frac{5\kappa_\lambda\kappa_V^3}{66} + \frac{19\kappa_V^4}{33} \right) \cdot \sigma_{\text{VBF}}(1, 3, 1) \\ & + \left(-\frac{16\kappa_{2V}\kappa_\lambda\kappa_V}{33} + \frac{16\kappa_{2V}\kappa_V^2}{33} + \frac{16\kappa_\lambda\kappa_V^3}{33} - \frac{16\kappa_V^4}{33} \right) \cdot \sigma_{\text{VBF}}(-5, 1, 0.5) \end{aligned} \quad (5.9)$$

The cross-section can thus be obtained by a linear combination of the six *basis* samples.

The *test* samples listed in Table 5.2 were used to validate the procedure, by comparing the distributions of events in the generated test samples to those obtained by applying the linear combination method to the *basis* samples. The diphoton invariant mass ($m_{\gamma\gamma}$) distributions of this validation procedure are displayed in Figure 5.1. Good agreement is observed between the generated distributions and those predicted by the linear combination method.

5.2.4 Simulation: Background

Table 5.4 summarizes the background MC event samples used in the analysis, including the cross-section values, generators, PDFs and tunes for hard-scattering and parton-shower simulation. The dominant backgrounds include the diphoton continuum background, also called irreducible background in the following, and all significant single Higgs production processes, as detailed in Section 1.2.1, with the Higgs boson decaying into the diphoton final state [139]. Diphoton continuum background events were generated using *Sherpa* 2.2.4, producing extra partons at NLO for up to one additional parton, and at LO for two and three additional partons. This process was expedited by a fast simulation of the ATLAS detector due to the large sample size. To enhance selection efficiency, a di-*b*-quark-filtered version using *Sherpa* 2.2.12 was designed, with a NLO exclusive matrix element. Radiation of additional partons is handled by the parton shower. Although the generated sample size was smaller, the improved filtering increased the equivalent luminosity by a factor of four. Due to its small size, this sample could be processed with the full ATLAS detector simulation.

5.3 Statistical Interpretation

In particle physics, statistical interpretation is crucial for deriving physical insights from observed events. The foundation of this interpretation is the likelihood function, which measures the probability of the observed data given specific values of the model parameters. This

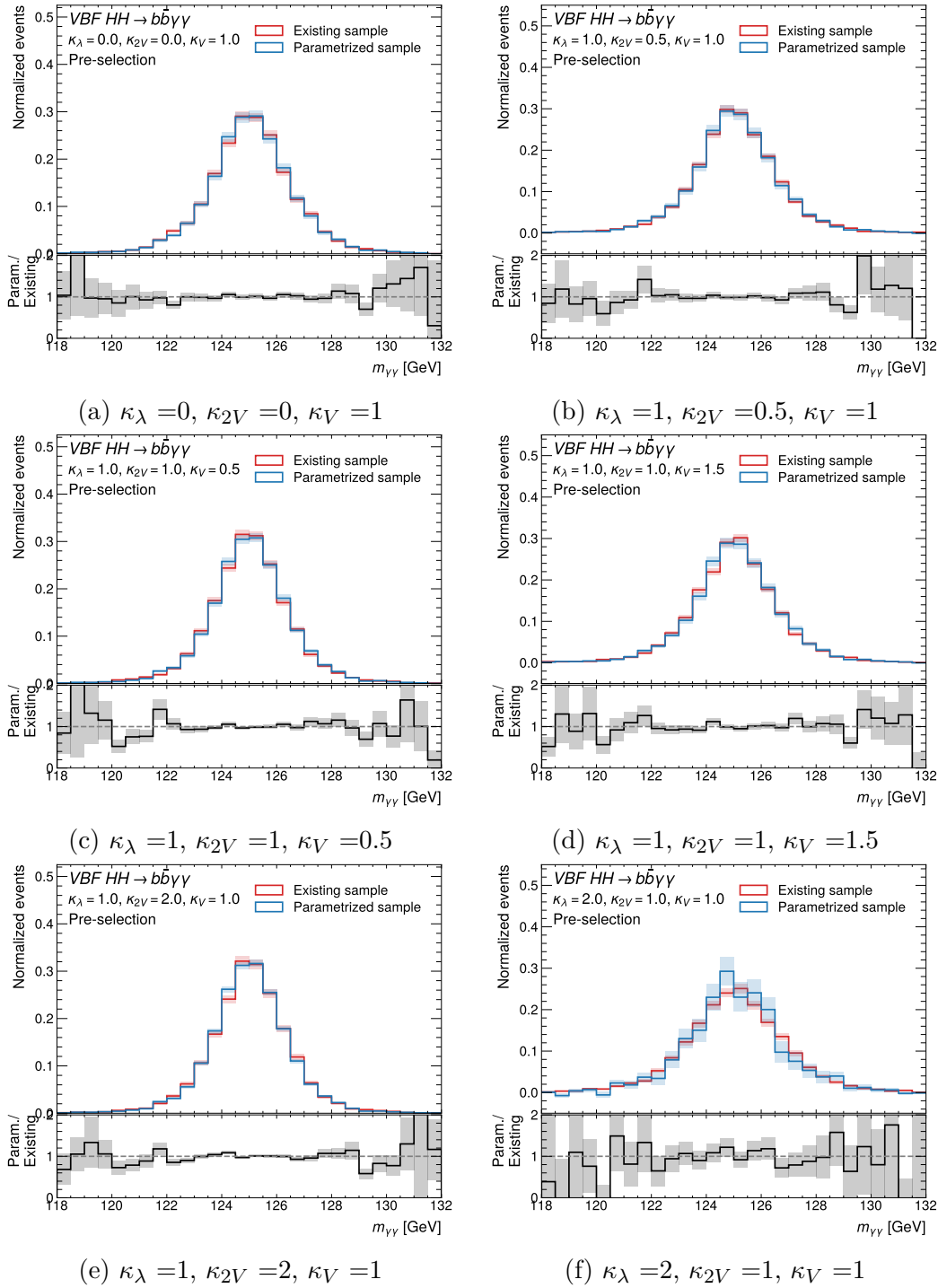


Fig. 5.1 Validation plots between the *test* samples (red) and the parameterized samples (blue) for the distribution of the diphoton invariant mass $m_{\gamma\gamma}$ in VBFHH events after the preselection applied.

approach provides a precise and quantitative link between theoretical models and experimental observations, ensuring that the data is properly interpreted and the results are reliable. Be-

Background Modes	Generator and Showering	PDF (ME)	PDF+Tuning (PS)	σ [pb]
Single Higgs Processes				
ggH	NNLOPS + PYTHIA8	PDFLHC	AZNLOCTEQ6	48.58
VBF	POWHEG + PYTHIA8	PDFLHC	AZNLOCTEQ6	3.78
W^+H	POWHEG MiNLO + PYTHIA8	PDFLHC	AZNLOCTEQ6	0.84
W^-H	POWHEG MiNLO + PYTHIA8	PDFLHC	AZNLOCTEQ6	0.53
$qq \rightarrow ZH$	POWHEG MiNLO + PYTHIA8	PDFLHC	AZNLOCTEQ6	0.76
$gg \rightarrow ZH$	POWHEG MiNLO + PYTHIA8	PDFLHC	AZNLOCTEQ6	0.12
$t\bar{t}H$	POWHEG + PYTHIA8	PDFLHC	A14NNPDF23	0.51
$b\bar{b}H$	POWHEG + PYTHIA8	PDFLHC	A14NNPDF23	0.49
$tHj\bar{b}$	MGMCatNLO + PYTHIA8	NNPDF	A14NNPDF23	0.07
tHW	MGMCatNLO + PYTHIA8	NNPDF	A14NNPDF23	0.02
Continuum Backgrounds				
$\gamma\gamma + 0, 1(\text{NLO}), 2, 3(\text{LO}), m_{\gamma\gamma} \in 90 - 175 \text{ GeV}$	SHERPA 2.2.4(ME@NLO+PS, AF2)			51.822
$\gamma\gamma + b\bar{b}(\text{NLO}), 3 + (\text{PS}), m_{\gamma\gamma} \in 90 - 175 \text{ GeV}$	SHERPA 2.2.12(ME@ NLO+PS, FullSim)			51.822
$t\bar{t}\gamma\gamma(\text{noallhad})$	MGMCatNLO + PYTHIA8			2.82
$t\bar{t}\gamma\gamma(\text{allhad})$	MGMCatNLO + PYTHIA8			1.77

Tab. 5.4 Summary of the background MC event samples used in the analysis, including their predicted cross-sections, generators, PDFs and tunes for hard-scattering and parton-shower simulation.

fore conducting the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis, it is imperative to outline the statistical model and methodology in detail. This involves specifying the likelihood function, defining the parameters of interest, and identifying the nuisance parameters. Additionally, the test statistics, limit setting procedure, and asymptotic approximation method will be discussed.

5.3.1 Fundamental Concepts

Parameters of Interest (POIs, μ) [140] represent the fundamental quantities to be measured or constrained using experimental data. These parameters typically include signal strengths (the ratio of the measured cross-section and the SM predicted cross-section), cross sections, coupling strength modifiers, particle masses, and branching ratios, which are crucial for testing SM predictions and probing potential new physics beyond the SM. Specifically, in the context of the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis, POIs involve the production cross section of Higgs boson pairs, expressed as signal strengths (μ_{HH} , μ_{HH}^{ggF} , μ_{HH}^{VBF}), the Higgs self-coupling modifier (κ_λ), and the strength modifiers (κ_{2V} , κ_V) of the couplings between the Higgs boson and the weak gauge bosons. Accurate measurement of these POIs is essential for validating the SM and exploring new phenomena beyond the SM.

Nuisance Parameters (NPs, θ) [140] describe the impact of various sources of systematic uncertainties and background estimates. These parameters are not of primary interest but must be accounted for in the likelihood function to properly interpret the experimental data. NPs include uncertainties related to detector calibration, energy scales, resolutions, efficiencies, theoretical predictions, and background modeling. In the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis, the most significant NPs encompass uncertainties in photon identification efficiency, jet energy scale, and background estimation, which will be elaborated upon in Section 5.9. Effectively managing and profiling these NPs can mitigate their impact on the POIs, leading to more precise and robust measurements, thereby enhancing overall confidence in the experimental results.

During the fitting process using the likelihood function, the POIs and NPs are floated in order to find the values that maximize the level of agreement between the data and the model. NPs can be divided into unconstrained and constrained parameters. Unconstrained NPs lack strong prior information or external constraints and are allowed to vary freely within the fit. These often denote uncertainties like background shapes for which there is limited prior knowledge or those that need to be determined directly from the data. In contrast, constrained NPs depend on prior knowledge or external constraints, typically derived from auxiliary measurements or theoretical predictions. These parameters are essential for quantifying the impact in the data of systematic uncertainties. Each constrained NP is associated with a given probability distribution, for instance a Gaussian function where the mean represents the global observable reflecting the observed value of the auxiliary measurement.

5.3.2 Construction of the Likelihood Function

The likelihood function [140] serves as the cornerstone of statistical analysis in particle physics. It quantifies the probability of observing the data under certain theoretical parameters, enabling researchers to test hypotheses and estimate parameters with a high degree of precision. This method bridges the gap between theory and experiment, allowing for rigorous testing of theoretical predictions against empirical evidence.

In the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis, statistical outcomes are derived by performing a simultaneous unbinned maximum likelihood fit to the $m_{\gamma\gamma}$ spectra of the reconstructed event categories within the [105,160] GeV range. The total likelihood function for the full dataset is expressed as follows:

$$\mathcal{L} = \prod_c \mathcal{L}_c, \quad \mathcal{L}_c = \text{Pois}(n_c | N_c(\boldsymbol{\theta})) \cdot \prod_{i=1}^{n_c} f_c(m_{\gamma\gamma}^i, \boldsymbol{\theta}) \cdot G(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}}), \quad (5.10)$$

$$\text{Pois}(n_c | N_c(\boldsymbol{\theta}_{\text{yield}})) = \frac{N_c(\boldsymbol{\theta}_{\text{yield}})^{n_c} e^{-N_c(\boldsymbol{\theta}_{\text{yield}})}}{n_c!}.$$

The likelihood function ($\mathcal{L}$) for the entire dataset is written as the product of the likelihood functions ($\mathcal{L}_c$) for each category c . $\text{Pois}(n_c | N_c(\boldsymbol{\theta}_{\text{yield}}))$ represents the probability of observing n_c events in category c , given an expected number of events N_c with nuisance parameters ($\boldsymbol{\theta}_{\text{yield}}$). The probability of each event i in category c is described by a probability density function (PDF) $f_c(m_{\gamma\gamma}^i, \boldsymbol{\theta})$, which depends on the $m_{\gamma\gamma}$ distribution and $\boldsymbol{\theta}$. The joint probability of observing all N_c events is obtained by multiplying the individual probabilities. $G(\boldsymbol{\theta}, \tilde{\boldsymbol{\theta}})$ represents the Gaussian constraint term $G(\tilde{\boldsymbol{\theta}} = 0 | \boldsymbol{\theta}, 1)$, involving $\boldsymbol{\theta}$ and their global observables $\tilde{\boldsymbol{\theta}}$. These observables are determined by maximizing the likelihood function, providing the best fit to the observed data within the given model.

The expected number of events N_c is given by:

$$N_c(\boldsymbol{\theta}_{\text{yield}}) = \mu \cdot N_c^{\text{HH}}(\kappa_\lambda, \kappa_{2V}, \kappa_V, \boldsymbol{\theta}_{\text{yield}}^{\text{HH}}) + N_c^{\text{H}}(\boldsymbol{\theta}_{\text{yield}}^{\text{H}}) + N_c^{\gamma\gamma} + N_c^{\text{SS}} \cdot \boldsymbol{\theta}_c^{\text{SS}} \quad (5.11)$$

It is calculated as the sum of the yields of di-Higgs boson events (N_c^{HH}), single-Higgs boson events (N_c^{H}), irreducible background ($N_c^{\gamma\gamma}$), as well as an extra term called spurious signal ($N_c^{\text{SS}} \cdot \boldsymbol{\theta}_c^{\text{SS}}$) that describes the uncertainty in the signal yield from the chosen continuum background model. One of the POIs, the signal strength modifier (μ), scales the expected number of signal

events. Additional POIs (κ_λ , κ_{2V} , κ_V) are incorporated into the statistical model, influencing the expected di-Higgs boson yields. Various sources of systematic uncertainties, represented by θ_{yield} , affect the expected yields for both di-Higgs and single-Higgs boson events. The yields of the irreducible background in each category are characterized by unconstrained NPs, which are determined by the fit to the data together with the POI(s). Yields from spurious signals are evaluated by the product of the expected SS yield (N_c^{SS}) and a NP (θ_c^{SS}) describing its uncertainty, as discussed later in Section 5.8.

The probability density function $f_c(m_{\gamma\gamma}, \theta)$ is given by:

$$\begin{aligned} f_c(m_{\gamma\gamma}, \theta) = & [\mu \cdot N_c^{\text{HH}}(\theta_{\text{yield}}^{\text{HH}}) \cdot f_c^{\text{HH}}(m_{\gamma\gamma}, \theta_{\text{shape}}^{\text{HH}}) \\ & + N_c^{\text{H}}(\theta_{\text{yield}}^{\text{H}}) \cdot f_c^{\text{H}}(m_{\gamma\gamma}, \theta_{\text{shape}}^{\text{H}}) \\ & + N_c^{\gamma\gamma} \cdot f_c^{\gamma\gamma}(m_{\gamma\gamma}, \theta_{\text{shape}}^{\gamma\gamma}) \\ & + N_c^{\text{SS}} \cdot \theta_c^{\text{SS}} \cdot f_c^{\text{HH}}(m_{\gamma\gamma}, \theta_{\text{shape}}^{\text{HH}})] / N_c(\theta_{\text{yield}}) \end{aligned} \quad (5.12)$$

The PDFs are normalized to the expected number of event yields in each category. θ_{shape} indicates the NPs related to the uncertainties in the shape of the signal and background distributions. The $m_{\gamma\gamma}$ distributions of di-Higgs and single-Higgs boson events are found empirically to be well modeled by Double-Sided Crystal Ball (DSCB) functions, incorporating systematic uncertainties (such as on the photon energy scale and resolution) and model parameter uncertainties as NPs within the PDFs. The Higgs boson mass is set to 125.00 GeV. Its uncertainty (240 MeV) and the difference (90 MeV) with respect to the central value of the ATLAS+CMS Run 1 measurement give a negligible impact on the results. The $m_{\gamma\gamma}$ distribution of the irreducible background is represented by analytic exponential functions, with the shape parameters being entirely unconstrained and allowed to float during the fit. The models of these shapes will be discussed in Section 5.5.3.

5.3.3 Profiled Likelihood Ratio Test Statistics

In a statistical analysis of the data that tries to establish the presence of a signal over a given background, two hypotheses are tested [140]: the null hypothesis (H_b) symbolizing the background-only model and the alternative hypothesis (H_μ) representing the signal-plus-background model. To perform the hypothesis tests, the profile likelihood ratio ($\Lambda(\mu)$) and the test statistic (q_μ) are defined as [141]:

$$\Lambda(\mu) = \frac{\mathcal{L}(\mu, \hat{\theta}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\theta})}, \quad t_\mu = -2\ln\Lambda(\mu) \quad (5.13)$$

where μ and θ are the POIs and NPs, respectively. The numerator $\mathcal{L}(\mu, \hat{\theta}(\mu))$ stands for the profile likelihood function, where $\hat{\theta}(\mu)$ denotes the value of θ that maximizes the likelihood function for a given μ , also known as the conditional maximum likelihood estimator (MLE). The denominator $\mathcal{L}(\hat{\mu}, \hat{\theta})$ signifies the global maximum of the likelihood function, where $\hat{\mu}$ and $\hat{\theta}$ are the best-fit values of μ and θ , respectively, referred to as the unconditional MLE. From Equation 5.13, higher values of the test statistic t_μ correspond to larger disagreement between the data and the hypothesized value of the POI (μ).

Since $\mu \geq 0$, if one finds data such that $\hat{\mu} < 0$, then the best level of agreement between the data and any physical value of μ occurs for $\mu = 0$. The profile likelihood ratio can thus be modified as follows:

$$\tilde{\Lambda}(\mu) = \begin{cases} \frac{\mathcal{L}(\mu, \hat{\boldsymbol{\theta}}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\boldsymbol{\theta}})}, & \hat{\mu} \geq 0, \\ \frac{\mathcal{L}(\mu, \hat{\boldsymbol{\theta}}(\mu))}{\mathcal{L}(0, \hat{\boldsymbol{\theta}}(0))}, & \hat{\mu} < 0, \end{cases} \quad (5.14)$$

and the test statistic becomes:

$$\tilde{t}_\mu = -2\ln\tilde{\Lambda}(\mu) = \begin{cases} -2\ln\frac{\mathcal{L}(\mu, \hat{\boldsymbol{\theta}}(\mu))}{\mathcal{L}(0, \hat{\boldsymbol{\theta}}(0))} & \hat{\mu} < 0, \\ -2\ln\frac{\mathcal{L}(\mu, \hat{\boldsymbol{\theta}}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\boldsymbol{\theta}})} & \hat{\mu} \geq 0. \end{cases} \quad (5.15)$$

To test (and exclude) the $\mu = 0$ hypothesis, i.e. for the discovery of a new signal, the test statistic then reduces to

$$q_0 = \tilde{t}_0 = \begin{cases} -2\ln\Lambda(0) & \hat{\mu} \geq 0, \\ 0 & \hat{\mu} < 0. \end{cases} \quad (5.16)$$

The level of disagreement between the data and the hypothesis of $\mu = 0$ is determined by calculating the p -value of the observed value of q_0 ,

$$p_0 = \int_{q_{0,obs}}^{\infty} f(q_0|\mu=0)dq_0. \quad (5.17)$$

5.3.4 Upper Limit Setting Procedure

To set upper limits on μ , the hypotheses to be rejected are those for which μ is greater than a given (positive) value. The test statistic used in this case is [140]:

$$\tilde{q}_\mu = \begin{cases} \tilde{t}_\mu = -2\ln\tilde{\Lambda}(\mu) & \hat{\mu} < \mu, \\ 0 & \hat{\mu} > \mu. \end{cases} \quad (5.18)$$

This is because by definition the largest values of μ that are excluded must be greater than the observed one $\hat{\mu}$. Substituting the definition of $\tilde{\Lambda}(\mu)$ into the previous equation yields:

$$\tilde{q}_\mu = \begin{cases} -2\ln\frac{\mathcal{L}(\mu, \hat{\boldsymbol{\theta}}(\mu))}{\mathcal{L}(0, \hat{\boldsymbol{\theta}}(0))} & \hat{\mu} < 0, \\ -2\ln\frac{\mathcal{L}(\mu, \hat{\boldsymbol{\theta}}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\boldsymbol{\theta}})} & 0 \leq \hat{\mu} \leq \mu, \\ 0 & \hat{\mu} > \mu \end{cases} \quad (5.19)$$

The upper limit on the signal strength (μ_{up}), related to the Higgs boson pair production cross-section, is constrained at the 95% Confidence Level (CL) using the CL_s technique [142]:

$$\begin{aligned} CL_s(\mu) &= \frac{CL_{s+b}}{CL_b} = \frac{p_\mu}{1 - p_b}, \\ CL_{s+b} &= p_\mu = P(\tilde{q}_\mu \geq \tilde{q}_\mu^{\text{obs}} \mid H_\mu) = \int_{\tilde{q}_\mu^{\text{obs}}}^{\infty} f(\tilde{q}_\mu \mid \mu, \hat{\boldsymbol{\theta}}_\mu^{\text{obs}}) d\tilde{q}_\mu, \\ CL_b &= 1 - p_b = P(\tilde{q}_\mu \geq \tilde{q}_\mu^{\text{obs}} \mid H_b) = \int_{q_0^{\text{obs}}}^{\infty} f(\tilde{q}_\mu \mid 0, \hat{\boldsymbol{\theta}}_0^{\text{obs}}) d\tilde{q}_\mu \end{aligned} \quad (5.20)$$

$$\mu_{\text{up}} = \hat{\mu} + \sigma\Phi^{-1}(1 - \alpha) \quad (5.21)$$

where $\hat{\mu}$ and σ are the best-fit value and the standard deviation of the signal strength modifier, respectively, and $\Phi^{-1}(1 - \alpha)$ is the critical value of the inverse of the cumulative distribution function of the standard normal distribution evaluated at $1 - \alpha$.

Two $\tilde{q}_\mu$ distributions, $f(\tilde{q}_\mu | 0)$ for H_b and $f(\tilde{q}_\mu | \mu)$ for H_μ , are required to calculate CL_b and CL_{s+b} . These can be generated using either the asymptotic approximation or toy MC pseudo-experiments. The asymptotic approximation assumes that $\tilde{q}_\mu$ follows a χ^2 distribution with one degree of freedom [140], which combines a delta function at zero and a χ^2 distribution. Alternatively, the distributions can be constructed from the observed test statistics ($\tilde{q}_\mu^{\text{obs}}$) and the observed NPs ($\hat{\theta}_0^{\text{obs}}$ and $\hat{\theta}_\mu^{\text{obs}}$) through toy MC pseudo-experiments. The value of $\tilde{q}_\mu^{\text{obs}}$ is calculated for a given signal strength μ under the alternative hypothesis H_μ . The values of $\hat{\theta}_0^{\text{obs}}$ and $\hat{\theta}_\mu^{\text{obs}}$ are obtained from the observed data by maximizing likelihood functions under the H_b and H_μ hypotheses. The p -value of the H_μ hypothesis is then derived by integrating the $\tilde{q}_\mu$ distribution, giving p_μ and $1 - p_b$ for H_μ and H_b in Equation 5.20. Finally, the μ_{up} at a certain μ and $CL_s \leq \alpha$ is obtained by making $p_\mu = \alpha$ and solving for μ , as described in Equation 5.21. The asymptotic approximation is valid for large sample sizes, but not suitable for small datasets, where the toy MC approach is preferred. In this analysis, the asymptotic approximation was adopted but checks with toy MC pseudo-experiments were performed.

5.3.5 Coupling Modifier Constraints

After obtaining the upper limit by the asymptotic approximation, the coupling modifiers (κ_λ , κ_{2V} , κ_V) can be constrained using the test statistic method described above. Each value of the couplings is evaluated by the upper limit on the signal strength (μ_{up}) at the 95% CL, and various values of the couplings are scanned to determine the constraints. The constraints on the modifiers are determined by the region where the cross-section is lower than the theoretically predicted value. When each POI is individually fit, the other POIs are fixed to their SM prediction, ensuring that the fit reflects the impact of the varied parameter alone. Furthermore, these couplings can be also measured from the negative log-likelihood (NLL, $-2\Delta\ln L(\kappa, \theta)$) scan as described in Equation 5.13. The best-fit values of the modifiers can be obtained by minimizing the NLL with respect to free POIs and NPs. From the scanned couplings, the constraints are derived by 68% and 95% CL.

The evaluation of uncertainties detailed in Section 5.10.3 is conducted through profiling, where NPs are set to values that maximize the likelihood for given values of the POIs. This process identifies the overall uncertainty in the POIs. To perform error decomposition, different groups of uncertainties are fixed to their unconditional fit values to analyze their individual contributions. Statistical uncertainty is determined by fixing all NPs to their best-fit values, except those related to background shape parameters and normalization. Theoretical or experimental uncertainty is then calculated by subtracting the experimental (or theoretical) and statistical uncertainties in quadrature from the total uncertainty. This approach provides a detailed understanding of the sources of uncertainty.

To avoid potential biases, the blind-analysis technique [143] is employed to evaluate the performance of the analysis strategy. This method involves optimizing the analysis (including

performing fits to the data to determine background shapes and yields for estimating the analysis sensitivity) while masking the signal region (SR). The “blind” results will be presented in Section 5.5.4 and Section 5.6.4. The SR is “unblinded” only after the analysis procedure is optimized and validated. The final results will be described in Section 5.10.1.

5.3.6 Workspace and Fit Tools

The construction of the statistical model necessitates the parameterization of the expected yields, $m_{\gamma\gamma}$ distributions, and systematic uncertainty constraints for all signals and backgrounds. These elements are integrated into a workspace, a comprehensive container holding all the information (POIs and NPs) essential for performing the statistical analysis. The workspace is created using the HistFactory tool [144], a component of the RooStats package [145].

In the baseline $HH \rightarrow b\bar{b}\gamma\gamma$ analysis, the workspace creation and the fitted results for the official strategy are executed using the *QuickStats* package. The alternative analysis strategy employs the *xmlAnaWSBuilder* package to generate the workspace, with the statistical results derived using the *quickFit* package. Both packages, designed by the HiggsGam group, facilitate blinding and unblinding analyses. They have been validated against each other, both yielding identical results when using the same inputs. These tools can evaluate the upper limits at 95% CL on the signal strength of SM ggFHH and SM VBFHH. Additionally, both 1D and 2D constraints on the coupling modifiers (κ_λ , κ_{2V} , κ_V) are determined from the cross-section upper limits and the negative log-likelihood (NLL) scan. The impacts on the constraints of POIs from the systematic uncertainties are presented in Section 5.10.3.

5.4 Event Preselection

Events passing the trigger requirements are fully reconstructed offline. Particle candidates (leptons, photons, jets) are reconstructed according to the methodologies outlined in Section 3.2. The primary vertex of the event is identified by the ANN algorithm introduced in Section 3.2.7. The missing transverse momentum E_T^{miss} is reconstructed from the negative vector sum of the transverse momentum of all above selected objects with the calibration matched to the primary vertex. The Track-based Soft Term (TST) algorithm is chosen to build the soft term collection. The details of the TST algorithm are provided in Section 3.2.6.

Additional selection requirements are applied by this analysis to reconstructed photons and jets to reduce the fraction of misidentified particles and to identify jets from the hadronization of b -quarks or from the scattering quarks in the VBFHH process. Subsequently, an event-level preselection is applied to suppress backgrounds and enhance the signal-to-background ratio. This section elaborates on the object-level selection and the event-level preselection.

5.4.1 Photon and Jet selection criteria

Photon candidates must have pseudorapidity $|\eta| < 2.37$, excluding the transition region between 1.37 and 1.52, and pass the “tight” identification criteria. Photon candidates must be isolated from nearby hadronic activity: they should pass a calorimeter isolation requirement, $E_T^{\text{topocone20}} < 0.065 \times p_T$, and a track-based isolation requirement, $p_T^{\text{cone20}} < 0.05 \times p_T$. The two p_T -leading photon candidates passing the previous requirements are retained. Their invariant

mass is required to be within the range $105 < m_{\gamma\gamma} < 160$ GeV. The transverse momenta of the leading and sub-leading photon must be larger than 0.35 and 0.25 times the diphoton invariant mass, respectively. These selections determine the $H \rightarrow \gamma\gamma$ candidates.

Jets, reconstructed with the anti- k_T algorithm using a radius $R = 0.4$, must satisfy the following kinematic requirements: $p_T > 25$ GeV, $|y| < 4.4$. A tight jet-vertex tagger requirement is applied to suppress jets from pile-up, and additional quality requirements are applied to suppress jets from sporadic calorimeter noise. Jets with $p_T \geq 40$ GeV and $|\eta| < 2.5$ are classified as central jets, which are instrumental in triggering and identifying $H \rightarrow b\bar{b}$ candidates. Jets with $p_T > 30$ GeV and $|\eta| \geq 2.5$ are classified as forward jets. They are considered candidates for the two jets from the hadronization of the scattering quarks in VBFHH events. The object-level requirements applied to photons and jets are summarized in Table 5.5.

Objects	Kinematics Requirements
photons	Tight ID, $ \eta < 2.37$ excluding the crack region $1.37 < \eta < 1.52$
	(Sub-)leading photon with $p_T/m_{\gamma\gamma} > (0.25)0.35$
	$E_T^{\text{topocone20}} < 0.065 \times p_T$ and $p_T^{\text{cone20}} < 0.05 \times p_T$ at FixedCutLoose Isolation WP
jets	$105 < m_{\gamma\gamma} < 160$ GeV
	$p_T > 25$ GeV, Anti- k_T $R = 0.4$, $ y < 4.4$
	Tight JVT WP, LooseBad Jet cleaning WP
	Central jets with $p_T \geq 40$ GeV and $ \eta < 2.5$
	Forward jets with $p_T \geq 30$ GeV and $ \eta \geq 2.5$

Tab. 5.5 Definition of photons and jets from the reconstruction.

5.4.2 b -jet Tagging and Calibration

Jets are categorized as b -jets, c -jets, or light-flavour jets (u , d , s or gluons) by the *DL1r* flavor tagging algorithm discussed in Section 3.2.4.3. To identify $H \rightarrow b\bar{b}$ candidates, events must contain exactly two b -jets tagged by *DL1r* at a 77% working point. These b -jets are ranked as leading and sub-leading based on their pseudo-continuous binned b -tagging scores. In cases where the selected b -jets have identical b -tagging scores, they are further sorted by p_T to determine the leading and sub-leading jets.

The energy of the b -jet candidates is corrected as follows, with the aim of improving the $m_{b\bar{b}}$ resolution. If a jet is within an angular distance $\Delta R(\mu, \text{jet})$ lower than $\min(0.4, 0.04 + 10/p_T^\mu [\text{GeV}])$ of a muon candidate with $p_T > 4$ GeV, $|\eta| < 2.5$, and passing the medium working point of the muon identification algorithm, then the four-vector of the reconstructed muon track is added to that of the b -jet to account for the muon's energy loss inside high- p_T jets. To avoid double counting, the estimated energy deposited by the muon in the calorimeter is subtracted from the b -jet energy. To take into account the missing energy due to the neutrinos from the semi-leptonic decays of b -hadrons, as well as out-of-cone effects (soft radiation), correction factors derived from $t\bar{t}$ events are employed. These factors correct the reconstructed p_T of b -jets in logarithmic bins of the true jet p_T . The combined effect of these two corrections, collectively called “BJetCalibration”, is an approximate 22% improvement in the $m_{b\bar{b}}$ resolution of reconstructed $H \rightarrow b\bar{b}$ decays, as illustrated in Fig. 5.2.

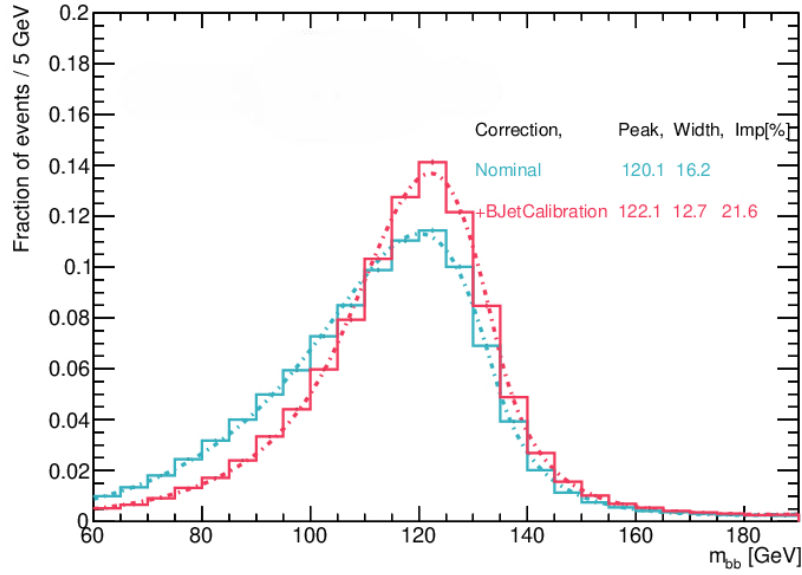


Fig. 5.2 Comparison of m_{bb} distributions of reconstructed $H \rightarrow b\bar{b}$ decays in the simulation: calibrated jets (red) versus nominal jet energy scale (blue). A Bukin function is used to fit the distributions, with peak values, resolutions, and relative improvements provided in the legend.

5.4.3 VBF-jet Selection

The VBFHH production mode is characterized by the presence of two forward jets with high transverse momenta (p_T) and significant pseudorapidity separation. Traditionally, the invariant mass of two jets ($m_{j_1 j_2}$) is used to identify VBF di-jets. In this study, a specialized VBF-jets tagger was developed to accurately distinguish VBFHH events using BDT algorithms trained on both signal and background events. Signal events are defined by pairs of jets with an angular separation ΔR of less than 0.3 between the reconstructed jets and the true VBF jets, identified through a truth-matching procedure. Jet pairs that do not meet the ΔR threshold are classified as background events. To capture the characteristics of VBF di-jets from the SM VBFHH sample, sixteen kinematic variables related to the VBFHH system were utilized in the training process. Performance, depicted in Figure 5.3, was evaluated by comparing the fraction of truth-matched VBF jets in events with at least four jets for both the BDT-based tagger and the $m_{j_1 j_2}$ -based method. The distribution of Δm_{jj} is fitted with a Double-Sided Crystal Ball (DSCB) function, and goodness of fit is quantified with a χ^2 test. The BDT-based tagger demonstrated a substantial improvement in the identification of VBF jets compared to the traditional $m_{j_1 j_2}$ -based method.

5.4.4 Event-level Preselection

Beyond the object-level selections described in the previous sections, an event-level preselection is applied to identify events consistent with the $HH \rightarrow b\bar{b}\gamma\gamma$ signature. This preselection aims at reducing background contamination, thereby enhancing the signal-to-background ratio within the analyzed phase space. To suppress the $t\bar{t}H$ background, especially from leptonic de-

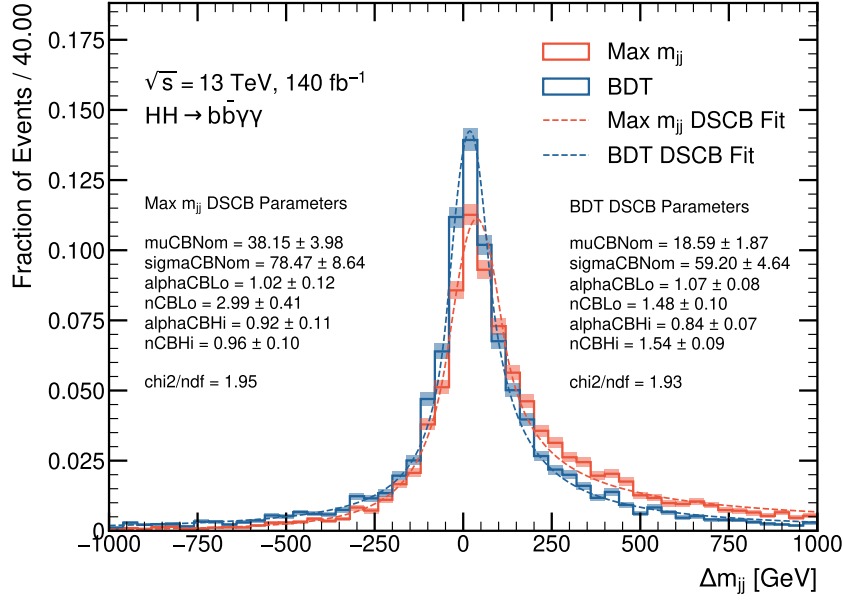


Fig. 5.3 Comparison of Δm_{jj} distributions for the two VBF jet candidates selected by maximizing m_{jj} (red) or using a BDT-based tagger (blue). The selection $N_{\text{jets}} > 4$ is required. The distributions are fitted with a DSCB function and the best-fit parameters are overlaid.

cays of top quarks ($t \rightarrow Wb \rightarrow \ell\nu b$), events are required to have zero leptons ($N_{\text{lep}} = 0$). To ensure the presence of the final state jets, events must contain more than two central jets ($N_{\text{central, jets}} > 2$). To suppress $t\bar{t}H$ events with hadronic decays of both top quarks ($t \rightarrow Wb \rightarrow qq'b$), a maximum of five central jets ($N_{\text{central, jets}} < 6$) is imposed. Selecting events with exactly two b -jets ($N_{\text{btag, WP77\%}} = 2$) further refines the sample.

The yield and efficiency resulting from this preselection for both ggFHH and VBFHH simulated event samples, as well as for data events in the sidebands of the diphoton invariant mass distribution ($m_{\gamma\gamma} \in [105, 160]$ GeV excluding $[120, 130]$ GeV), are detailed in Table 5.6, after each step of the preselection. The lower efficiency observed in the $H \rightarrow \gamma\gamma$ selection for VBFHH compared to ggFHH is anticipated due to the larger pseudorapidity of the two Higgs bosons in VBFHH and thus the lower transverse momentum of the photons from the $H \rightarrow \gamma\gamma$ decay. While the expected efficiency of the $N_{\text{btag, WP77\%}} = 2$ requirement for a b -tagging working point with a nominal efficiency of 77% is around 60%, Table 5.6 indicates a significantly lower efficiency of $\approx 40\%$ for ggFHH and $\approx 29\%$ for VBFHH. This is due to the fact that the kinematic distributions ($p_T, |\eta|$) of jets from $H \rightarrow b\bar{b}$ in ggFHH and VBFHH are significantly different from those of b -jets from $t\bar{t}$ events, for which the selected WP of the b -tagging algorithm yields an average efficiency of 77%. The b -jets from signal events in the HH analysis tend to have lower transverse momentum and/or larger pseudorapidity, populating regions of phase space in which the b -tagging algorithm is less efficient than the average value.

Event-level Selections	SM ggFHH		SM VBFHH		Data SideBands	
	Yield	Efficiency [%]	Yield	Efficiency [%]	Yield	Efficiency [%]
All events	12.600	100.00	0.7222	100.00	86537305	100.00
Pass trigger	9.368	74.35	0.4460	61.76	59711892	69.00
Has primary vertex	9.368	74.35	0.4460	61.76	59711892	69.00
2 loose photons	6.875	54.57	0.3442	47.66	59711892	69.00
$e - \gamma$ ambiguity	6.872	54.54	0.3440	47.64	59711892	69.00
Trigger match	6.833	54.23	0.3415	47.29	59117608	68.31
Photons tight ID cut	5.974	47.41	0.2977	41.22	14331082	16.56
Photons isolation cut	5.332	42.31	0.2655	36.77	5641625	6.52
Rel. p_T cuts	4.788	38.00	0.2381	32.97	4923920	5.69
$m_{\gamma\gamma} \in [105, 160]$ GeV	4.782	37.95	0.2369	32.81	937473	1.08
$N_{\text{lep}} = 0$	4.759	37.77	0.2355	32.62	935623	1.08
$N_{\text{jets}} \geq 2$	4.221	33.50	0.2240	31.05	199003	0.23
$N_{\text{central, jets}} < 6$	4.118	32.68	0.2228	30.85	197982	0.23
$N_{\text{btag, WP77\%}} = 2$	1.628	12.92	0.0635	8.80	1479	0.002

Tab. 5.6 Expected yields and efficiencies after each step of the event preselection for SM HH simulated events and data events in the diphoton invariant mass sidebands ($m_{\gamma\gamma} \in [105, 160]$ GeV, excluding $[120, 130]$).

5.5 Baseline Analysis Strategy

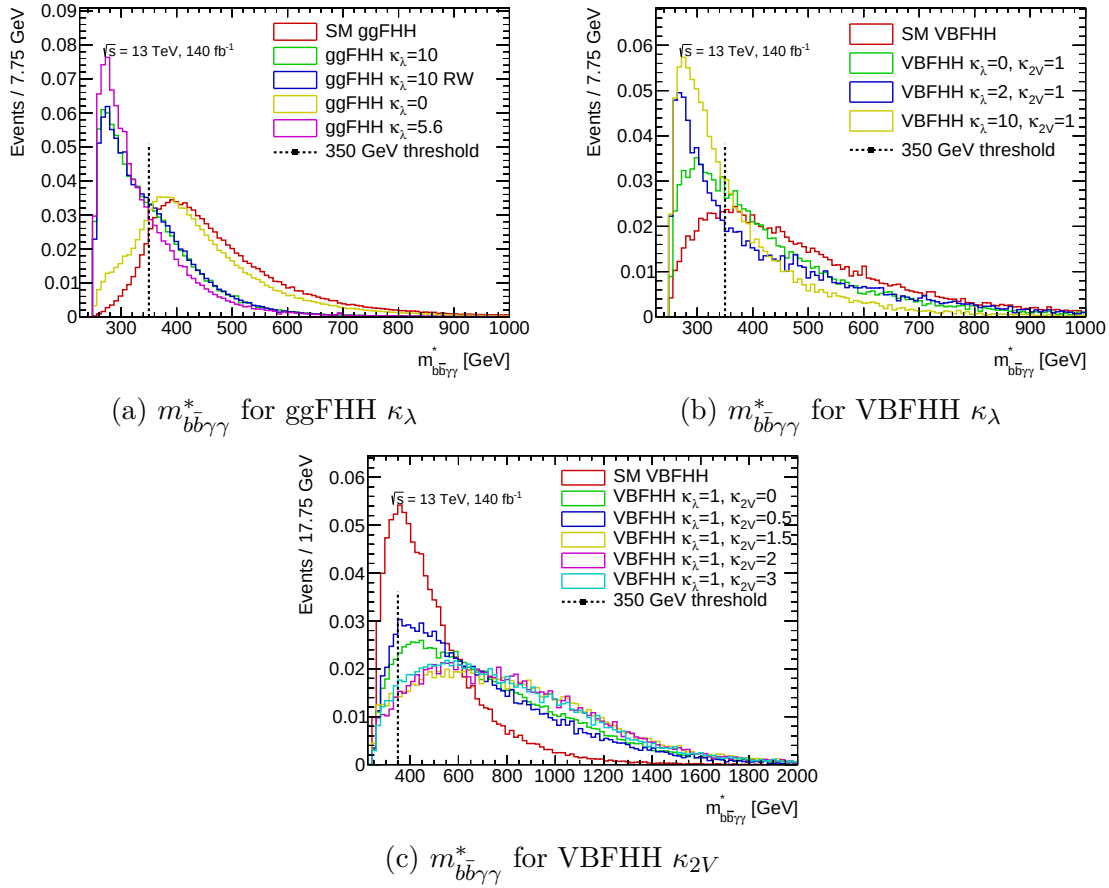
After the trigger and the basic preselection requirements of the previous sections, events with a $HH \rightarrow b\bar{b}\gamma\gamma$ signature are passed through additional selection and classification algorithms to further separate the signals from the backgrounds and increase the statistical significance of the signal being sought for. The events are firstly classified into two regions according to the “reduced” invariant mass of the $b\bar{b}\gamma\gamma$ system ($m_{b\bar{b}\gamma\gamma}^*$), defined as:

$$m_{b\bar{b}\gamma\gamma}^* = m_{b\bar{b}\gamma\gamma} - (m_{b\bar{b}} - 125 \text{ GeV}) - (m_{\gamma\gamma} - 125 \text{ GeV}), \quad (5.22)$$

where shifting the $b\bar{b}\gamma\gamma$ invariant mass by the differences between the invariant masses of the two Higgs boson candidates ($m_{b\bar{b}}$ and $m_{\gamma\gamma}$) and the Higgs boson mass (125 GeV) leads to a better resolution for $m_{b\bar{b}\gamma\gamma}^*$ than for $m_{b\bar{b}\gamma\gamma}$. A “low-mass” region is defined by the requirement $m_{b\bar{b}\gamma\gamma}^* \leq 350$ GeV, while a “high-mass” region is defined by $m_{b\bar{b}\gamma\gamma}^* > 350$ GeV. These region definitions are explained by the $m_{b\bar{b}\gamma\gamma}^*$ distributions exhibited in Figure 5.4, where it can be noticed that the SM process, as well as BSM scenarios with $\kappa_\lambda = 1$ and anomalous values of κ_{2V} , tend to produce Higgs boson pairs with large invariant mass, populating more the high-mass region. Anomalous values of κ_λ lead to events with lower $m_{b\bar{b}\gamma\gamma}^*$, more concentrated in the low-mass region.

5.5.1 Classification Strategy

To further enhance the separation between signals and backgrounds, two binary classifiers implemented and trained with the XGBoost package [146] for the low and high mass regions, respectively. As described in Section 5.2.4, dominant backgrounds include single Higgs and

**Fig. 5.4**

Distribution of the reduced invariant mass $m_{b\bar{b}\gamma\gamma}^*$ for simulated (a) ggFHH events with different values of κ_λ , (b) VBFHH events with different values of κ_λ , while κ_{2V} is set to one, and (c) VBFHH events with $\kappa_\lambda = 1$ and different values of κ_{2V} . In (a), both the distributions from the generated $ggFHH \kappa_\lambda = 10$ sample and one obtained with the κ_λ reweighting technique for the same value of κ_λ (denoted by "RW" in the legend) are shown, exhibiting good agreement with each other. The expected distributions for $\kappa_\lambda = 0$ and $\kappa_\lambda = 5.6$ are also shown. The threshold at 350 GeV (dashed line) shows a good separation between SM-like (≈ 1) and BSM values of κ_λ .

continuum processes summarized in Table 5.4. For the training, distinct HH production modes are regarded as signals in the two mass regions. In the low mass region, the signal training sample contains simulated BSM ggFHH events with $\kappa_\lambda = 10$ as well as events with $\kappa_\lambda = 5.6$ obtained by reweighting the SM ggFHH sample. In the high mass region, the signal training sample is formed by simulated SM ggFHH and SM VBFHH events. Additionally, some BSM VBFHH samples with $(\kappa_\lambda, \kappa_{2V}, \kappa_V) = (0, 1, 1), (10, 1, 1), (1, 1.5, 1), (1, 3, 1)$ and $(-5, 1, 0.5)$ are considered for training in both the low and high mass regions.

The two BDT classifiers use as input a large number of kinematic features, focusing on variables related to photons, b -jets, VBF-jets, MET and di-Higgs candidates. These variables are chosen to effectively capture the $b\bar{b}\gamma\gamma$ final state signature and to reject special background

processes. The H_T , χ_{Wt} , E_T^{miss} and ϕ^{miss} variables in particular are dedicated to suppress $t\bar{t}H$ and ZH backgrounds. Event-shape variables such as $S_\perp$, p_f and p_T^{balance} for rejecting $t\bar{t}H$ and ZH are also used to enhance the separation between signals and backgrounds by inspecting the properties of the event as a whole. The full list of input variables is summarized in Table 5.7. The events in the low and high-mass regions will be further categorized into different categories based on the output scores of the two BDT discriminants.

Variables	Description
Photons and Jets	$p_T/m_{\gamma\gamma}$, η , and ϕ of the two photons
	p_T , η , ϕ and pseudo-continuous b -tag score of each b -jet
	p_T , η , ϕ and pseudo-continuous b -tag score of the 3 rd and 4 th b -jets
	$p_T^{b\bar{b}}$, $\eta^{b\bar{b}}$, $\phi^{b\bar{b}}$, $m_{b\bar{b}}$ of two b -jets system
	H_T : scalar sum of p_T of all jets
	χ_{Wt} : single-topness variable $\min\left(\sqrt{(\frac{m_{j_1j_2}-m_W}{m_W})^2 + (\frac{m_{j_1j_2j_3}-m_t}{m_t})^2}\right)$
VBF-Jets	E_T^{miss} and ϕ^{miss} : magnitude and azimuthal angle of the MET
	$\Delta\eta_{j_1j_2}$: pseudo-rapidity separation of two VBF-jets
HH System	$m_{j_1j_2}$: invariant mass of two VBF-jets
	$m_{b\bar{b}\gamma\gamma}^*$: reduced invariant mass of the di-Higgs boson system
	$\Delta R(\gamma_1\gamma_2)$: angular separations between the two photon candidates
Event Shape	$\Delta R(b_1b_2)$: angular separations between the two b -jet candidates
	$S_\perp$: transverse sphericity [147], p_f : planar flow [148]
	p_T^{balance} : p_T balance defined by $\frac{ \vec{p}_T^{\gamma_1} + \vec{p}_T^{\gamma_2} + \vec{p}_T^{j_1} + \vec{p}_T^{j_2} }{ \vec{p}_T^{\gamma_1} + \vec{p}_T^{\gamma_2} + \vec{p}_T^{j_1} + \vec{p}_T^{j_2} }$

Tab. 5.7 Description of the input features used in binary classification to distinguish the HH signal from background.

5.5.2 Events Categorization

Before training each BDT classifier, hyperparameter tuning is conducted for each mass region using a Bayesian optimization algorithm. This process optimizes the per-process weight and the hyperparameter of the BDT classifier to maximize the expected combined Asimov significance [140], expressed as:

$$Z_{\text{tot}} = \sum_{k \in \text{bin}} \sqrt{2 \cdot \left[(S_k + B_k) \cdot \log\left(1 + \frac{S_k}{B_k}\right) - S_k \right]}, \quad (5.23)$$

where S_k and B_k are the expected signal and background yields in each bin k of the histogram of the BDT score distribution, respectively.

After the training, the events are classified in a given number of orthogonal categories based on the output score of the BDT. The number of categories and the thresholds in BDT output score used to separate the events are determined by maximizing the combined number counting significance, defined as in Eq. 5.23, where S_k and B_k are the expected signal and background

yields in each category k . The low-mass region is divided into four categories while the events in high mass region are classified into three categories. The BDT distributions for signals, backgrounds and data sideband events in low and high mass regions are illustrated in Figure 5.5. The corresponding BDT thresholds are depicted with dashed line in Figure 5.5 and listed in Table 5.8. The leftmost region in each BDT distribution, which exhibits background-like behavior, is excluded from the analysis. The whole analysis strategy after the preselection is described in Figure 5.6.

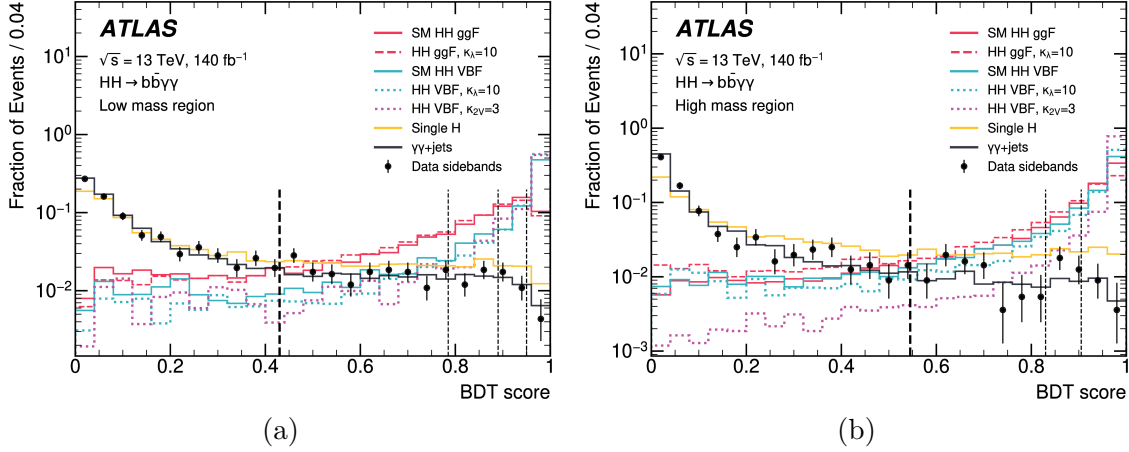


Fig. 5.5 Normalized BDT distributions for simulated ggFHH and VBFHH signal events and dominant backgrounds in the low-mass (a) and high-mass (b) regions (histograms). Data sideband events are also shown as black points. The dashed lines denote the BDT thresholds used to define the final categories. Events in the leftmost region in each plot are excluded from the analysis.

Category Name	Mass Region	Categories from BDT score
Low Mass 1 (LM 1)	$m_{b\bar{b}\gamma\gamma}^* \leq 350 \text{ GeV}$	$0.430 \leq \text{BDT score} < 0.785$
Low Mass 2 (LM 2)	$m_{b\bar{b}\gamma\gamma}^* \leq 350 \text{ GeV}$	$0.785 \leq \text{BDT score} < 0.890$
Low Mass 3 (LM 3)	$m_{b\bar{b}\gamma\gamma}^* \leq 350 \text{ GeV}$	$0.890 \leq \text{BDT score} < 0.950$
Low Mass 4 (LM 4)	$m_{b\bar{b}\gamma\gamma}^* \leq 350 \text{ GeV}$	$0.950 \leq \text{BDT score}$
High Mass 1 (HM 1)	$m_{b\bar{b}\gamma\gamma}^* > 350 \text{ GeV}$	$0.545 \leq \text{BDT score} < 0.830$
High Mass 2 (HM 2)	$m_{b\bar{b}\gamma\gamma}^* > 350 \text{ GeV}$	$0.830 \leq \text{BDT score} < 0.905$
High Mass 3 (HM 3)	$m_{b\bar{b}\gamma\gamma}^* > 350 \text{ GeV}$	$0.905 \leq \text{BDT score}$

Tab. 5.8 Thresholds in $m_{b\bar{b}\gamma\gamma}^*$ and BDT scores to define the final categories.

Figure 5.7 illustrates the efficiency of each category for ggFHH and VBFHH events for various values of the coupling modifiers. The third high-mass category and the fourth low-mass category exhibit the highest efficiencies for signal events, depending on the values of κ_λ and κ_{2V} . The expected yields with their statistic uncertainties in each category for ggFHH and VBFHH processes for different values of the coupling modifiers are calculated and summarized

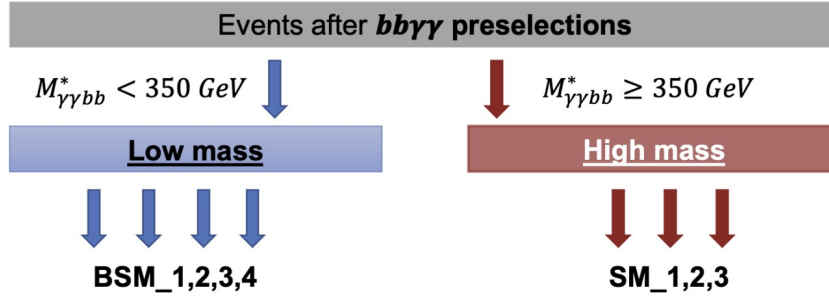
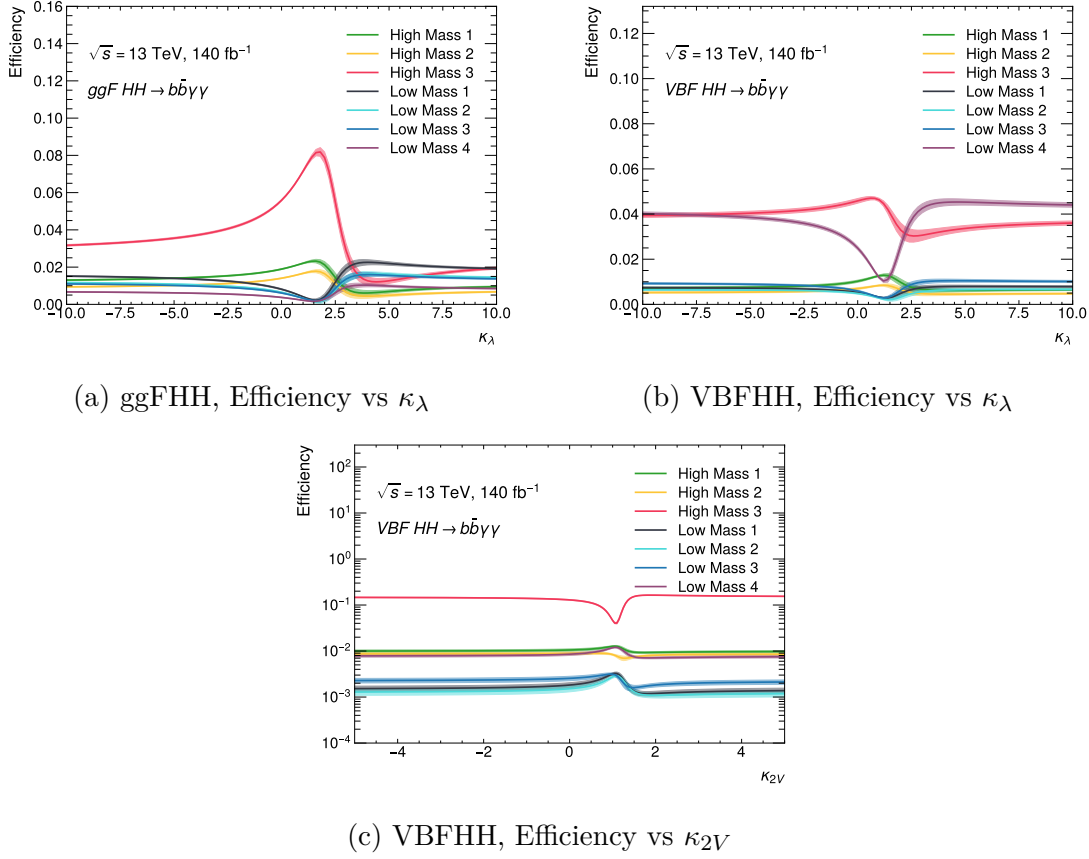


Fig. 5.6 Strategy of BDT-based classification after preselections applied for low and high mass regions.

in Table 5.9. The MC yields for dominant backgrounds are presented in Table 5.10, where data sideband events are also shown. The continuum background yield $\gamma\gamma + \gamma j + jj$ is obtained by rescaling the yield from the simulated $\gamma\gamma$ event sample by a factor 1.34 to account for the fraction estimated in data of nonresonant background (about 25%) from jets misidentified as photons (γ -jet and jet-jet events).

**Fig. 5.7**

Efficiency versus the coupling modifiers for each category for $ggFHH$ as a function of κ_λ (a), $VBFHH$ as a function of κ_λ (b) and $VBFHH$ as a function of κ_{2V} (c) processes. The target coupling modifier is various while the others are fixed to SM values.

Production Modes	κ_λ	κ_t	HM 1	HM 2	HM 3	LM 1	LM 2	LM 3	LM 4
ggFHH	1	1	0.254 ± 0.003	0.191 ± 0.003	0.822 ± 0.006	0.047 ± 0.001	0.037 ± 0.001	0.038 ± 0.001	0.025 ± 0.001
	10	1	2.35 ± 0.06	1.66 ± 0.05	4.94 ± 0.09	4.81 ± 0.09	3.64 ± 0.08	3.40 ± 0.07	2.08 ± 0.06
	0	1	0.494 ± 0.006	0.366 ± 0.006	1.46 ± 0.01	0.211 ± 0.008	0.168 ± 0.007	0.159 ± 0.006	0.097 ± 0.005
	5.6	1	0.350 ± 0.005	0.246 ± 0.004	0.783 ± 0.007	1.13 ± 0.08	0.87 ± 0.06	0.73 ± 0.05	0.40 ± 0.05
	20	1	13.7 ± 0.4	9.8 ± 0.3	29.9 ± 0.6	23.2 ± 0.4	17.6 ± 0.4	16.6 ± 0.4	10.2 ± 0.3
VBFHH	κ_λ	κ_{2V}	κ_V						
	0	1	1	0.0175 ± 0.0008	0.0119 ± 0.0007	0.078 ± 0.002	0.0089 ± 0.0006	0.0082 ± 0.0006	0.043 ± 0.001
	2	1	1	0.0056 ± 0.0003	0.0037 ± 0.0002	0.0165 ± 0.0005	0.0031 ± 0.0002	0.0024 ± 0.0002	0.0152 ± 0.0004
	10	1	1	0.24 ± 0.01	0.17 ± 0.01	1.31 ± 0.03	0.29 ± 0.02	0.24 ± 0.01	0.37 ± 0.02
	1	0	1	0.101 ± 0.003	0.087 ± 0.003	1.27 ± 0.01	0.018 ± 0.001	0.016 ± 0.001	0.023 ± 0.002
	1	0.5	1	0.039 ± 0.002	0.031 ± 0.002	0.393 ± 0.006	0.0063 ± 0.0007	0.0056 ± 0.0007	0.0080 ± 0.0008
	1	1.5	1	0.0117 ± 0.0006	0.0092 ± 0.0005	0.190 ± 0.002	0.0017 ± 0.0002	0.0016 ± 0.0002	0.0020 ± 0.0002
	1	2	1	0.047 ± 0.003	0.038 ± 0.002	0.86 ± 0.01	0.0055 ± 0.0009	0.0053 ± 0.0009	0.008 ± 0.001
	1	3	1	0.23 ± 0.01	0.20 ± 0.01	3.85 ± 0.05	0.031 ± 0.004	0.027 ± 0.004	0.049 ± 0.005
	1	1	0.5	0.040 ± 0.002	0.032 ± 0.002	0.584 ± 0.007	0.0080 ± 0.0009	0.0065 ± 0.0008	0.0092 ± 0.0009
	1	1	1.5	0.29 ± 0.01	0.21 ± 0.01	2.50 ± 0.04	0.071 ± 0.006	0.052 ± 0.005	0.068 ± 0.006
	0	0	1	0.132 ± 0.006	0.115 ± 0.006	1.51 ± 0.02	0.038 ± 0.003	0.032 ± 0.003	0.046 ± 0.004
	-5	1	0.5	0.0108 ± 0.0008	0.0086 ± 0.0007	0.273 ± 0.004	0.0106 ± 0.0008	0.0113 ± 0.0008	0.0147 ± 0.0009
									0.055 ± 0.002

Tab. 5.9 Expected ggFHH and VBFHH event yields with MC statistic uncertainties in each category for different values of the coupling modifiers.

Main Backgrounds	HM 1	HM 2	HM 3	LM 1	LM 2	LM 3	LM 4
ggFH	0.46 ± 0.04	0.15 ± 0.02	0.25 ± 0.03	0.29 ± 0.03	0.08 ± 0.02	0.07 ± 0.02	0.04 ± 0.01
$b\bar{b}H$	0.010 ± 0.008	0.002 ± 0.006	-0.006 ± 0.005	0.09 ± 0.02	0.03 ± 0.01	0.017 ± 0.007	0.024 ± 0.007
VBFH	0.081 ± 0.008	0.030 ± 0.005	0.040 ± 0.005	0.023 ± 0.004	0.016 ± 0.004	0.007 ± 0.002	0.009 ± 0.003
W^+H	0.007 ± 0.002	0.015 ± 0.0007	0 ± 0	0.013 ± 0.002	0.003 ± 0.001	0.0013 ± 0.0007	0.0003 ± 0.0003
W^-H	0.0045 ± 0.0010	0.0020 ± 0.0007	0.0023 ± 0.0007	0.005 ± 0.001	0.0017 ± 0.0006	0.0007 ± 0.0004	0.0004 ± 0.0003
$q\bar{q} \rightarrow ZH$	0.409 ± 0.008	0.109 ± 0.004	0.116 ± 0.004	0.462 ± 0.008	0.143 ± 0.005	0.062 ± 0.003	0.023 ± 0.002
$g\bar{g} \rightarrow ZH$	0.217 ± 0.007	0.067 ± 0.004	0.075 ± 0.004	0.037 ± 0.003	0.010 ± 0.002	0.008 ± 0.001	0.005 ± 0.001
$t\bar{t}H$	0.308 ± 0.006	0.070 ± 0.003	0.064 ± 0.003	0.791 ± 0.009	0.219 ± 0.005	0.102 ± 0.003	0.049 ± 0.002
tHj b	0.06 ± 0.02	0.051 ± 0.010	0.03 ± 0.01	0.04 ± 0.01	0.035 ± 0.009	0.019 ± 0.008	0.006 ± 0.008
tWH	0.006 ± 0.002	0.0025 ± 0.0010	0.001 ± 0.001	0.015 ± 0.003	0.004 ± 0.002	0.001 ± 0.001	0.0001 ± 0.0009
single H	1.57 ± 0.05	0.48 ± 0.02	0.58 ± 0.03	1.77 ± 0.04	0.55 ± 0.02	0.29 ± 0.02	0.16 ± 0.02
$\gamma\gamma + \gamma j + j\bar{j}$	47.8 ± 2.0	12.4 ± 1.0	12.9 ± 1.0	159.6 ± 4.0	483 ± 20	22.7 ± 1.0	11.1 ± 0.9
$\gamma\gamma + b\bar{b}$	36.0 ± 0.8	10.4 ± 0.4	12.0 ± 0.5	84.8 ± 1.0	29.2 ± 0.8	17.1 ± 0.6	9.6 ± 0.5
$t\bar{t}\gamma\gamma(\text{allhad})$	0.29 ± 0.01	0.055 ± 0.006	0.041 ± 0.005	1.53 ± 0.03	0.38 ± 0.02	0.19 ± 0.01	0.078 ± 0.007
$t\bar{t}\gamma\gamma(\text{noallhad})$	0.23 ± 0.02	0.035 ± 0.008	0.025 ± 0.006	1.62 ± 0.06	0.42 ± 0.03	0.23 ± 0.02	0.08 ± 0.01
Data Sideband	44 ± 6.6	13 ± 3.6	11 ± 3.3	145 ± 12	42 ± 6.5	17 ± 4.1	5 ± 2.2

Tab. 5.10 Expected yields in each category for all single Higgs production modes and continuum backgrounds. The events in data sideband are shown in the last row. Statistic uncertainties are reported.

5.5.3 Signal and Background Modeling

As described in Section 5.3.2, constructing the likelihood function requires the probability density functions (f_c) of the observable under study, i.e. the invariant mass of the diphoton system. According to Equation 5.12, f_c is related to three PDFs: f_c^{HH} for di-Higgs boson events, f_c^H for single-Higgs boson events, and $f_c^{\gamma\gamma}$ for continuum background. These are collectively referred to as signal and background modeling. This section will give the details about the signal and background modeling using different analytic functions.

5.5.3.1 Signal and Resonant Background

The Higgs boson pair signal is modeled using a Double-Sided Crystal Ball (DSCB) function [149] in Equation 5.24 and Figure 5.8 (a). The DSCB function combines a Gaussian core with two sided power-law tails, which are connected smoothly at the core-tail transition points. The function is determined by six parameters μ_{CB} and σ_{CB} for the mean and width of the Gaussian core, α_{CB}^{Low} , n_{CB}^{Low} , α_{CB}^{High} , and n_{CB}^{High} for the low and high power-law tails. The Gaussian distribution captures the core of the signal peak, while the power-law tails represent the tails, accounting for the photon energy loss due to pair production with bremsstrahlung in the ID [150]. The parameters of the DSCB function for each event category are derived by executing a point-by-point fit within the $m_{\gamma\gamma}$ range of [115, 135] GeV on SM ggFHH and SM VBFHH MC events after the preselection in Table 5.6 and event selection in Table 5.8 applied. These results are shown in Figure 5.8 for the high mass region and Figure 5.9 for the low mass region. It is observed in the simulation that single-Higgs boson events exhibit similar diphoton invariant mass distributions to the HH signal in the same category. For this reason, the same PDFs with the same values of the parameters are used for single-Higgs boson background and HH signal within a given category.

$$f(t) = N \times \begin{cases} e^{-\frac{1}{2}t^2} & \text{if } -\alpha_{CB}^{Low} \leq t \leq \alpha_{CB}^{High} \\ e^{-\frac{1}{2}(\alpha_{CB}^{Low})^2} \left[\frac{\alpha_{CB}^{Low}}{n_{CB}^{Low}} \left(\frac{n_{CB}^{Low}}{\alpha_{CB}^{Low}} - \alpha_{CB}^{Low} - t \right) \right]^{-n_{CB}^{Low}} & \text{if } t < -\alpha_{CB}^{Low} \\ e^{-\frac{1}{2}(\alpha_{CB}^{High})^2} \left[\frac{\alpha_{CB}^{High}}{n_{CB}^{High}} \left(\frac{n_{CB}^{High}}{\alpha_{CB}^{High}} - \alpha_{CB}^{High} + t \right) \right]^{-n_{CB}^{High}} & \text{if } t > \alpha_{CB}^{High} \end{cases} \quad (5.24)$$

where N as the normalization factor and $t = \frac{m_{\gamma\gamma} - \mu_{CB}}{\sigma_{CB}}$.

5.5.3.2 Nonresonant Background

The nonresonant background exhibits a continuous diphoton invariant mass distribution that is fit well by an exponential function ($Ne^{p_0 m_{\gamma\gamma}}$). The evaluation of the alternative functional forms are discussed in Section 5.8. The parameters of the function itself are sensitive to the exact amount of reducible background from photon misidentification, the kinematic dependence of the photon reconstruction and selection efficiency, as well as of theoretical input parameters used for the generation. For this reason, the parameters of the background distribution are not fixed from the simulation, but determined directly from the data. For the analysis optimization, the data $m_{\gamma\gamma}$ spectra of the sidebands are fit, excluding events within the mass window [120, 130] GeV, and the parameters from the fit are used to estimate the expected background and the analysis sensitivity. The parameters in each category are illustrated in Figure 5.10. In the

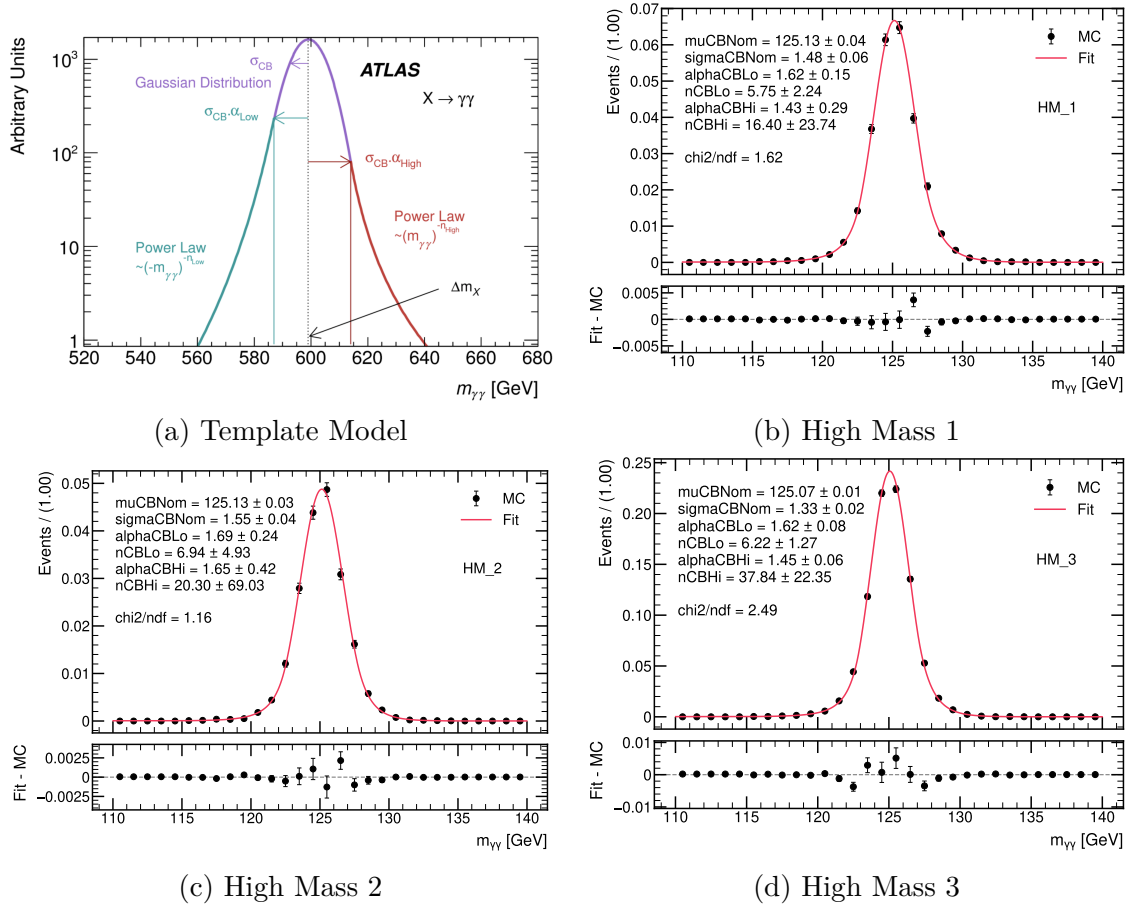
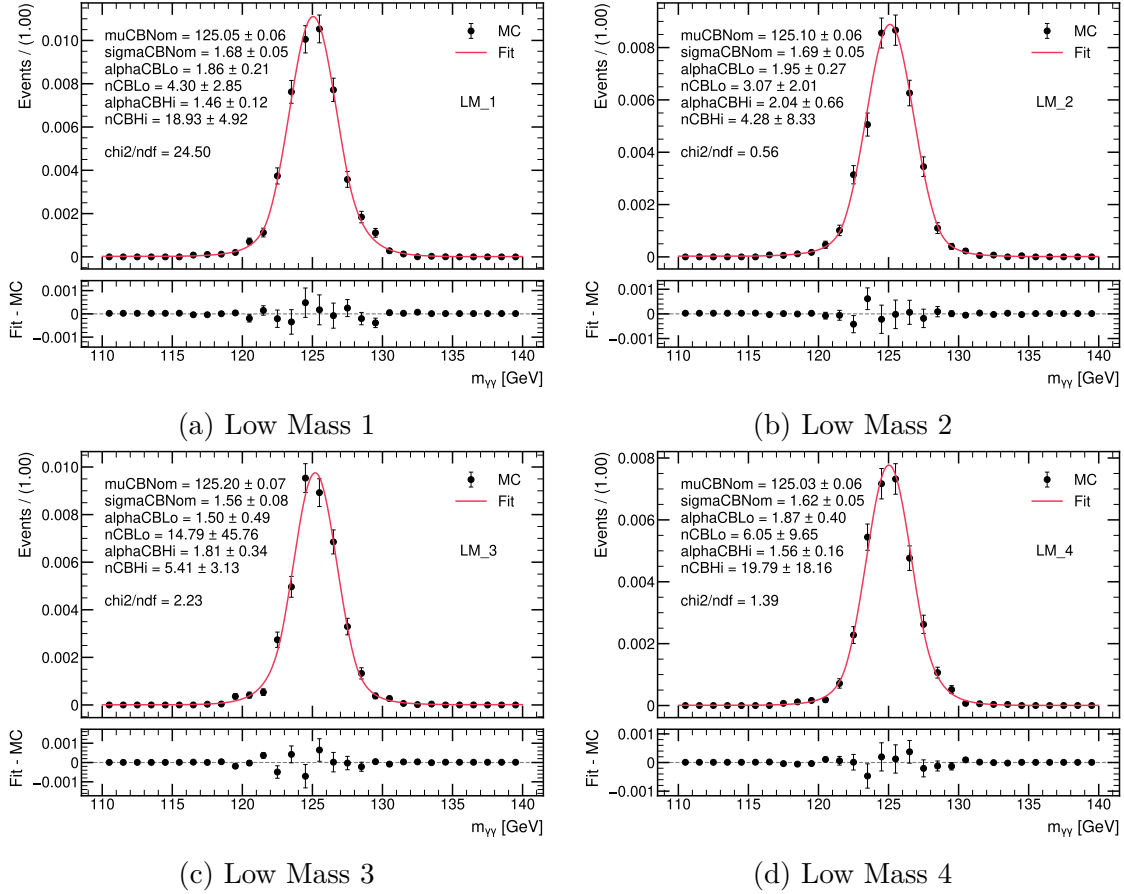


Fig. 5.8 Distribution of diphoton invariant mass $m_{\gamma\gamma}$: (a) Schematic depiction of the DSCB function; (b), (c) and (d): models for the three high-mass region categories. The MC events (black points) of SM ggFHH and SM VBFHH after the preselection and event selection are fitted using the DSCB function (red line). The parameters with the corresponding uncertainties are listed on the plots. The residuals between the model and the simulation are shown in the bottom panels.

final fit to the data, the nonresonant background parameters are floated during the fit and thus constrained by the data themselves.

**Fig. 5.9**

Distribution of diphoton invariant mass $m_{\gamma\gamma}$ for the four categories of the low mass region. The MC events (black points) of SM ggFHH and SM VBFHH after the preselection and event selection are fitted using the DSCB function (red line). The parameters with the corresponding uncertainties are listed on the plots. The residuals between the model and the simulation are shown in the bottom panels.

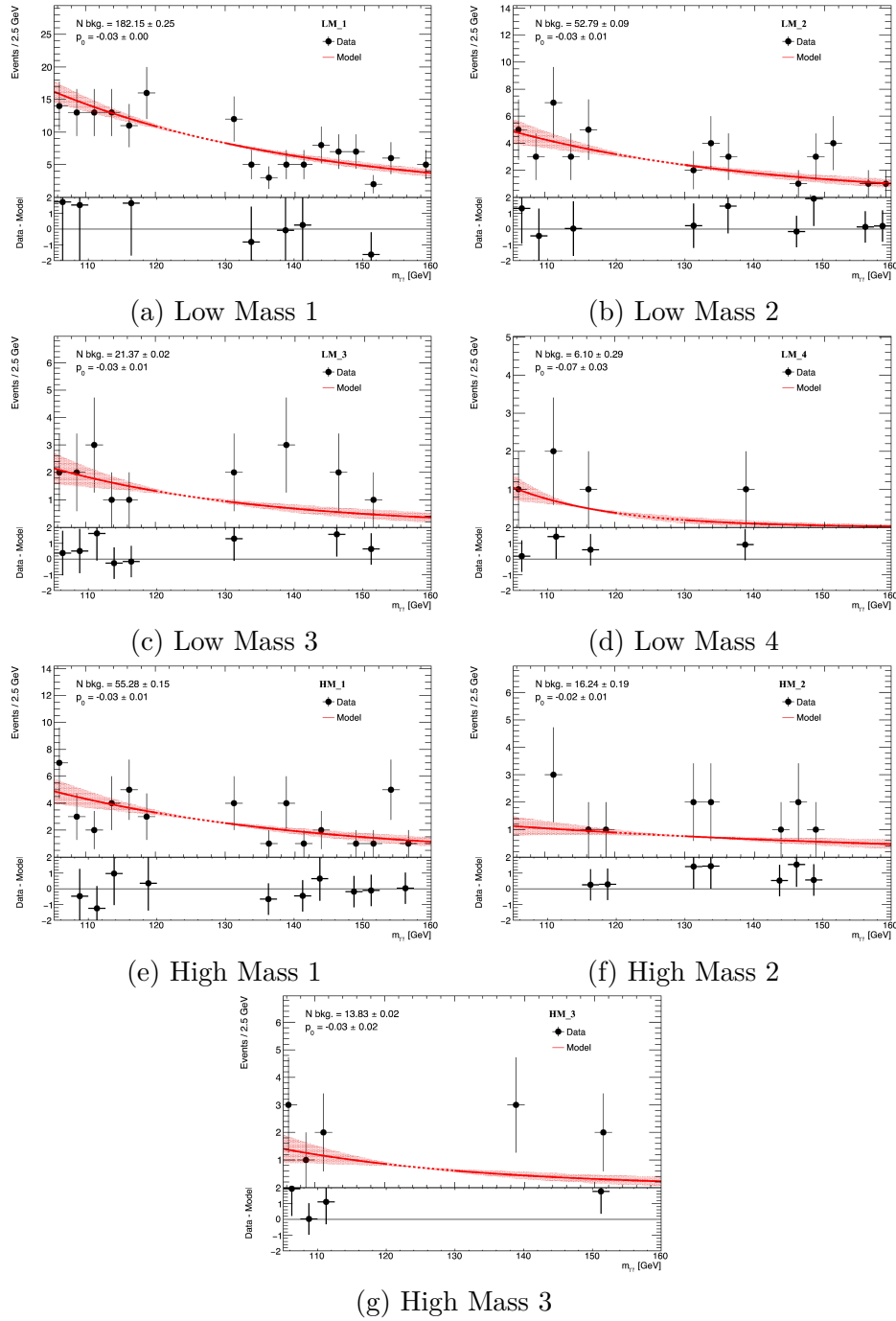


Fig. 5.10 Distribution of diphoton invariant mass $m_{\gamma\gamma}$ for seven categories after the pre-selection and event selection. The events (black points) within the data sideband regions are fitted using an exponential function (red line). The red band shows the envelope of the background model from the 1σ uncertainties in the background parameters. The residuals between the data and the model are shown in the bottom panels.

5.5.4 Expected Results

Following the procedures outlined in Section 5.3, expected upper limits on the HH signal strength were obtained by fitting the Asimov dataset [140], generated under the background-only hypothesis ($\mu=0$). The expected signal and background yields and shape parameters were used for the generation of the dataset and to normalize the signal strengths. Only statistical uncertainties are included in this study. The exclusion limits are set at a 95% confidence level. The expected upper limits on the HH production cross-section consider the contributions from both ggFHH and VBFHH. The expected value of μ_{HH}^{up} is 4.95. Using an Asimov dataset with ggFHH but not VBFHH ($\mu_{HH}^{\text{VBF}}=0$), an expected upper limit on $\mu_{HH}^{\text{VBF}}=132.27$ is obtained. The expected upper limits on the cross-sections are calculated by multiplying the signal strength times the SM prediction. Both the expected upper limits for μ_{HH} and μ_{HH}^{VBF} and the corresponding cross-sections, along with $\pm 1\sigma$ and $\pm 2\sigma$ error bands, are summarized in Table 5.11.

Signal Strength or Cross-Sections	Expected Upper Limits with Error Bands				
	-2σ	-1σ	Median	$+1\sigma$	$+2\sigma$
μ_{HH} (ggFHH + VBFHH)	2.66	3.57	4.95	7.32	10.94
Expected σ_{HH} [fb]	87.19	117.02	162.26	239.95	358.61
μ_{HH}^{VBF} (only VBFHH)	70.99	95.30	132.27	196.47	295.25
Expected σ_{HH}^{VBF} [fb]	122.53	164.49	228.30	339.11	509.60

Tab. 5.11 Expected upper limits at 95% CL on the signal strength μ_{HH} for ggFHH and VBFHH production modes, while μ_{HH}^{VBF} for only VBFHH, from the baseline analysis. The expected cross-sections are given by the signal strength multiplied by the SM prediction (32.78 fb for HH and 1.726 fb for VBFHH). Their corresponding $\pm 1\sigma$ and $\pm 2\sigma$ error bands are also listed.

As discussed in Section 5.3.5, the coupling modifiers can be constrained from the expected upper limits of the HH cross-sections. The expected one-dimensional constraints for κ_λ and κ_{2V} , with statistical uncertainties only, are shown respectively in Figure 5.11 (a) and (b). The dashed curve indicates the expected upper limit of the HH or VBFHH cross-section at 95% CL. The green band represents the $\pm 1\sigma$ error band, while the yellow band represents the $\pm 2\sigma$ error band. The predicted cross-sections (black solid curve) of ggFHH and VBFHH with the uncertainties (red bands) in SM theory are also illustrated in Figure 5.11 (a) and (b). The allowed intervals of κ_λ and κ_{2V} are determined from the crossing points between the expected cross-section and the theoretical predictions. These effective ranges are listed in Table 5.12.

Furthermore, two-dimensional constraints for κ_λ vs κ_{2V} can be set. The expected results with their error bands are shown in Figure 5.12.

5.6 Alternative Analysis Strategy

Following the preselections, in alternative to the event selection and classification detailed in Section 5.5, a novel analysis strategy for event selection and classification has been investigated.

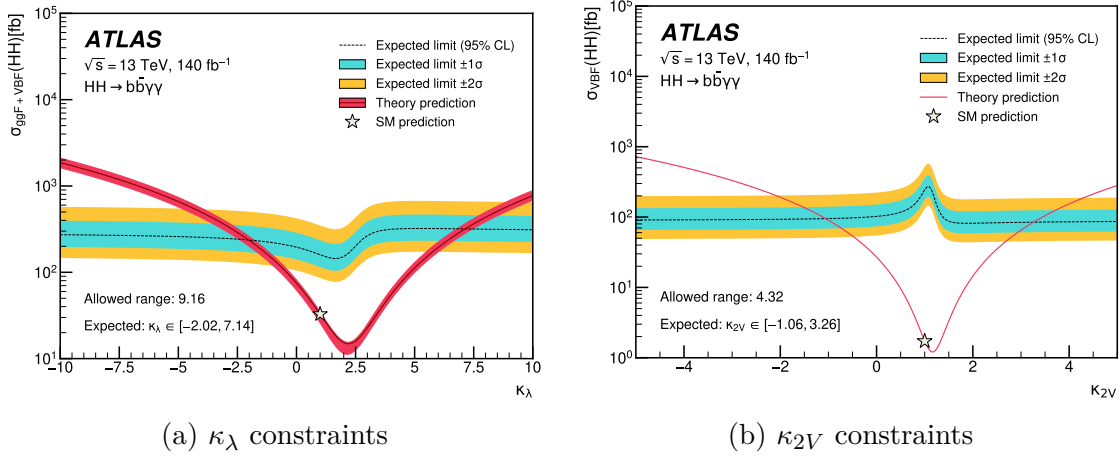


Fig. 5.11 Constraints on (a) κ_λ and (b) κ_{2V} from the expected upper limits of the HH and VBFHH cross-section at 95% CL, from the baseline analysis. The dashed curve indicates the expected upper limit, with the green band representing the $\pm 1\sigma$ error band and the yellow band representing the $\pm 2\sigma$ error band. The solid curve and the surrounding red band represent the predicted cross-sections and their associated uncertainties for κ_λ . Theoretical error bands for κ_{2V} are not displayed, as the scale uncertainties (0.05%) are minimal [36]. The allowed intervals are derived from the crossing points between the expected limits and the theoretical ones. Only statistical uncertainties are considered.

Coupling Modifiers	Allowed range	Size of allowed range
κ_λ	[-2.02, 7.13]	9.15
κ_{2V}	[-1.06, 3.27]	4.33

Tab. 5.12 Allowed ranges of κ_λ and κ_{2V} from the expected 95% CL upper limits on the HH and VBFHH cross-sections, from the baseline analysis. Only statistical uncertainties are considered.

The baseline analysis separates events into low- and high-mass regions, as defined by $m_{b\bar{b}\gamma\gamma}^*$, based on the relationship between κ_λ and the kinematics of the $b\bar{b}\gamma\gamma$ system, and then defines categories for each region based on binary BDT classifiers trained to distinguish HH production from the background. The alternative strategy uses a multi-output classifier to identify the ggFHH and VBFHH production modes for various κ_λ and κ_{2V} scenarios. After this initial step, a binary classifier developed for each output class of the multi-classifier is used to separate the HH signal from the background. The classifiers are trained with the Scikit-learn software implementation [151] of the XGBoost algorithm [146]. This section will present the methodology and results for this alternative classification strategy.

5.6.1 Classification Strategy

First, a multi-classifier BDT with four output classes is developed to differentiate between ggFHH and VBFHH production for SM and BSM values of the κ_λ and κ_{2V} coupling modifiers.

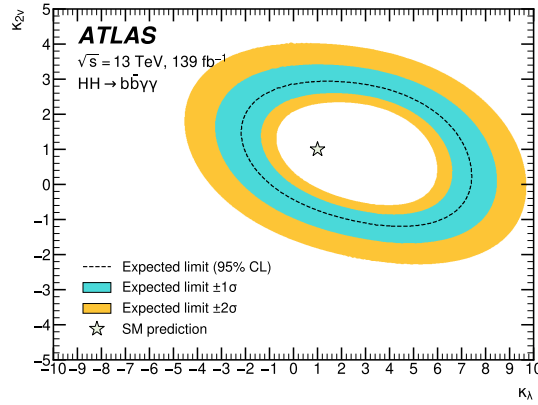


Fig. 5.12 Two-dimensional constraints of κ_λ and κ_{2V} from the expected upper limits of the HH and VBF HH cross-sections at 95% CL. The dashed line represents the expected upper limit, with the green band representing the $\pm 1\sigma$ error band and the yellow band representing the $\pm 2\sigma$ error band. The star symbolizes the SM prediction. Only statistical uncertainties are considered.

As a second step, a binary-classifier BDT for each class is trained to further discriminate HH events from single-Higgs production and continuum backgrounds. The events are then categorized into eight distinct regions based on the output scores of these boosted decision trees, as illustrated in Figure 5.13.

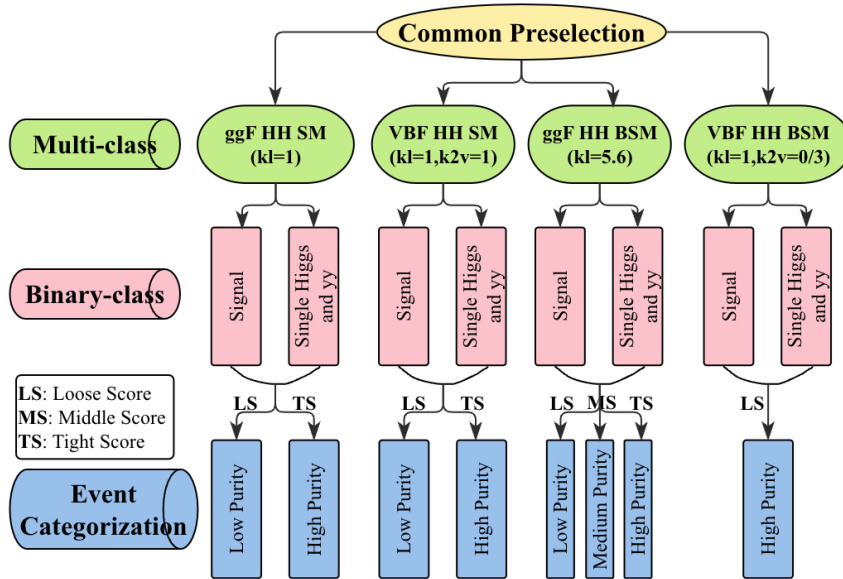


Fig. 5.13 Flow of the alternative analysis strategy designed by a multi-output classifier (green) with four classes and four binary classifiers (pink). The events are finally classified into eight distinct regions (blue) according to the BDT output scores.

The input features used in the multi-classifier and binary-classifier BDTs are summarized in Table 5.13. They include the kinematic variables of photons, b -jets, VBF-jets, missing momen-

tum, HH candidates, and event-level quantities describing the overall event shape or designed to suppress specific background event topologies. In the $t\bar{t}H$ ($t \rightarrow Wb$) and ZH backgrounds, W and Z bosons can undergo hadronic decay into two jets or leptonic decay into two leptons, with neutrinos potentially produced. Electrons or muons are excluded by requiring no leptons in the preselections. The suppression of $t\bar{t}H$ and ZH with hadronic decay is achieved using H_T and χ_{Wt} as additional input variables in the classifier. The magnitude (E_T^{miss}) and azimuthal angle (ϕ^{miss}) of the missing transverse momentum vector are utilized as inputs to reduce the presence of $t\bar{t}H$ and ZH events with invisible decays. Event-shape variables such as $S_\perp$, p_f , and p_T^{balance} are employed to enhance the separation between signals and backgrounds. The minimum angular separation ($\min(\Delta R_{(\gamma, \text{jet})})$, $\min(\Delta R_{(b, \text{jet})})$) between the candidate photon or b -jet and each candidate VBF-jet, the cross product of the pseudo-rapidity between two VBF-jets, and the Zeppenfeld variable (Z_η^*), which describes the rapidity difference between the $b\bar{b}\gamma\gamma$ system and the two VBF forward jets, are introduced to enhance the identification of VBFHH events. The distributions of these four latter variables, not used in the baseline analysis, are illustrated in Figure 5.14 for simulated ggFHH and VBFHH events with various values of the coupling strength modifiers. The distributions show good separation of VBFHH processes from ggFHH modes.

5.6.1.1 Hyper-parameter Optimization

All simulated events are divided into four groups based on the remainder of EventNumber%4: training dataset for training the classifiers, validation dataset for optimizing the hyper-parameters, public test dataset for evaluating the MVA performance, and private test dataset for determining the MVA strategy. 50% of the events are used for training and validation, named train-valid dataset, 25% for public testing, and 25% for private testing. Before finalizing the models for the multi-classifier and binary classifiers, hyper-parameters are tuned to derive the optimal parameters using the bayesian algorithm in Hyperopt [154]. The training process for each set of hyper-parameters incorporates five-fold cross-validation, where each fold utilizes 80% of the train+validation events for training and 20% for validation. For the multi-classifier, the average accuracy from the five folds is employed as the performance metric and maximized to ascertain the optimal parameters, which are then utilized on the complete train+validation dataset to construct the final model. For the binary classifiers, the average combined number counting significance in Equation 5.23 from the five folds is leveraged as the performance metric and maximized to determine the optimal hyper-parameters, which are subsequently applied to the entire train-valid dataset to derive the final model. Final evaluations are performed in the public testing dataset. All the procedures are illustrated in Figure 5.15.

5.6.1.2 Multi-Classifier Training

The multi-classifier is designed to differentiate ggFHH from VBFHH, for SM vs BSM values of the coupling strength modifiers. Simulated events in the signal regions ($m_{\gamma\gamma} \in [120, 130]$ GeV) are considered to perform the training process. Four output classes are defined, corresponding to the following MC samples used in the BDT training: *ggFHH SM*, trained with SM ggFHH events; *ggFHH BSM*, trained with ggFHH $\kappa_\lambda = 5.6$ events; *VBFHH SM*, trained with SM VBFHH samples; and *VBFHH BSM*, trained with VBFHH samples with $\kappa_{2V} = 0$ or $\kappa_{2V} = 3$. The ggFHH $\kappa_\lambda = 5.6$ event sample is obtained from the reweighting of the SM ggFHH sample, as introduced

Discriminating Variables	Definitions and Descriptions
Photons and b -jets	$p_T/m_{\gamma\gamma}$, η , ϕ of each photon $\Delta p_T^{\gamma_1\gamma_2}$, $\Delta R_{\gamma_1\gamma_2}$, $\Delta\eta_{\gamma_1\gamma_2}$ and $\Delta\phi_{\gamma_1\gamma_2}$ of two photons p_T , η , ϕ and b_{Tag} pseudo-continuous score of each b -jet $p_T^{b\bar{b}}$, $\eta^{b\bar{b}}$, $\phi^{b\bar{b}}$, $m_{b\bar{b}}$ of two b -jets system H_T : scalar sum of p_T of all jets with $p_T > 30$ GeV χ_{Wt} : single-topness variable, as defined in Table 5.7 E_T^{miss} and ϕ^{miss} : MET energy and azimuthal angle
VBF-Jets	p_T , η , ϕ of each VBF-jet $\Delta\eta_{j_1j_2}$: pseudo-rapidity separation between two VBF-jets $\Delta\phi_{j_1j_2}$: angular between two VBF-jets $m_{j_1j_2}$: invariant mass of two VBF-jets $\min(\Delta R_{(\gamma,\text{jet})})$: $\min \Delta R$ of γ and each VBF-jet [152] $\min(\Delta R_{(b,\text{jet})})$: $\min \Delta R$ of b -jet and each VBF-jet [152] $\eta_{j_1} \times \eta_{j_2}$: cross product of the pseudo-rapidity of two VBF-jets [152] N_{jets} : number of jets in an event
HH System	$m_{b\bar{b}\gamma\gamma}^*$: reduced invariant mass of the HH candidate $\Delta R_{b\bar{b}\gamma\gamma}$: angular separation between diphoton and di- b -jet
Event Shape	$S_{\perp}$: transverse sphericity [147], p_f : planar flow [148] p_T^{balance} : p_T balance, as defined in Table 5.7 $Z_{\eta}^* = y_{b\bar{b}\gamma\gamma} - \frac{ (y_{jet,1} + y_{jet,2}) }{2}$: rapidity difference [153] between the HH system and VBF-jets

Tab. 5.13 Definitions of input features used in the classifiers for the alternative analysis strategy. Fundamental kinematics, special signatures and event-shape variables are included to enhance the discrimination of the signals or suppress specific backgrounds.

in Section 5.2.2.2. Training weights of the events are calculated by scaling the event weights to the statistics of all training samples.

The performance of the multi-classifier is evaluated by the cross-entropy loss function and the error rate during the training. The confusion matrix is displayed in Figure 5.16, which shows that the accuracy is around 68%. The overfitting is checked by comparing the BDT score distributions on the training dataset and validation dataset of targeted signals and other modes considered as “backgrounds”. The results for four classes are illustrated in Figure 5.17. The Kolmogorov-Smirnov test values indicate that the model is not obviously overfitted. The model shows a good performance on both targeted signals and backgrounds in all four classes.

The determined model is then applied to the events of the public testing dataset, assigning each event four scores. Each event is classified into the class with the highest score, ensuring that all events are categorized into one of the four classes. These procedures are also performed for all background samples.

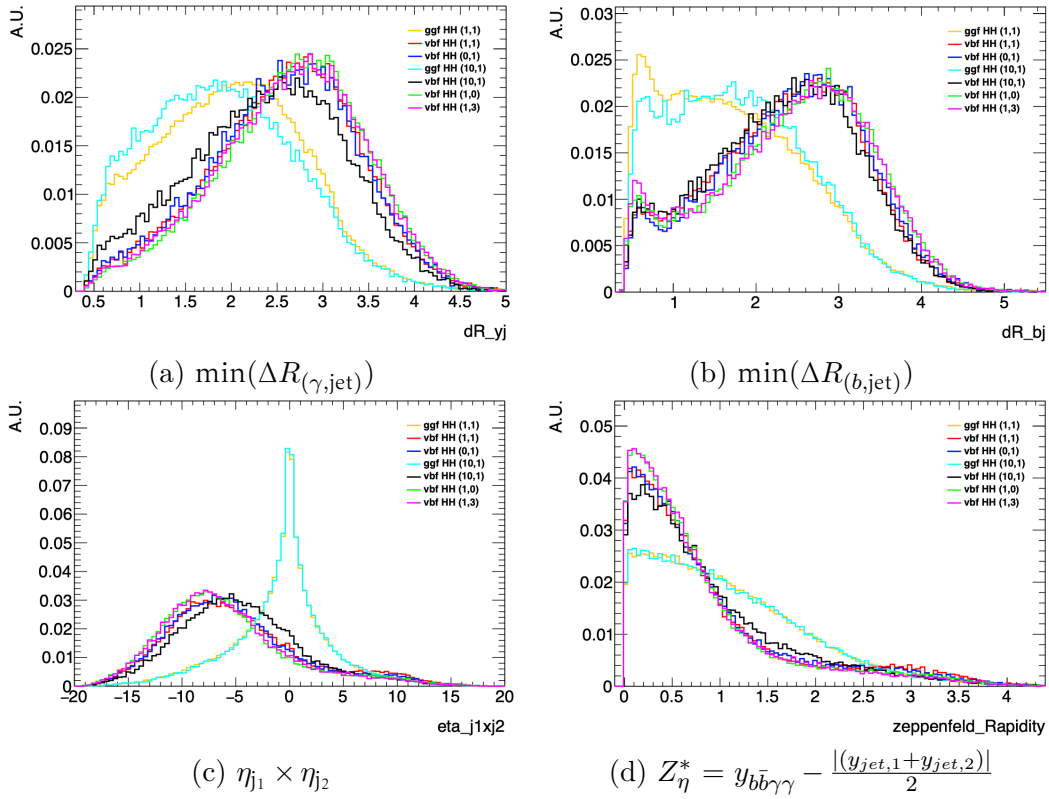


Fig. 5.14

Distributions of VBFHH-oriented variables for simulated ggFHH and VBFHH events with various $(\kappa_{\lambda}, \kappa_{2V})$ values. The minimum angular separation between the candidate photon or b -jet and each candidate VBF-jet are shown in (a) and (b). The cross product of the pseudo-rapidities of the two VBF-jets, and the Zeppenfeld variable, are illustrated in (c) and (d). Good separation of VBFHH events from ggFHH ones is observed.

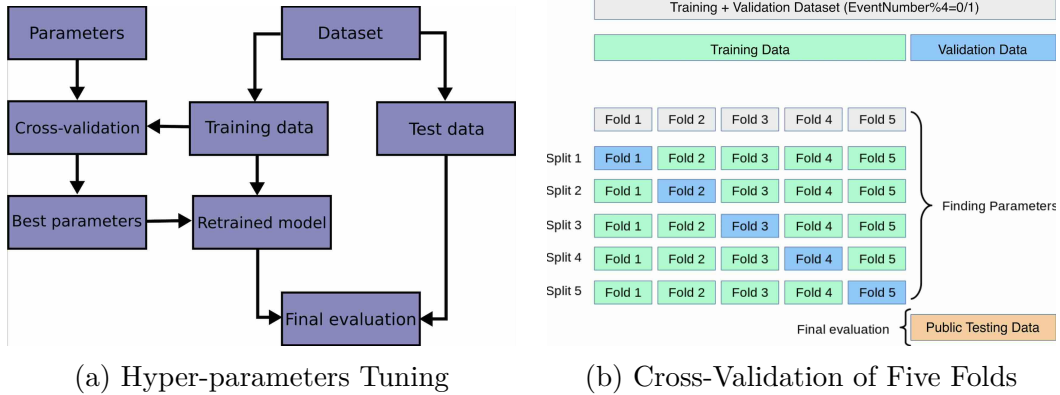


Fig. 5.15

Schematic illustration of the hyper-parameters tuning (a) and the cross validation (b) procedures. Modified from: [Scikit-learn](https://scikit-learn.org/).

Hyper Parameters	Multi-Classifer	Binary-Classifiers			
		ggFHH SM	VBFHH SM	ggFHH BSM	VBFHH BSM
max_depth	2	21	2	10	3
learning_rate	0.12	0.002	0.42	0.002	0.003
max_bin	295	190	244	164	256
max_delta_step	18	11	18	17	0
min_child_weight	64	64	88	13	1
gamma	5.75	6.18	3.39	9.46	0.009
reg_alpha	0.24	0.14	0.91	0.73	0.03
reg_lambda	5.80	1.54	8.36	9.66	0.02
subsample	0.82	0.12	0.31	0.82	0.15
colsample_bylevel	0.55	0.88	0.76	0.97	0.07
colsample_bynode	0.88	0.23	0.78	0.79	0.996
colsample_bytree	0.44	0.80	0.90	0.82	0.17

Tab. 5.14 Optimal hyper-parameters of the multi-classifier with maximum accuracy and binary classifiers with best combined significance for four classes after the hyper-tuning.

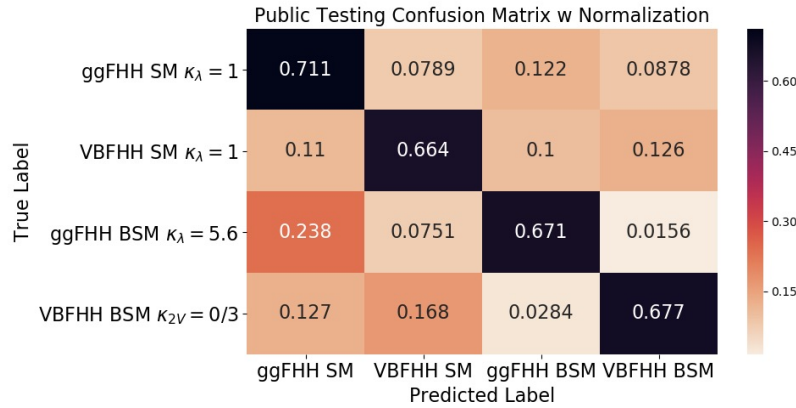


Fig. 5.16 Confusion matrix of the predicted labels on x-axis and truth labels on y-axis for four classes. The values along the diagonal are the accuracy, while others represents the misidentification rate. The results are from the public testing dataset and normalized.

5.6.1.3 Binary-Classifier Training

The multi-classifier has been designed to identify various production modes of HH signals. It is trained only on HH signal events, but it is evaluated on all signal and background samples (and, later, on data). Each class thus contains the targeted signals along with some background events. To further distinguish targeted HH signal from single-Higgs boson production and continuum background, four binary classifiers have been developed, one for each class.

The signal and background events within each class are used to train the classifier. Their training weights are obtained by scaling the event weights to the relevant statistics of signals and backgrounds for all train+validation datasets. All the variables enumerated in Table 5.13

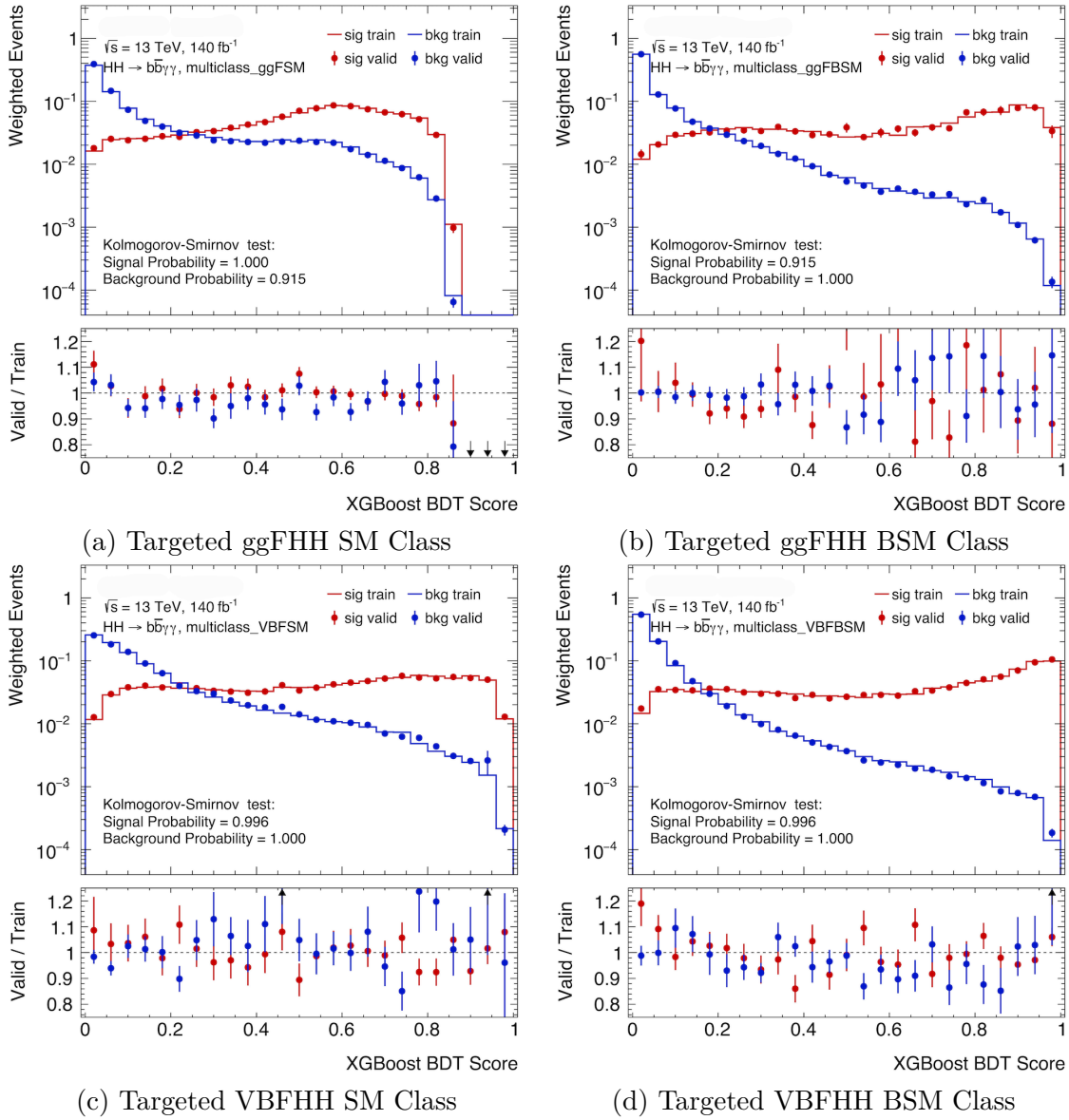


Fig. 5.17 Distributions of BDT scores for each class between the training set (lines) and validation set (points) for the multi-classifier. Targeted production mode is regarded as signal (red), while other signals are considered as "backgrounds" (blue). The ratios between validation and training distributions are illustrated in the bottom panels.

are used as input to each binary classifier. The hyper-parameters of each classifier are optimized following the procedure outlined in Section 5.6.1.1. This approach aims at maximizing the combined number counting significance as a metric, considering specific categorizations. The parameters yielding the best performance are listed in Table 5.14. The classifier model is trained on the full train+validation dataset with the optimized hyper-parameters. Over-training checks, verifying the consistency of the performance on training and validation sets for signal and back-

ground for the four models, are illustrated in Figure 5.18. Kolmogorov-Smirnov test values, calculated and displayed in these figures, demonstrate that these models are not significantly overfitted, aside from discrepancies in the tail due to small number of simulated events there.

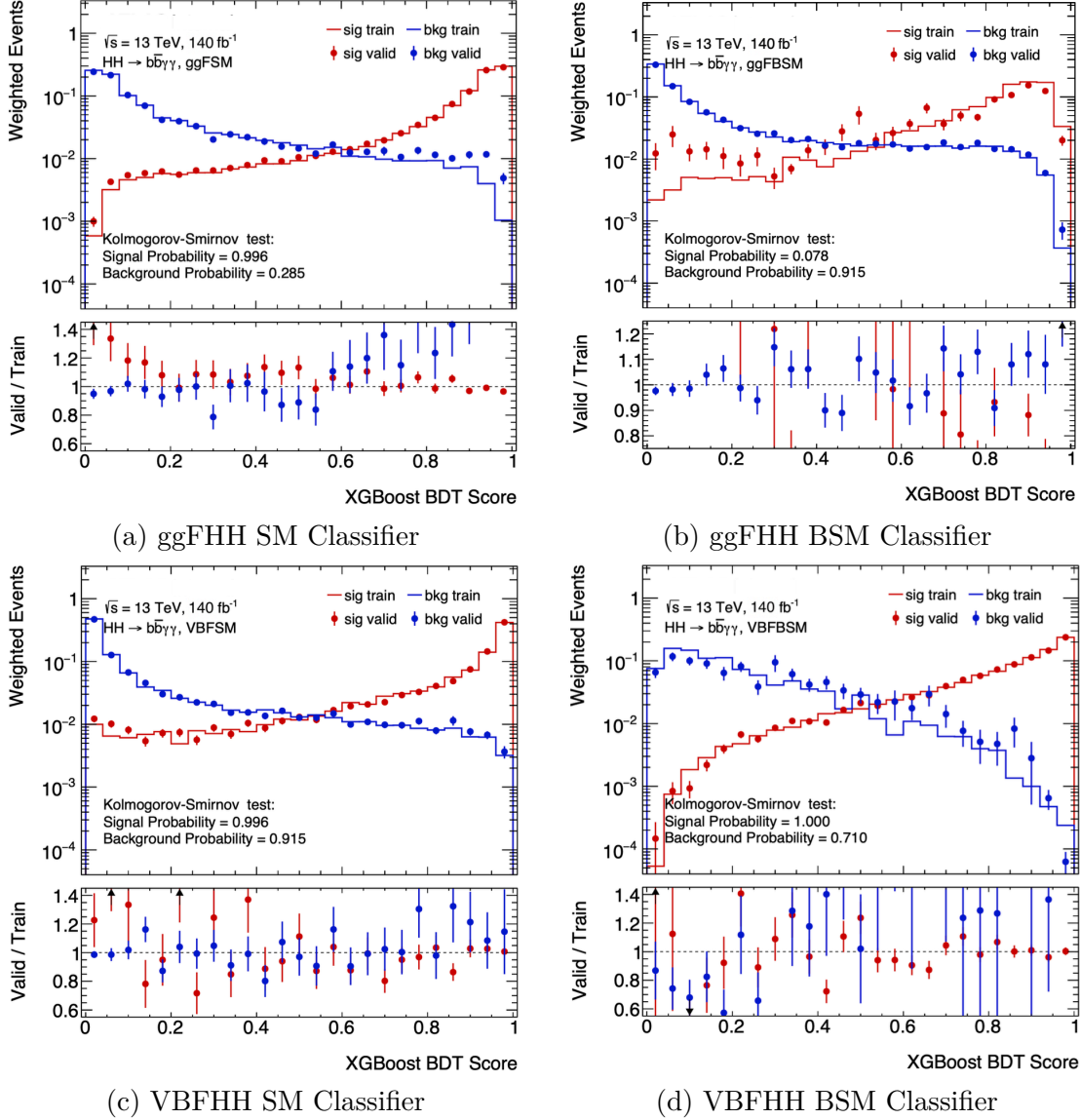


Fig. 5.18 Distributions of BDT scores for the training set (lines) and validation set (points) of signals and backgrounds for the binary-classifiers. The events of the targeted HH processes in each class are considered as signals (red), while the events of single-Higgs boson production and continuum background in each class are seen as backgrounds (blue). The ratios between validation and training distributions are illustrated in the bottom panels.

The four trained binary classifiers are applied to the events in the public testing dataset of signals and backgrounds. The BDT score is then used to categorize the events into orthogonal regions as described in the following section.

5.6.2 Events Categorization

To construct the statistical model, all samples in the public testing dataset are categorized after applying the multi-classifier and four binary classifiers. This categorization is based on the BDT score distributions of the signal and background events from the binary classifiers. The BDT score in each class is scanned across 200 bins with a step size of 0.005. The requirements for the BDT thresholds are at least 11 weighted irreducible background ($\gamma\gamma + \gamma jet + jetjet$) events in each bin and the best combined number counting significance defined in Equation 5.23. The $\gamma\gamma + \gamma jet + jetjet$ yields are obtained by scaling the $\gamma\gamma$ yields by a factor of 1.34, as derived from the background decomposition of the $\gamma\gamma$, γjet , and jet-jet components [130]. Accurate modeling requires $\gamma\gamma + \gamma jet + jetjet$ yields to be at least 11. Before the grid scan, the number of BDT thresholds in each class must be specified. During the scan, the combined significance is calculated using the signal and background yields in each region under a set of BDT thresholds. The BDT thresholds that result in the highest combined significance are determined as the final categorization strategy.

Figure 5.19 illustrates the BDT score distributions of signals and backgrounds in each class. The data sideband events are also shown as black points, which is consistent with the irreducible background ($\gamma\gamma + \gamma jet + jetjet$). Considering the significance and statistics, different categories are defined for each class. Both the ggFHH SM class and the VBFHH SM class are further split into low and high purity categories. The ggFHH BSM class is further divided into low, medium, and high purity categories. Meanwhile, the VBFHH BSM class remains as a single category due to lack of the statistics of the irreducible background. The events with lower than the lowest BDT threshold are discarded because of background-like behavior. Eight categories are defined in total for the statistical model, which are shown in Table 5.15.

Classes	Defined Categories			$Z_{\text{comb, sig}}$
	Low Purity (LP)	Medium Purity (MP)	High Purity (HP)	
ggFHH SM	$0.670 \leq \text{BDT}_{\text{score}} < 0.850$	-	$0.850 \leq \text{BDT}_{\text{score}}$	0.227
ggFHH BSM	$0.160 \leq \text{BDT}_{\text{score}} < 0.775$	$0.775 \leq \text{BDT}_{\text{score}} < 0.885$	$0.885 \leq \text{BDT}_{\text{score}}$	0.278
VBFHH SM	$0.610 \leq \text{BDT}_{\text{score}} < 0.855$	-	$0.855 \leq \text{BDT}_{\text{score}}$	0.008
VBFHH BSM	$0.170 \leq \text{BDT}_{\text{score}}$	-	-	1.160

Tab. 5.15 Summary of BDT thresholds to determine the final categories. The events with BDT scores less than the lowest threshold are excluded from the analysis. "-" indicates that the category is not defined.

According to the construction of the likelihood function 5.10 in Section 5.3.2, the signal and background yields in each category are required. The expected yields with statistic uncertainties for ggFHH and VBFHH with various coupling modifiers are calculated and summarized in Table 5.16. The expected MC yields for dominant backgrounds are presented in Table 5.17, where data sideband events are also shown. The $\gamma\gamma$ samples are scaled by 1.34 to account for the γ -jet and jet-jet components, which are both considered as continuum backgrounds.

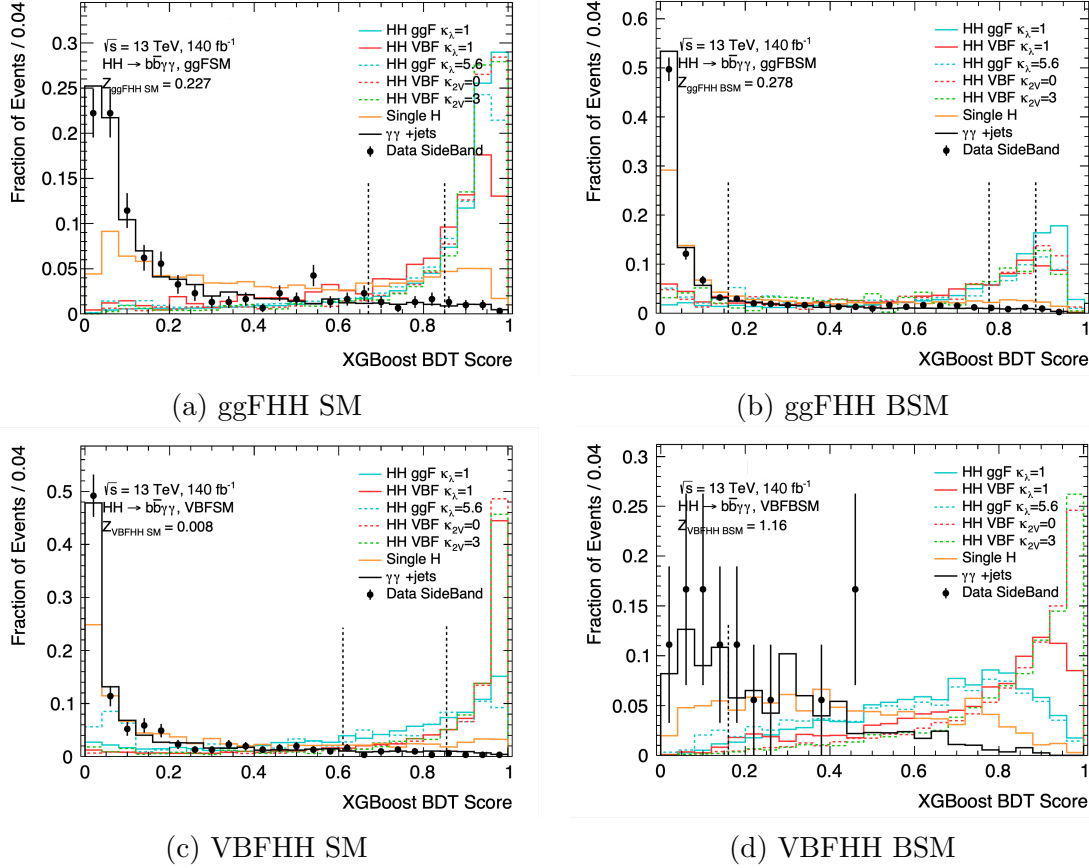


Fig. 5.19 Distributions of BDT score for HH signals and dominant backgrounds in each class. The events of diHiggs and single Higgs are selected at signal region [120, 130] GeV. The $\gamma\gamma$ yields within [105, 160] GeV are scaled by 1.34 to account for the γ -jet and jet-jet components. The data sideband events with the error bars are shown as black points. The BDT thresholds are exhibited as dashed vertical lines.

Production Modes		ggFHH SM LP	ggFHH SM HP	VFHH SM LP	VFHH SM HP	ggFHH BSM LP	ggFHH BSM MP	ggFHH BSM HP	VFHH BSM
SM ggF HH	SM ggF HH	0.164118 ± 0.00264	0.817260 ± 0.00603	0.040257 ± 0.00126	0.051464 ± 0.00146	0.067694 ± 0.00163	0.052973 ± 0.00144	0.072561 ± 0.00171	0.130511 ± 0.00253
	Reweight SM ggF HH to $\kappa_\lambda = 5.6$	0.209411 ± 0.00397	0.805033 ± 0.00687	0.111149 ± 0.01295	0.128716 ± 0.01209	1.653105 ± 0.11119	0.832736 ± 0.05157	0.734404 ± 0.03234	0.073202 ± 0.00158
SM VBF HH	SM VBF HH	0.001534 ± 0.00010	0.003550 ± 0.00016	0.007190 ± 0.00023	0.028764 ± 0.00046	0.002738 ± 0.00014	0.001609 ± 0.00011	0.001077 ± 0.00009	0.007685 ± 0.00024
	VBF HH $\kappa_\lambda = 0, \kappa_{2V} = 1, \kappa_V = 1$	0.005186 ± 0.00046	0.014310 ± 0.00075	0.018652 ± 0.00085	0.076260 ± 0.00173	0.014485 ± 0.00075	0.006816 ± 0.00051	0.006803 ± 0.00052	0.029608 ± 0.00110
	VBF HH $\kappa_\lambda = 2, \kappa_{2V} = 1, \kappa_V = 1$	0.000896 ± 0.00011	0.001827 ± 0.00016	0.007809 ± 0.00032	0.022579 ± 0.00055	0.004615 ± 0.00024	0.001722 ± 0.00015	0.000991 ± 0.00012	0.006043 ± 0.00029
	VBF HH $\kappa_\lambda = 10, \kappa_{2V} = 1, \kappa_V = 1$	0.092540 ± 0.00880	0.358293 ± 0.01717	0.411957 ± 0.01856	1.526171 ± 0.03579	0.491481 ± 0.02010	0.212683 ± 0.01318	0.200302 ± 0.01281	0.638685 ± 0.02334
	VBF HH $\kappa_\lambda = 1, \kappa_{2V} = 0, \kappa_V = 1$	0.031507 ± 0.00187	0.158989 ± 0.00427	0.060521 ± 0.00263	0.280521 ± 0.00569	0.029640 ± 0.00183	0.015502 ± 0.00133	0.017093 ± 0.00139	0.986037 ± 0.01076
	VBF HH $\kappa_\lambda = 1, \kappa_{2V} = 0.5, \kappa_V = 1$	0.011458 ± 0.00096	0.049210 ± 0.00203	0.025418 ± 0.00144	0.112212 ± 0.00305	0.010797 ± 0.00093	0.005957 ± 0.00069	0.005876 ± 0.00071	0.275371 ± 0.00481
	VBF HH $\kappa_\lambda = 1, \kappa_{2V} = 1.5, \kappa_V = 1$	0.003965 ± 0.00033	0.017444 ± 0.00070	0.005341 ± 0.00039	0.020650 ± 0.00077	0.002601 ± 0.00027	0.001315 ± 0.00019	0.000897 ± 0.00016	0.017448 ± 0.00224
	VBF HH $\kappa_\lambda = 1, \kappa_{2V} = 2, \kappa_V = 1$	0.019097 ± 0.00171	0.083104 ± 0.00358	0.020176 ± 0.00175	0.099850 ± 0.00396	0.010746 ± 0.00128	0.004572 ± 0.00079	0.005339 ± 0.00092	0.756268 ± 0.01088
	VBF HH $\kappa_\lambda = 1, \kappa_{2V} = 3, \kappa_V = 1$	0.085158 ± 0.00676	0.431836 ± 0.01554	0.109418 ± 0.00779	0.482160 ± 0.01647	0.049044 ± 0.00531	0.026320 ± 0.00384	0.020444 ± 0.00331	3.266269 ± 0.04309
	VBF HH $\kappa_\lambda = 0, \kappa_{2V} = 0, \kappa_V = 1$	0.044738 ± 0.00367	0.208400 ± 0.00812	0.096751 ± 0.00552	0.432240 ± 0.01165	0.060833 ± 0.00435	0.039193 ± 0.00349	0.029941 ± 0.00300	1.099089 ± 0.01871
	VBF HH $\kappa_\lambda = 1, \kappa_{2V} = 1, \kappa_V = 0.5$	0.015740 ± 0.00122	0.071189 ± 0.00256	0.018873 ± 0.00131	0.097703 ± 0.00302	0.012512 ± 0.00108	0.006641 ± 0.00078	0.006194 ± 0.00076	0.502155 ± 0.00692
	VBF HH $\kappa_\lambda = 1, \kappa_{2V} = 1, \kappa_V = 1.5$	0.087430 ± 0.00691	0.357631 ± 0.01416	0.184893 ± 0.01022	0.798722 ± 0.02121	0.093688 ± 0.00714	0.051540 ± 0.00524	0.056852 ± 0.00570	1.864105 ± 0.03275
	VBF HH $\kappa_\lambda = 5, \kappa_{2V} = 1, \kappa_V = 0.5$	0.002072 ± 0.00063	0.012085 ± 0.00082	0.014587 ± 0.00089	0.047440 ± 0.00161	0.019679 ± 0.00103	0.008162 ± 0.00067	0.006646 ± 0.00060	0.267598 ± 0.00388

Tab. 5.16 Expected yields for the analysis categories with 140 fb^{-1} for signal ggF HH and VBF HH processes in the SM case and for different values of the coupling modifiers κ_λ , κ_{2V} , and κ_V .

Main Backgrounds		ggFHH SM LP	ggFHH SM HP	VFHH SM LP	VFHH SM HP	ggFHH BSM LP	ggFHH BSM MP	ggFHH BSM HP	VFHH BSM
ggFHH + $b\bar{b}H$	ggFHH	0.226341 ± 0.02516	0.270974 ± 0.02741	0.154639 ± 0.02234	0.089324 ± 0.01586	0.624099 ± 0.04533	0.112230 ± 0.01972	0.070790 ± 0.01557	0.171832 ± 0.02151
	VBFH	0.023278 ± 0.00438	0.022307 ± 0.00411	0.026021 ± 0.00428	0.037183 ± 0.00527	0.055669 ± 0.00669	0.012885 ± 0.00342	0.010792 ± 0.00289	0.038384 ± 0.00549
	WH	0.008521 ± 0.00159	0.005827 ± 0.00134	0.000763 ± 0.00044	0.000974 ± 0.00051	0.026875 ± 0.00287	0.002323 ± 0.00080	0.000922 ± 0.00056	0.004798 ± 0.00121
	$q\bar{q} \rightarrow ZH + g\bar{g} \rightarrow ZH$	0.529508 ± 0.00980	0.490172 ± 0.00948	0.036867 ± 0.00262	0.034587 ± 0.00260	0.768932 ± 0.01110	0.155758 ± 0.00500	0.80353 ± 0.00360	0.141134 ± 0.00505
	$t\bar{t}H$	0.349136 ± 0.00581	0.321977 ± 0.00560	0.142055 ± 0.00377	0.084172 ± 0.00287	1.330627 ± 0.01129	0.254588 ± 0.00493	0.107445 ± 0.00321	0.236604 ± 0.00502
$t\bar{t}H$	$t\bar{t}H$	0.040584 ± 0.01051	0.015802 ± 0.00979	0.092211 ± 0.01636	0.100586 ± 0.01721	0.087104 ± 0.01635	0.012296 ± 0.00714	0.004775 ± 0.00418	0.039277 ± 0.01265
	$t\bar{t}H$	0.006735 ± 0.00235	0.008139 ± 0.00232	0.004690 ± 0.00168	0.002948 ± 0.00125	0.018967 ± 0.00428	0.004901 ± 0.00153	0.001101 ± 0.00113	0.004377 ± 0.00206
	$t\bar{t}H$	12.664914 ± 0.91086	8.519275 ± 0.67032	18.520327 ± 1.01166	8.368397 ± 0.73444	166.993725 ± 3.24277	20.294947 ± 1.05680	8.232354 ± 0.66578	8.254892 ± 0.70942
$\gamma\gamma + \gamma jet + jetjet$	$\gamma\gamma$	16.970984 ± 1.22055	11.415829 ± 0.89822	24.817238 ± 1.35562	11.213652 ± 0.98416	223.771592 ± 4.34531	27.195230 ± 1.41611	11.031354 ± 0.89215	11.061555 ± 0.95062
	Data Sidebands	17 ± 4.1	10 ± 3.2	16 ± 4.0	3 ± 1.7	209 ± 14.5	22 ± 4.7	10 ± 3.2	8 ± 2.8

Tab. 5.17 Expected yields for the analysis categories with 140 fb^{-1} for main backgrounds. In order to account for the γjet and $jetjet$ components for the continuum background, the expected yields from the $\gamma\gamma$ MC sample is scaled by 1.34. The number of events in data sidebands for each category is also quoted.

The comparisons between data and MC simulations for the $m_{\gamma\gamma}$ distribution after applying specific event selection criteria are shown in Figure 5.20-5.22. Each plot represents different event categories, including common preselections, and varying purity levels (low, medium, high) of SM and BSM processes for ggFHH and VBFHH modes. The data points (black dots) are superimposed on MC predictions (colored histograms) that include contributions from SM Higgs boson pair production, single Higgs processes, and diphoton background events. The histograms are color-coded to differentiate these processes, with shaded areas indicating the statistical uncertainties of the MC predictions. The bottom panels of each plot show the ratio of data to the predicted MC values (Data/Pred.), showing a detailed examination of the agreement between observed data and the MC model. The consistency observed in the ratio plots, despite minor fluctuations, supports the reliability of the event selection process and the accuracy of the MC models used in this analysis.

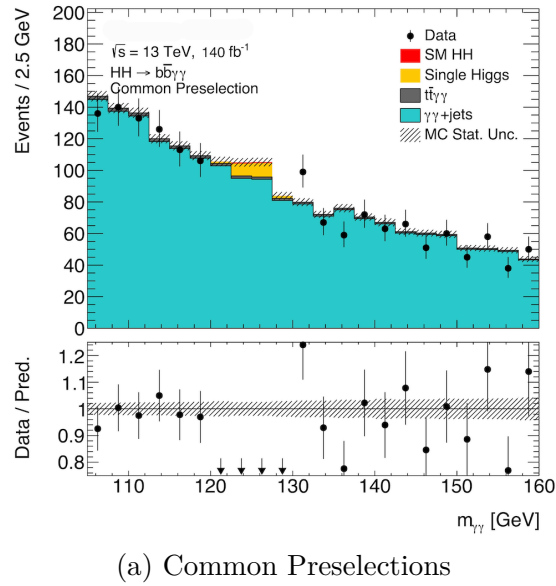


Fig. 5.20 Data versus MC comparison plots of the $m_{\gamma\gamma}$ distribution after common preselections applied. The plots compare data (black dots) with MC predictions. The colored histograms represent different processes: SM HH (red), single Higgs (orange), irreducible backgrounds (cyan), and $t\bar{t}\gamma\gamma$ (grey), with the hatched areas indicating MC statistical uncertainties. The lower panels show the ratio of data to MC values (Data/Pred.), providing insight into the agreement between observed data and the simulation.

5.6.3 Signal and Background Modeling

Similar analytic models to those employed in Section 5.5.3 are used for the signal and background to study the sensitivity of the alternative analysis strategy.

5.6.3.1 Signal and Resonant Background

Double-sided Crystal Ball functions are used to model the diphoton invariant mass distribution for both signal and resonant background. They are determined to fits form simulated signal

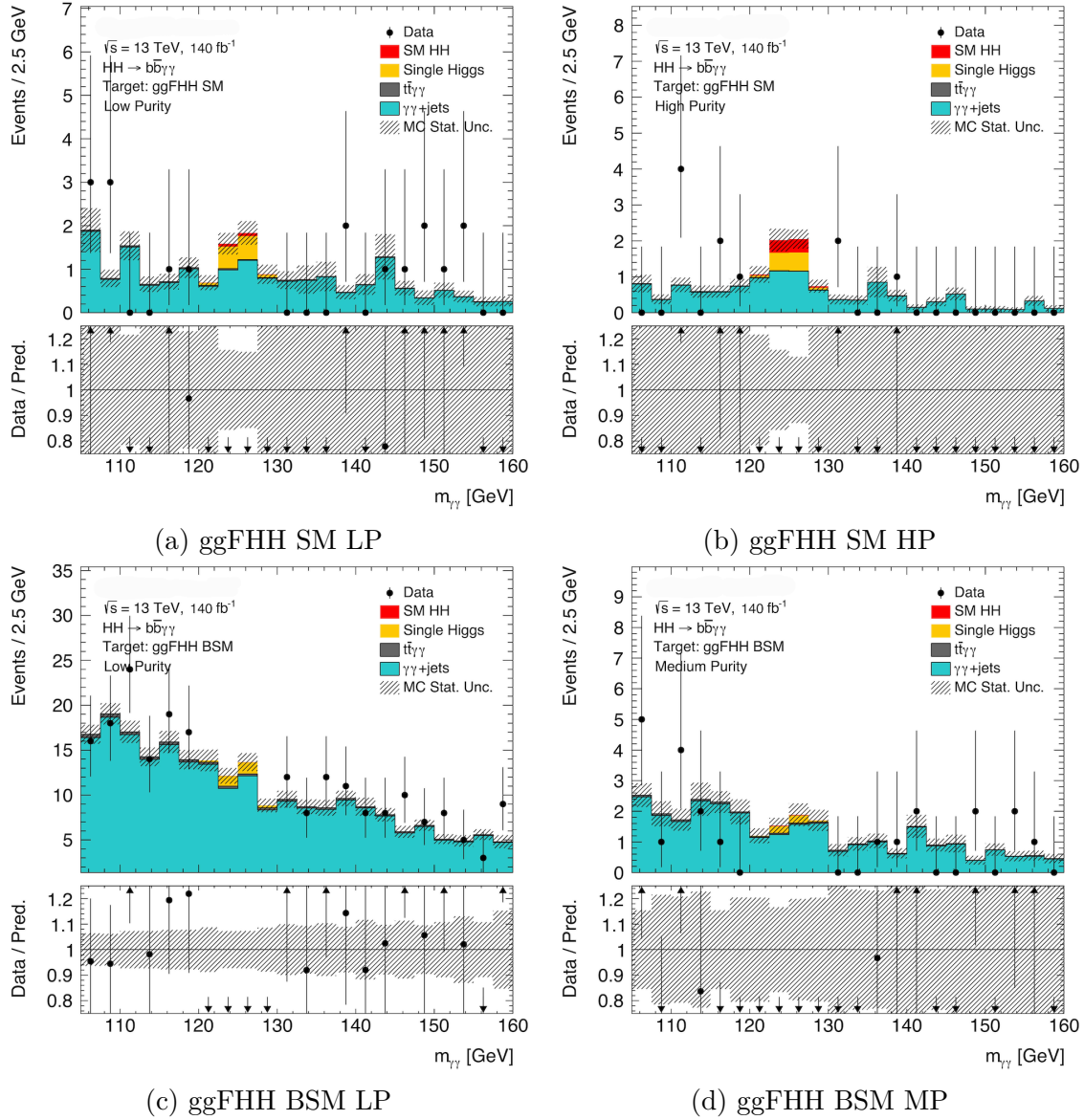


Fig. 5.21 Data versus MC comparison plots of the $m_{\gamma\gamma}$ distribution after event selection. The plots compare data (black dots) with MC predictions for various event categories, including lower purity, medium purity, and high purity events under both SM and BSM scenarios (a-d). The colored histograms represent different processes: SM HH (red), single Higgs (orange), irreducible backgrounds (cyan), and $t\bar{t}\gamma\gamma$ (grey), with the hatched areas indicating MC statistical uncertainties. The lower panels show the ratio of data to MC values (Data/Pred.), providing insight into the agreement between observed data and the simulation.

events in each category. The same model is found to describe equally well the resonant background. The plots showing the fits to the signal for each of the eight final event categories are shown in Figure 5.23-5.24. The black data points represent the simulated ggFHH and VBFHH events, while the red curves depict the fitted DSCB function. Key fit parameters, such as the

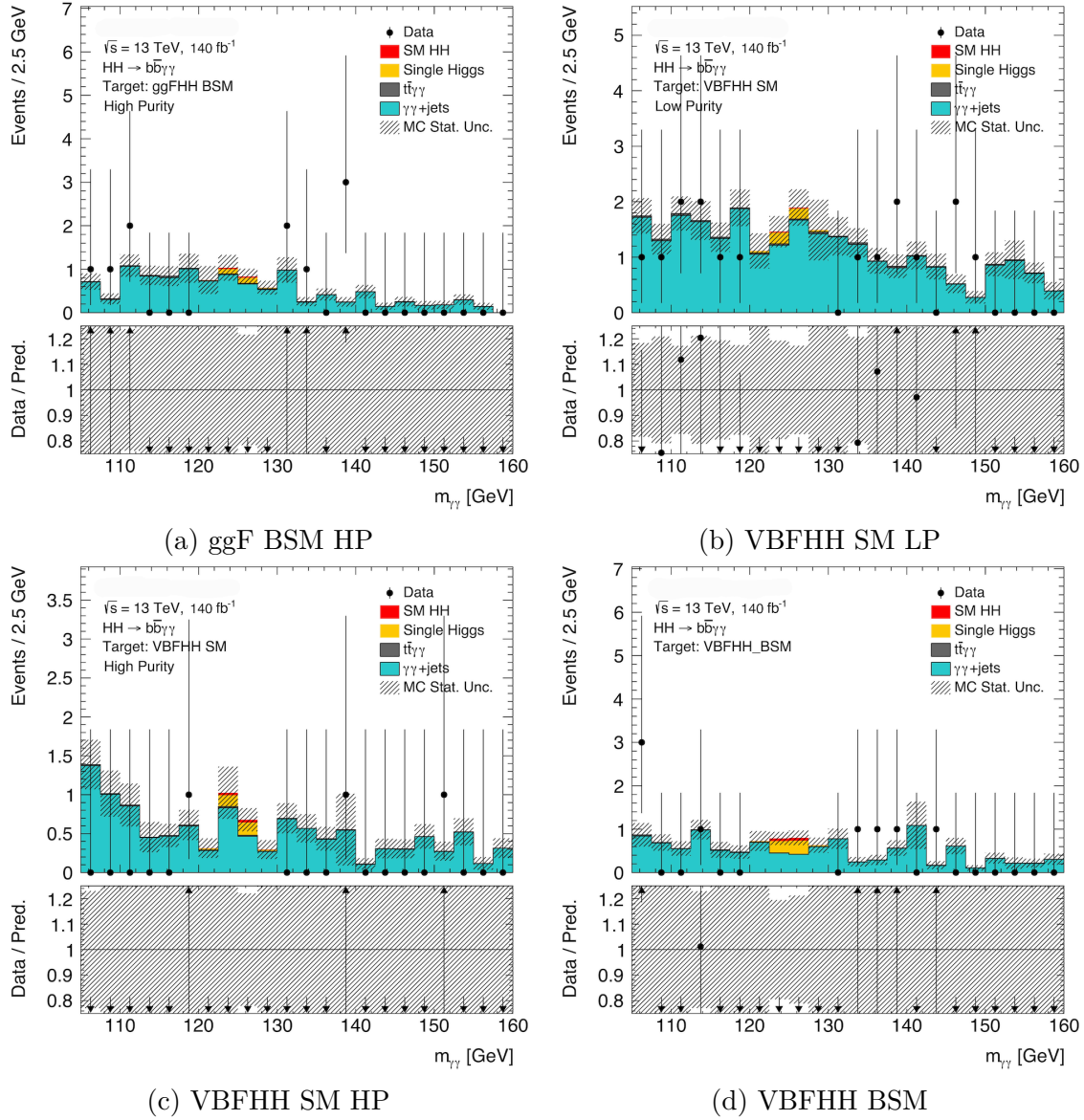
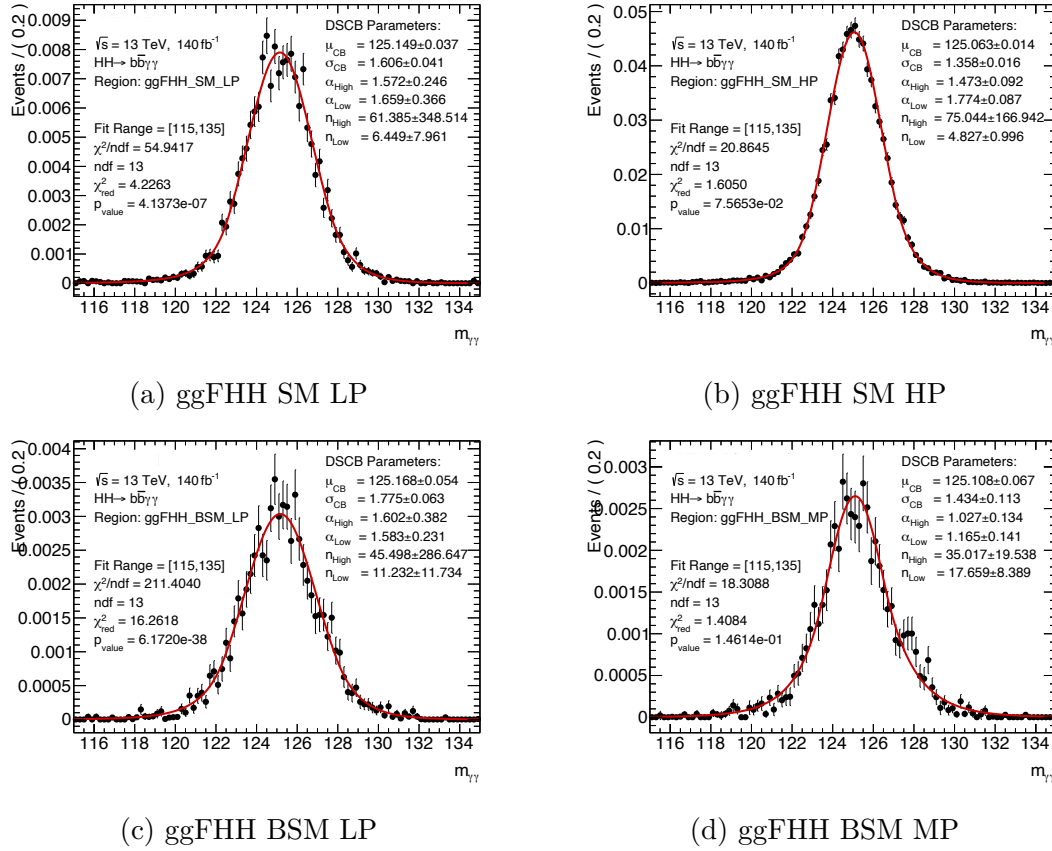


Fig. 5.22 Data versus MC comparison plots of the $m_{\gamma\gamma}$ distribution after event selection. The plots compare data (black dots) with MC predictions for various event categories, including lower purity and high purity events under both SM and BSM scenarios (a-d). The colored histograms represent different processes: SM HH (red), single Higgs (orange), irreducible backgrounds (cyan), and $t\bar{t}\gamma\gamma$ (grey), with the hatched areas indicating MC statistical uncertainties. The lower panels show the ratio of data to MC values (Data/Pred.), providing insight into the agreement between observed data and the simulation.

DSCB parameters, fit range, chi-squared per degree of freedom (χ^2/ndf), and p-values, are annotated on each plot. The excellent agreement between the fitted models and the simulated data points across all categories highlights the robustness of the signal extraction methodology, which is pivotal for accurately identifying and analyzing potential $HH \rightarrow b\bar{b}\gamma\gamma$ events.

**Fig. 5.23**

Distribution of diphoton invariant mass $m_{\gamma\gamma}$ for the signal for four categories of the alternative analysis strategy. The MC events (black points) of SM ggFHH and SM VBFHH after the preselection and event selection are fitted using the DSCB function (red line). The parameters with the corresponding uncertainties are listed on the plots. The agreement between the signal models and the data points validates the robustness of the signal extraction methods.

5.6.3.2 Nonresonant Background

The nonresonant background diphoton invariant mass distribution is modelled with an exponential function. The parameters, used afterwards to generate the background Asimov datasets, are obtained by fitting the data in the sidebands, as illustrated in Figure 5.25-5.26, where data are indicated by the black dots, and the fitted models by the red curves. The fit parameters, including the background yield ($\text{Yield}_{\text{bkg}}$) and the slope of the exponential function ($\text{Slope}_{\text{Bkg}}$), are calculated and displayed for each event category. This method allows for an accurate estimation of the background contribution directly from the data, minimizing reliance on simulation and thereby enhancing the robustness of the background model. The resulting fits show a good agreement with the data, validating the approach and ensuring that the background is well understood for the subsequent signal extraction and analysis.

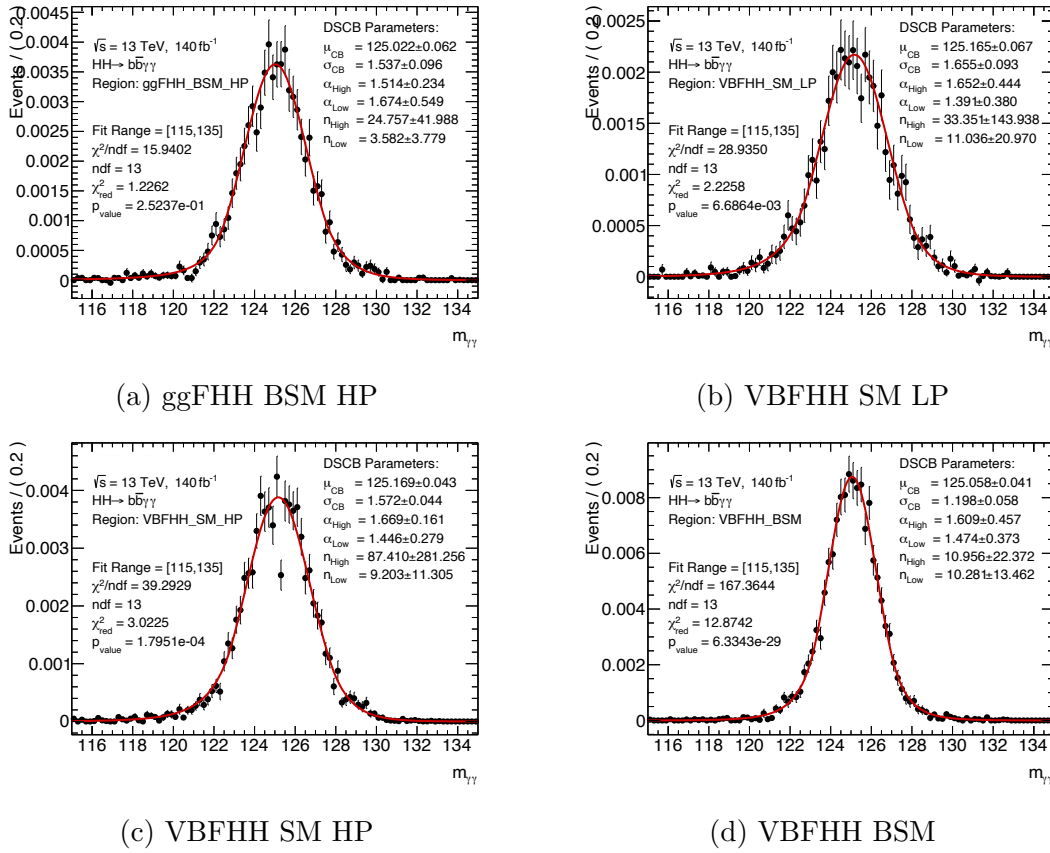


Fig. 5.24

Distribution of diphoton invariant mass $m_{\gamma\gamma}$ for the signal for four categories of the alternative analysis strategy. The MC events (black points) of SM ggFHH and SM VBFHH after the preselection and event selection are fitted using the DSCB function (red line). The parameters with the corresponding uncertainties are listed on the plots. The agreement between the signal models and the data points validates the robustness of the signal extraction methods.

5.6.4 Expected Results

The workspace for the statistical model is constructed using eight categories and includes the parameters of interest (POIs), yields, PDFs, and blinded data for each of them. Systematic uncertainties are not incorporated, and the results are derived considering only statistical uncertainties. The expected upper limits on the signal strengths (μ_{HH} and μ_{HH}^{VBF}) are extracted by fitting the Asimov dataset generated under the background-only hypothesis ($\mu_{HH} = 0$ and $\mu_{HH}^{VBF} = 0$). Exclusion limits are consistently established at a 95% confidence level. Cross-section upper limits are calculated by multiplying the signal strengths by the SM predictions. The expected upper limits for μ_{HH} and μ_{HH}^{VBF} , along with the corresponding cross-sections and the $\pm 1\sigma$ and $\pm 2\sigma$ standard deviation error bands, are summarized in Table 5.11.

The coupling modifiers κ_λ and κ_{2V} are constrained from the expected results and the predicted HH cross-sections. The results are illustrated in Figure 5.27 (a) and (b). The black dashed line shows the expected upper limits at a 95% CL, with the green band indicating the

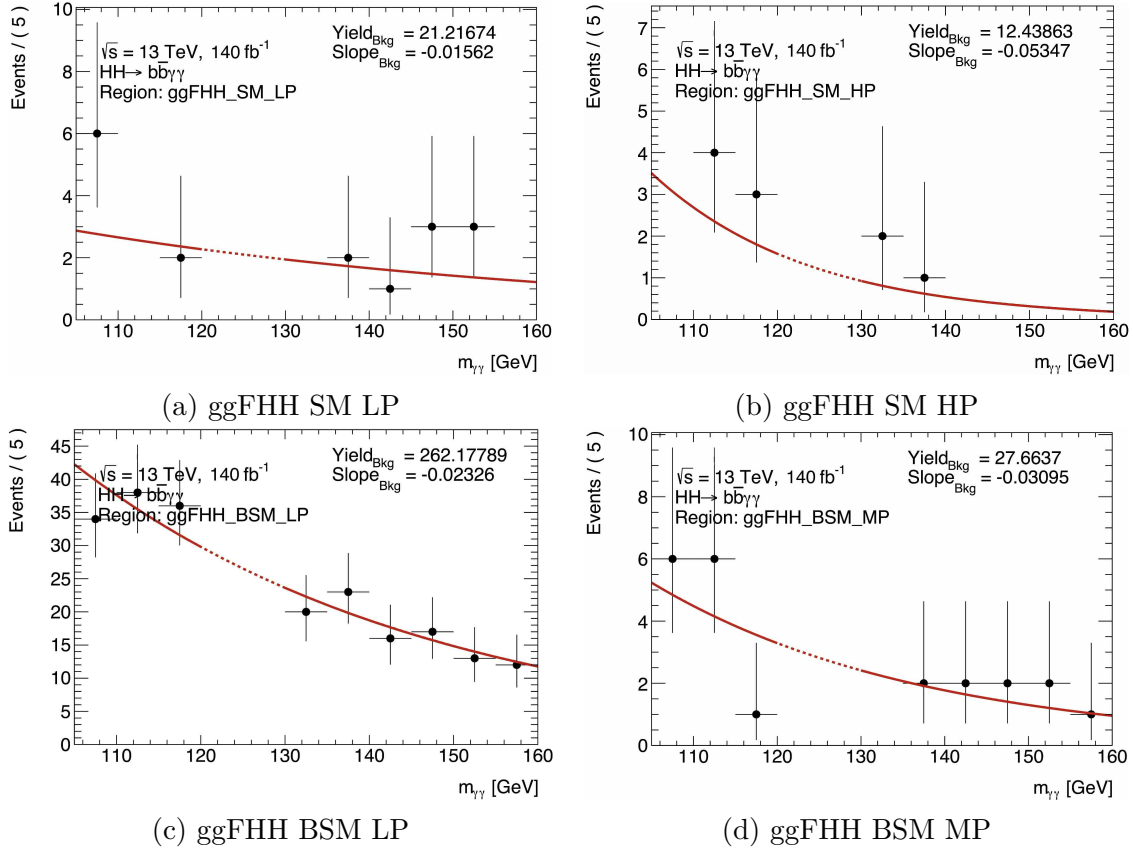


Fig. 5.25 Background modeling of the $m_{\gamma\gamma}$ distribution for four various event categories. The plots depict the data sideband events (black points) fitted with an exponential function (red line) using a data-driven method. Each plot corresponds to a distinct category defined by the event selections. The fit parameters, including the background yield ($\text{Yield}_{\text{bkg}}$) and the slope of the exponential function ($\text{Slope}_{\text{Bkg}}$), are displayed in each plot. The close agreement demonstrates the backgrounds are accurately modeling.

$\pm 1\sigma$ standard deviation error band and the yellow band illustrating the $\pm 2\sigma$ standard deviation error band. The red curve, along with its error bands, depicts the theoretical prediction of the cross-sections. Values of κ_λ and κ_{2V} that lie outside the intersection points between the predictions and the expectations are excluded at a 95% CL. The allowed ranges for κ_λ and κ_{2V} are provided in Table 5.12.

Figure 5.28 shows the expected two-dimensional constraints on κ_λ vs κ_{2V} . The shaded regions indicate the expected limits at $\pm 1\sigma$ (green) and $\pm 2\sigma$ (yellow) standard deviation error bands, while the red dashed line represents the expected 95% CL limit. The black star denotes the SM prediction.

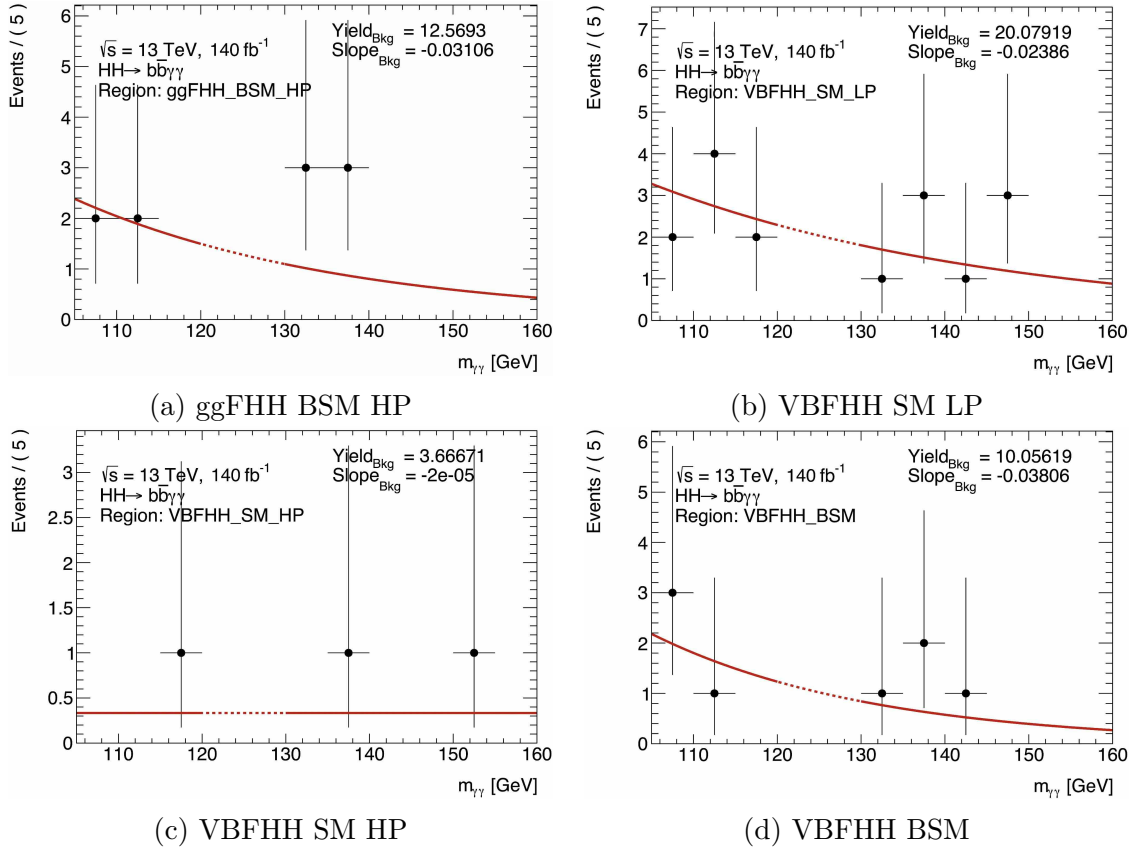


Fig. 5.26 Background modeling of the $m_{\gamma\gamma}$ distribution for four various event categories. The plots depict the data sideband events (black points) fitted with an exponential function (red line) using a data-driven method. Each plot corresponds to a distinct category defined by the event selections. The fit parameters, including the background yield ($Yield_{bkg}$) and the slope of the exponential function ($Slope_{Bkg}$), are displayed in each plot. The close agreement demonstrates the backgrounds are accurately modeling.

5.7 Analysis Strategy Comparison

The section compares the sensitivity of the alternative strategy with that of the official strategy. The primary statistical-only results are summarized in Table 5.20, focusing on the expected upper limits on signal strength (μ_{HH} and μ_{HH}^{VBF}) and the constraints on the coupling modifiers (κ_λ and κ_{2V}). The results for both strategies are quite similar, with relative differences of a few percent observed in the table. Notably, the alternative strategy shows a significant improvement of 20% in the μ_{HH}^{VBF} expected upper limit. These can be explained by the inclusion of additional discriminating variables in the training features.

Significant differences exist in the design of each strategy. The alternative strategy employs a dedicated multi-classifier to identify distinct production modes for both SM and BSM of ggFHH and VBFHH, while the baseline analysis strategy uses the variable $m_{b\bar{b}\gamma\gamma}^*$ with a threshold of 350 GeV to separate events into low and high mass regions that probe BSM or SM-like

Signal Strength or Cross-Sections	Expected Upper Limits with Error Bands				
	-2σ	-1σ	Median	$+1\sigma$	$+2\sigma$
μ_{HH} (ggFHH + VBFHH)	2.69	3.60	5.00	7.34	10.78
Expected σ_{HH} [fb]	88.18	118.01	163.90	240.61	353.37
μ_{HH}^{VBF} (only VBFHH)	57.07	76.61	106.39	158.50	241.81
Expected σ_{HH}^{VBF} [fb]	98.50	132.23	183.63	273.57	417.36

Tab. 5.18 Expected upper limits at 95% CL on the signal strength μ_{HH} for SM ggFHH + VBFHH and μ_{HH}^{VBF} for only VBFHH, from the alternative analysis. The expected cross-sections are given by the signal strength multiplied by the SM prediction (32.78 fb for HH and 1.726 fb for VBFHH). Their corresponding $\pm 1\sigma$ and $\pm 2\sigma$ error bands are also listed.

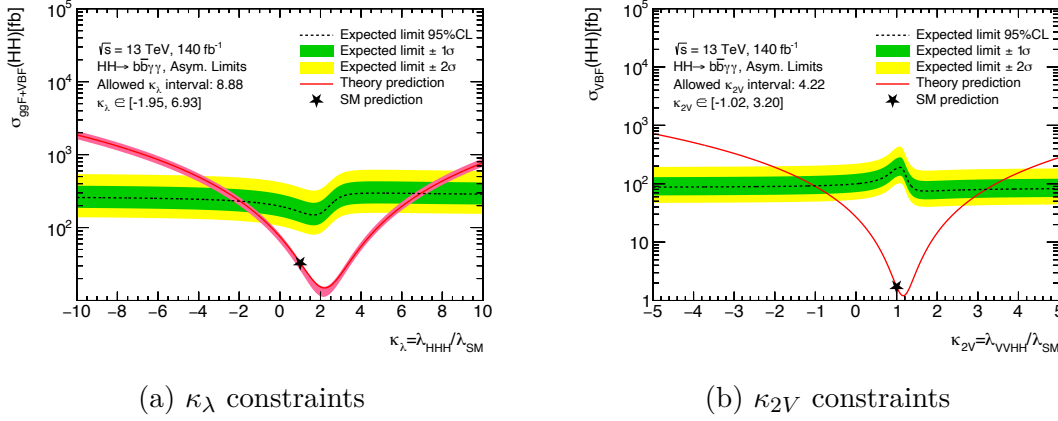


Fig. 5.27 Constraints on κ_λ (a) and κ_{2V} (b) from the expected upper limits of the HH and VBFHH cross-section at 95% CL, from the alternative analysis. The coupling modifier κ_λ is constrained by the cross-section of ggFHH + VBFHH, while κ_{2V} is constrained by that of VBFHH. The dashed curve indicates the expected upper limit, with the green band representing the $\pm 1\sigma$ error band and the yellow band representing the $\pm 2\sigma$ error band. The solid curve and the surrounding red band represent the predicted cross-sections and their associated uncertainties for κ_λ . Theoretical error bands for κ_{2V} are not displayed, as the scale uncertainties (0.05%) are minimal [36]. The allowed intervals are derived from the crossing points between the expected limits and the theoretical ones. Only statistical uncertainties are considered.

events, respectively. Additional discriminating variables for VBFHH, as shown in Figure 5.14, are added into the training features for the alternative analysis. These enhancements improve the identification of VBFHH, affecting the signal strength μ_{HH}^{VBF} . Furthermore, a dedicated category for κ_{2V} is introduced to enhance the sensitivity of the VBFHH signal, resulting in a 2.54% improvement in κ_{2V} . While the official results of the published analysis are based on the

Coupling Modifiers	Allowed range	Size of allowed range
κ_λ	[-1.95, 6.93]	8.88
κ_{2V}	[-1.02, 3.20]	4.22

Tab. 5.19 Allowed ranges of κ_λ and κ_{2V} from the expected 95% CL upper limits on the HH and VBFHH cross-sections, from the alternative analysis. Only statistical uncertainties are considered.

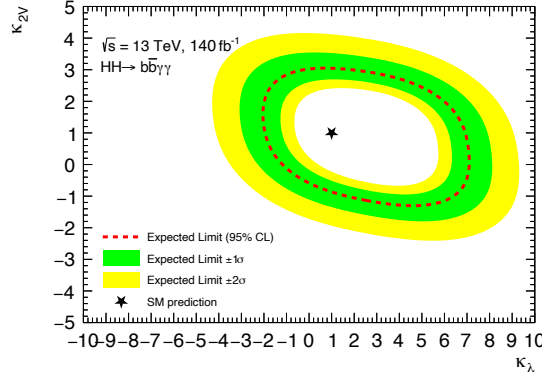


Fig. 5.28 Expected limits at 95% CL on the HH production cross-section as a function of κ_λ and κ_{2V} . The plot shows the expected limits with $\pm 1\sigma$ (green) and $\pm 2\sigma$ (yellow) uncertainty bands. The red dashed contour represents the expected 95% CL limit. The black star denotes the SM prediction.

baseline approach, this alternative analysis strategy introduces promising improvements for a future, more sensitive analysis.

5.8 Nominal Background Model and Spurious Signal

The continuum backgrounds are modeled in the likelihood function using a specific analytic function. The complexity of the function will directly impact the presence of signal. Too many parameters will lead to overfitting to submerge the signal, while less parameters will result in underfitting and mimic a fake signal. A study is thus performed to find the model with the minimum number of parameters that yields a reasonably small potential bias (called “spurious signal” in the following) on the fitted signal yield.

The study is based on fits to the diphoton invariant mass distributions of large background-only samples using the combined signal+background model in the range [105, 160] GeV. The signal PDF used in the fit is the nominal DSCB model with fixed parameters determined from fits to simulated signal events, while the background function is any function to be evaluated, with floating parameters. Multiple fits are performed where the position of the signal peak is varied in each fit by increments of 0.5 GeV, corresponding to Higgs boson masses ranging from 123 GeV to 127 GeV, to avoid that statistical fluctuations in the sample in the signal region lead to accidental underestimation of the bias if only one specific value of the Higgs boson mass is

POIs	Strategy	Expected Upper Limits [95% C.L.]	
μ_{HH} (ggFHH + VBFHH)	Official	4.95	
	Alternative	5.00	
	Rel. Diff.	1.01%	
		Allowed Constraints	Length
κ_λ	Official	[-2.02, 7.13]	9.15
	Alternative	[-1.95, 6.93]	8.88
	Rel. Diff.	-2.95%	
		Expected Upper Limits [95% C.L.]	
μ_{HH}^{VBF} (only VBFHH)	Official	132.27	
	Alternative	106.39	
	Rel. Diff.	-19.57%	
		Allowed Constraints	Length
κ_{2V}	Official	[-1.06, 3.27]	4.33
	Alternative	[-1.02, 3.20]	4.22
	Rel. Diff.	-2.54%	

Tab. 5.20 Relative differences of the expected upper limits and the allowed intervals of κ_λ and κ_{2V} from the two strategies. Only uncertainties of statistical origin are included in the results.

considered. The maximum number of the fitted signal yield in these fits is taken as the expected spurious signal (N^{SS}). For a function to be considered a potential background model, the spurious signal is required to be less than 20% of the statistical uncertainty (σ_{bkg}) from the data sideband region, denoted as $|\max(N^{SS}/\sigma_{bkg})| < 0.2$. To deal with the small number of events in the background-only samples leading to statistical fluctuations being fitted as (spurious) signals, a looser criteria (ζ^{SS}) considering the statistical uncertainty on the SS ($\pm 2\Delta_{MC}$) is used:

$$\zeta^{SS} = \begin{cases} N^{SS} + 2\Delta_{MC}, & N^{SS} < -2\Delta_{MC} \\ 0, & -2\Delta_{MC} \leq N^{SS} \leq 2\Delta_{MC} \\ N^{SS} - 2\Delta_{MC}, & N^{SS} > 2\Delta_{MC}, \end{cases} \quad (5.25)$$

where ζ^{SS} still keeps the same criterion as N^{SS} .

To evaluate the spurious signal, the large simulated event sample of $\gamma\gamma$ + HF events is used. This samples is normalized to the data sideband events to account for the γjet and $jetjet$ components. It has been checked with the simulated inclusive $\gamma\gamma$ +jet sample that the background model and spurious signal are not affected significantly by the inclusion or exclusion of quark flavours other than b . The spurious signal results with $\gamma\gamma$ + HF are presented in Table 5.21. Both the exponential function ($Ne^{\alpha m_{\gamma\gamma}}$) and the power function ($Nm_{\gamma\gamma}^\alpha$) are analyzed for the spurious signal. The spurious signal yield, N^{SS} and the relative difference ($\max(N^{SS}/\sigma_{bkg})$) to the background uncertainty are displayed. The results for the $\max(\zeta^{SS})$ are less than 20%. The χ^2 probability is checked using the background-only fit with MC statistic uncertainties. Ultimately, the exponential function, which has the fewest parameters and the lowest spurious

signal events, is chosen as the background function. The spurious signal yield, N^{SS} , is then incorporated into the statistical model, as shown in Equation 5.11.

Category	Function	N^{SS}	$\max\left(N^{SS}/\sigma_{bkg}\right) [\%]$	$\max\left(\zeta^{SS}\right) [\%]$	Prob (χ^2) [%]
High Mass 1	Exponential	-0.143	-5.21	0	49.9
	Power	0.154	5.75	0	58.7
High Mass 2	Exponential	-0.17	-11.7	0	27.9
	Power	-0.122	-8.38	0	25.8
High Mass 3	Exponential	0.0513	3.89	0	11.5
	Power	0.0823	6.26	0	6.36
Low Mass 1	Exponential	-0.991	-19.8	0	30.8
	Power	0.643	13.3	0	31.4
Low Mass 2	Exponential	-0.327	-12.6	0	2.04
	Power	-0.137	-5.27	0	5.6
Low Mass 3	Exponential	0.0881	5.17	0	84.2
	Power	0.173	10.1	0	70.8
Low Mass 4	Exponential	0.0676	6.68	0	0.573
	Power	0.104	10.2	0	0.24

Tab. 5.21 Results of the spurious signal test across various categories for both high mass and low mass regions using exponential and power functions. The table presents the values of the spurious signal strength (N^{SS}), the maximum spurious signal significance ($\frac{N^{SS}}{\sigma_{bkg}}$), the maximum spurious signal fraction (ζ^{SS}), and the chi-squared probability (Prob(χ^2)). The test evaluates the impact of different background modeling functions on the fitted signal yield in the absence of a true signal.

5.9 Systematic Uncertainties

Uncertainties in the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis originate from statistical and systematic effects. While statistical uncertainties are predominant, systematic uncertainties also play a non negligible role and their incorporation as nuisance parameters in the likelihood function is essential for a proper interpretation of the data. These systematic uncertainties are classified into two categories: experimental and theoretical uncertainties. They mainly affect the expected signal yields or the $m_{\gamma\gamma}$ shape. Thorough evaluation of each systematic uncertainty is vital to ensure the robustness and reliability of the analysis. The only uncertainty associated with the irreducible background is the spurious signal, which impacts the yields, as discussed in the previous Section 5.8. This section provides an in-depth examination of the other sources of systematic uncertainties.

5.9.1 Experimental Uncertainties

Quantities that are determined experimentally with limited precision, such as photon and jet selection efficiency and calibration, can influence the expected yields of HH and single Higgs processes, as well as their $m_{\gamma\gamma}$ shape. In the simulation, these quantities – or the independent sources of uncertainties in them – can be varied independently by $\pm 1\sigma$, where σ is the experimental uncertainty from auxiliary measurements of those quantities. The relative modifications of yields and shape parameters for the HH signal and single-Higgs background that are induced by these variations are incorporated in the likelihood functions as pre-fit uncertainties associated to the corresponding nuisance parameters.

5.9.1.1 Uncertainties in the Yields

Experimental sources of uncertainty impacting the HH and single-Higgs boson yields are summarized in Table 5.22. They arise mainly from photon and jet reconstruction performance, with lesser impact from the E_T^{miss} reconstruction and impact of pile-up. Simulation samples with variations of these quantities by $\pm 1\sigma$ are used to calculate a corresponding uncertainty in the expected yields, defined as the relative difference $\delta N(\pm 1\sigma)$ of the yields between the nominal sample $N(\text{nom})$ and the alternative samples $N(\pm 1\sigma)$ in Equation 5.26.

Objects	Sources
Photons	diphoton trigger efficiency
	identification, isolation efficiency
	photon energy scale and resolution
Jets	jet energy scale (JES) and resolution (JER)
	jet vertex tagger efficiency
	flavour tagging efficiency
Others	E_T^{miss} soft term scale and resolution
	pile-up modeling

Tab. 5.22 Sources of systematic uncertainties affecting the yields.

$$\delta N(\pm 1\sigma) = \frac{N(\pm 1\sigma)}{N(\text{nom})} - 1 \quad (5.26)$$

The statistical uncertainty in δN is evaluated using the bootstrap method [155, 156]. The generated samples are replicated three thousand times for each event in the variation samples. An additional weight following a Poisson distribution with a mean value of unity is applied to each replica. These replicas are used to derive the category yields with $\pm 1\sigma$ variations. The mean and standard deviation of the replicas are considered as the central value and the statistical errors, respectively. The bootstrap method effectively handles potential correlations between the nominal events and variation events in the calculation of systematic uncertainties.

Several distinct correlation schemes in Table 5.23 are implemented to reduce the number of independent NPs in the statistical model. Pruning procedures are employed to retain in the likelihood function only systematic uncertainties that are non-negligible compared to statistical

uncertainties. The pruning process considers three scenarios: identifying and discarding systematic uncertainties where $\delta N(\pm 1\sigma) < 0.1\%$, eliminating systematic uncertainties if the relative effect of the statistical errors exceeds 100%, and retaining systematic uncertainties with the same signs for both up and down variations, symmetrizing them by the largest absolute value.

Sources of Uncertainty	Scheme Methods
Jet Energy Scale	CategoryReduction
Jet Energy Resolution	FullJER
Flavour Tagging	SFs Eigen, Medium Reduction Schemes, PCBT for the SFs
Photons	1 NP

Tab. 5.23 Schemes for different sources of systematic uncertainties.

The systematic uncertainties pertaining to JER require meticulous handling in simulations. When the JER in MC simulations is superior to that observed in experimental data, no smearing is applied to the MC jets. Conversely, if the JER in data surpasses that in MC, a Gaussian smearing is implemented to reconcile the MC with the data. This adjustment is executed bi-directionally for each source of systematic uncertainties: initially, to account for scenarios where the JER in MC exceeds that in data (MC smearing), and subsequently, for instances where the JER in MC is suboptimal compared to data (pseudo-data, PD smear). The resulting JER uncertainty encapsulates both the MC-smear and PD-smear components, preserving their anti-correlated nature. The final uncertainty incorporated into the statistical model is computed from the difference between the propagated $\pm 1\sigma$ variations of the MC-smear and PD-smear components. The total statistical uncertainty is ascertained by summing in quadrature these two components, thereby ensuring an exhaustive representation of the systematic uncertainties in JER.

The systematic uncertainties in the yields from the envelopes of various signal samples for ggFHH and VBFHH are displayed in Figure 5.29 (a) and (b). The results for significant single-Higgs boson background processes (ggH, ggZH, ZH, ttH) are also illustrated in Figure 5.30. The up and down variation in the most sensitive category are exhibited, with the statistical errors depicted as shaded bands in the figures.

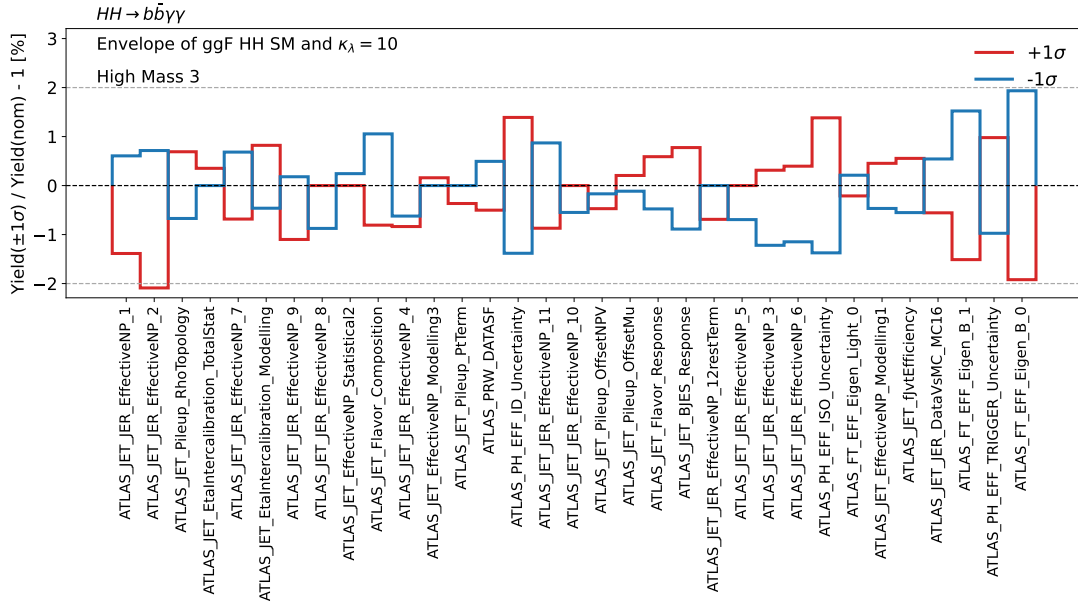
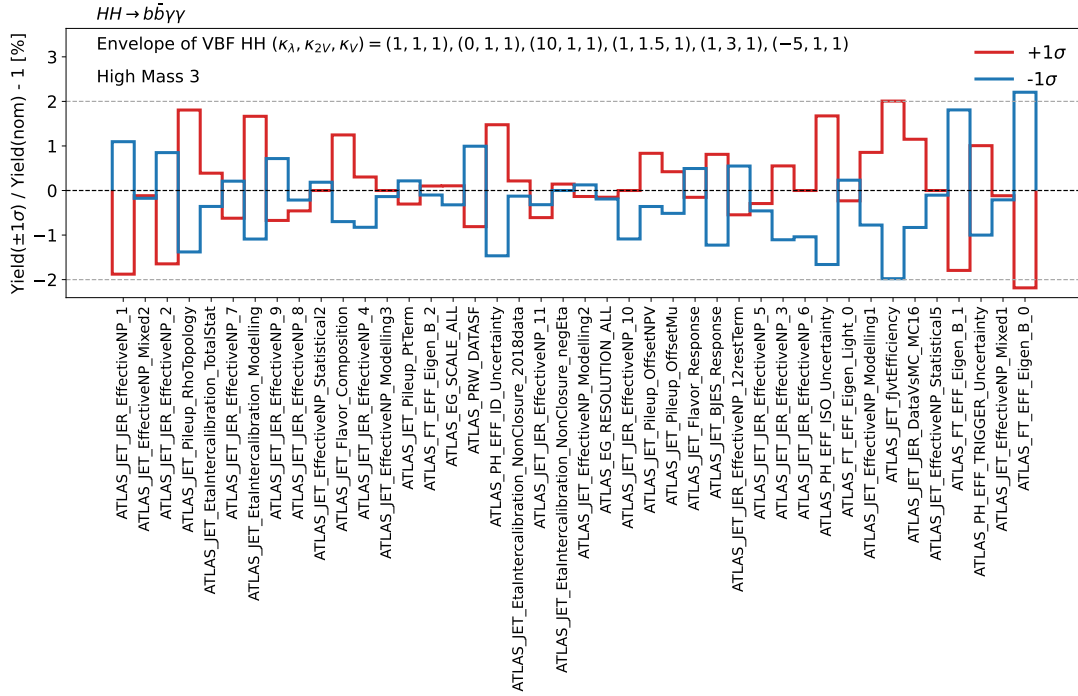
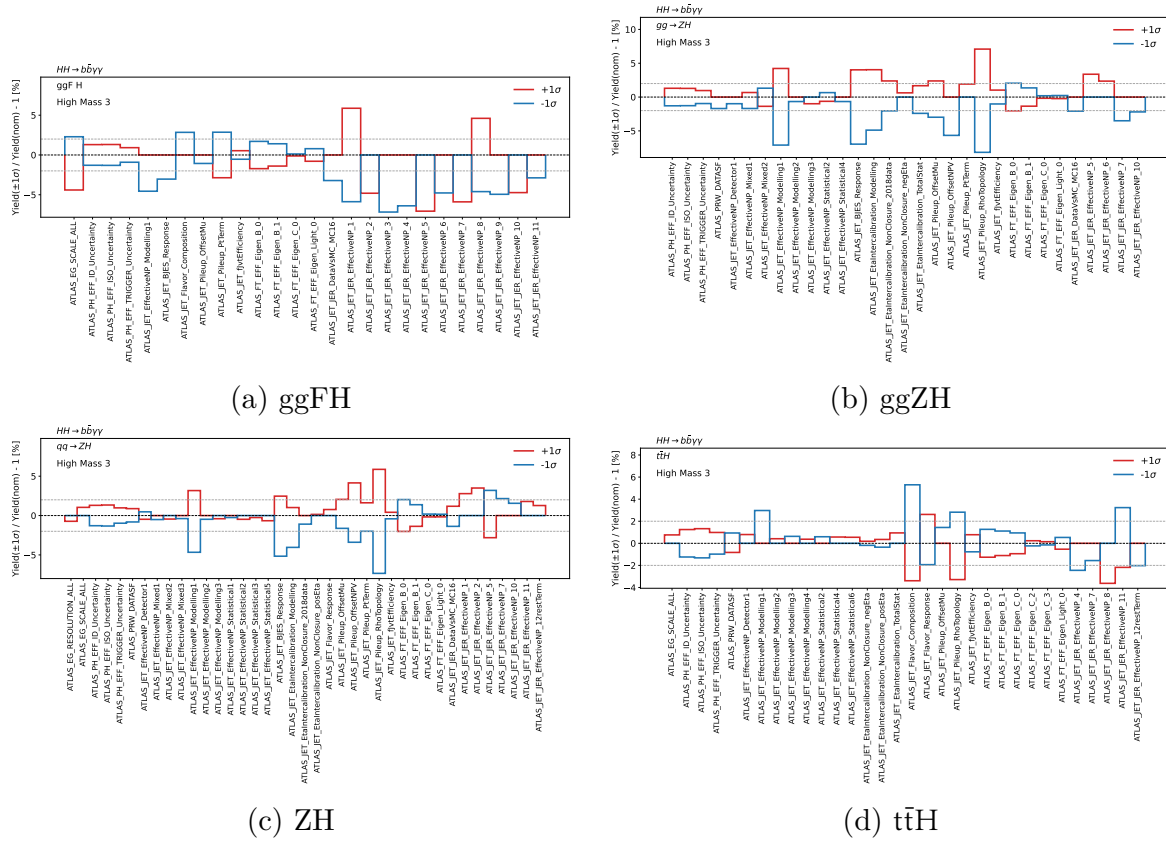
(a) Envelope of ggFHH SM and $\kappa_\lambda = 10$ (b) Envelope of VBFHH with various $(\kappa_\lambda, \kappa_{2V}, \kappa_V)$

Fig. 5.29 Expected experimental systematic uncertainties in the yields in the most sensitive category, for $\pm 1\sigma$ variations of the uncertainty sources. Only the significant sources of uncertainties are listed. The statistical errors are reported as the shaded bands. The uncertainties of ggFHH (a) and VBFHH (b) are enveloped using various signal samples with different values of the coupling modifiers.

**Fig. 5.30**

Expected experimental systematic uncertainties in the yields in the in the most sensitive category, for $\pm 1\sigma$ variations of the uncertainty sources. Only the significant sources of uncertainties are listed. The statistical errors are reported as the shaded bands. The yield uncertainties for single Higgs processes ggH (a), ggZH (b), ZH (c), and ttH (d), which constitute the main resonant backgrounds, are also shown.

5.9.1.2 Uncertainties in the Models

The parameters for the diphoton invariant mass models for signal and resonant background that can affect the results most significantly are peak position (μ_{CB}) and width (σ_{CB}) of the DSCB function. Such quantities can be affected by the photon energy scale (PES) and resolution (PER), respectively. Peak position uncertainties are measured by the relative difference in the $\langle m_{\gamma\gamma} \rangle$ mean value between the nominal sample and alternative samples in which the photon energy scale is varied by $\pm 1\sigma$.

$$\delta_{\mu_{CB}}(\pm 1\sigma) = \frac{\langle m_{\gamma\gamma} \rangle (\pm 1\sigma)}{\langle m_{\gamma\gamma} \rangle (\text{nom})} - 1 \quad (5.27)$$

For the peak width, uncertainties are determined by comparing the $m_{\gamma\gamma}$ interquartile range (IQR) of the nominal sample and alternative samples in which the photon energy resolution is varied by $\pm 1\sigma$.

$$\delta_{\sigma_{CB}}(\pm 1\sigma) = \frac{IQR_{m_{\gamma\gamma}}(\pm 1\sigma)}{IQR_{m_{\gamma\gamma}}(\text{nom})} - 1 \quad (5.28)$$

These uncertainties, calculated for all the categories for both signal (ggFHH and VBFHH) and main single-Higgs boson background (ggFH, $t\bar{t}H$, and ZH), are shown in Tables 5.24 and 5.25.

Systematic Uncertainties of PES on $m_{\gamma\gamma}$ peak position [%]							
Production Modes	LM 1	LM 2	LM 3	LM 4	HM 1	HM 2	HM 3
SM ggFHH	+0.45	+0.44	+0.45	+0.43	+0.52	+0.52	+0.53
	-0.45	-0.44	-0.45	-0.45	-0.52	-0.52	-0.53
SM VBFHH	+0.42	+0.44	+0.43	+0.44	+0.55	+0.54	+0.55
	-0.43	-0.44	-0.45	-0.44	-0.55	-0.55	-0.54
ggFH	+0.40	+0.48	+0.47	+0.36	+0.54	+0.52	+0.52
	-0.41	-0.46	-0.38	-0.61	-0.52	-0.56	-0.57
$t\bar{t}H$	+0.44	+0.44	+0.45	+0.44	+0.52	+0.52	+0.52
	-0.44	-0.44	-0.45	-0.45	-0.53	-0.52	-0.53
$qq \rightarrow ZH$	+0.44	+0.44	+0.46	+0.44	+0.55	+0.56	+0.55
	-0.44	-0.44	-0.45	-0.43	-0.55	-0.54	-0.55
$gg \rightarrow ZH$	+0.43	+0.43	+0.45	+0.28	+0.51	+0.51	+0.53
	-0.43	-0.43	-0.35	-0.45	-0.51	-0.51	-0.51

Tab. 5.24 Systematic Uncertainties in $m_{\gamma\gamma}$ peak position derived from $\pm 1\sigma$ variations of photon energy scale for SM ggFHH, SM VBFHH, ggFH, $t\bar{t}H$, and ZH processes.

Systematic Uncertainties of PER on $m_{\gamma\gamma}$ peak width [%]							
Production Modes	LM 1	LM 2	LM 3	LM 4	HM 1	HM 2	HM 3
SM ggFHH	+10.21	+10.09	+13.12	+12.58	+12.72	+14.00	+15.80
	-5.49	-9.03	-9.35	-9.40	-9.60	-10.52	-10.71
SM VBFHH	+9.60	+8.13	+7.71	+9.99	+12.04	+12.80	+14.02
	-7.04	-6.69	-11.69	-7.94	-7.48	-8.57	-9.77
ggFH	+0.00	+0.00	+15.96	+0.00	+18.91	+30.69	+12.32
	-5.42	-9.47	-29.42	-0.00	-10.86	-0.00	-10.80
$t\bar{t}H$	+10.09	+8.80	+12.91	+11.88	+14.42	+14.32	+16.24
	-7.89	-8.85	-5.81	-6.74	-11.84	-12.94	-7.45
$qq \rightarrow ZH$	+9.36	+8.41	+11.11	+6.76	+15.12	+10.56	+14.00
	-8.74	-5.12	-8.03	-7.12	-10.59	-7.86	-11.17
$gg \rightarrow ZH$	+11.86	+12.92	+0.00	+0.00	+14.04	+15.21	+16.80
	-10.40	-11.14	-0.00	-0.00	-9.19	-11.48	-10.83

Tab. 5.25 Systematic Uncertainties on $m_{\gamma\gamma}$ peak width obtained from $\pm 1\sigma$ variations of photon energy resolution for SM ggFHH, SM VBFHH, ggFH, $t\bar{t}H$, and ZH processes.

5.9.2 Theoretical Uncertainties

Two main sources of theoretical uncertainties are considered in the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis: QCD scale and PDF + α_S uncertainties. They have been found to affect primarily the expected

yields of both diHiggs and single Higgs processes. The scale (Scale) uncertainties arises from the choice of the nominal energy scales used in perturbative QCD calculations. The PDF + α_S uncertainties arise from the limited knowledge of the parton distribution functions and the strong coupling constant, α_S . Both uncertainties are evaluated using the envelope method, which involves calculating the relative differences between the expected yields of alternative samples and nominal samples for various values of the coupling modifiers and then taking the maximum difference as the uncertainty. The following section provides a detailed description of these theoretical uncertainties and how they are quantified.

5.9.2.1 QCD Scale Uncertainties

QCD scale uncertainty primarily arises in perturbative QCD calculations due to missing higher-order corrections, impacting the yields of resonant processes. This uncertainty is evaluated by comparing the relative differences in expected yields from various renormalization (μ_R) and factorization (μ_F) scales. Six alternative groups of μ_R and μ_F scales, $(\mu_R, \mu_F) = (0.5, 1.0)$, $(2.0, 1.0)$, $(0.5, 0.5)$, $(1.0, 0.5)$, $(1.0, 2.0)$, and $(2.0, 2.0)$, are applied to calculate the expected yields for each category and process, utilizing dedicated alternative MC weights. The relative differences between the six alternative yields and the nominal yields are computed, and the largest absolute difference is considered the QCD scale uncertainty for the respective category. The QCD scale uncertainties for ggFHH and VBFHH are summarized in Tables 5.26 and 5.27, respectively. Those for the dominant single-Higgs boson processes (ggFH and VBFH) are detailed in Table 5.28.

5.9.2.2 PDF and α_S Uncertainties

The uncertainties from the parton distribution function and the strong coupling constant are also estimated using the alternative weights related to different PDFs and α_S . The simulations of the ggFHH and single-Higgs boson processes rely on the PDF4LHC set, which contains 30 alternative PDFs and 1 nominal PDF. Whereas, the simulation of VBFHH events involves the NNPDF23LO set, including 100 alternative PDFs and 1 nominal PDF. The PDF uncertainty in each category for a certain process is computed by the square sum of the relative differences between the expected yields from the alternative PDFs and the nominal PDF. Additionally, the α_S uncertainty is the half difference ($\frac{\delta_{\text{down}} - \delta_{\text{up}}}{2}$) between two expected yields from two extra alternative weights corresponding to $\pm 1\sigma$ variations of the strong coupling constant. The combined PDF + α_S uncertainty is the sum in quadrature of the above two components. The uncertainties for ggFH and VBFH are presented in Tables 5.26 and 5.27. Those for the dominant single-Higgs boson processes (ggFH and VBFH) are listed in Table 5.28.

5.9.3 Other Uncertainties

An additional source of experimental uncertainty is the uncertainty in the integrated luminosity of the data (0.83% for full Run-2 data [69]), which affect the yields of all processes in the same way.

Theoretically, Scale and PDF + α_S uncertainties can also impact the cross-section and the branching ratios of the Higgs boson, as reported in Table 5.29. This overall rescaling of the yields is factorized from the impact of these sources of uncertainties on the fraction of HH and single- H events that populate each category, quantified in the previous section. The Scale uncertainty

ggFHH QCD Scale and PDF + α_S Uncertainties [%]								
Production Modes	Sources	HM 1	HM 2	HM 3	LM 1	LM 2	LM 3	LM 4
SM: $\kappa_\lambda = 1$	QCD Scale	0.370	0.527	1.325	2.658	2.449	2.684	3.023
	PDF + α_S	0.509	0.471	0.449	1.318	1.308	1.347	1.395
$\kappa_\lambda = 10$	QCD Scale	1.39	1.11	1.21	0.94	0.87	0.87	0.32
	PDF + α_S	0.27	0.30	0.40	0.42	0.41	0.44	0.42
Envelope	QCD Scale	1.39	1.11	1.325	2.658	2.449	2.684	3.023
	PDF + α_S	0.509	0.471	0.449	1.318	1.308	1.347	1.395

Tab. 5.26 QCD Scale and PDF + α_S uncertainties [%] on the yields using the envelope method for ggFHH SM and $\kappa_\lambda = 10$.

VBFHH QCD Scale and PDF + α_S Uncertainties [%]								
Production Modes	Sources	HM 1	HM 2	HM 3	LM 1	LM 2	LM 3	LM 4
SM: $\kappa_\lambda = 1, \kappa_{2V} = 1, \kappa_V = 1$	QCD Scale	0.992	0.690	1.567	5.125	4.675	3.989	1.534
	PDF + α_S	2.430	3.668	3.612	6.776	10.277	6.213	2.203
$\kappa_\lambda = 0, \kappa_{2V} = 1, \kappa_V = 1$	QCD Scale	0.365	0.058	2.042	4.089	3.365	2.980	0.819
	PDF + α_S	7.686	5.439	4.457	5.325	5.390	4.444	2.831
$\kappa_\lambda = 10, \kappa_{2V} = 1, \kappa_V = 1$	QCD Scale	0.318	0.705	2.727	2.862	2.875	2.561	0.202
	PDF + α_S	4.925	6.700	5.003	4.835	7.324	5.474	10.143
$\kappa_\lambda = 1, \kappa_{2V} = 1.5, \kappa_V = 1$	QCD Scale	3.414	2.657	0.614	7.951	7.899	7.770	4.491
	PDF + α_S	7.056	12.697	2.516	12.138	11.662	9.583	7.119
$\kappa_\lambda = 1, \kappa_{2V} = 3, \kappa_V = 1$	QCD Scale	3.161	2.567	0.578	7.349	7.095	7.094	4.218
	PDF + α_S	5.583	5.586	2.179	15.849	9.901	12.804	7.131
$\kappa_\lambda = 5, \kappa_{2V} = 1, \kappa_V = 1$	QCD Scale	1.008	0.643	2.299	7.720	7.453	7.547	4.908
	PDF + α_S	6.851	8.819	3.725	10.824	11.489	11.611	7.382
Envelope	QCD Scale	3.414	2.657	2.727	7.951	7.899	7.770	4.908
	PDF + α_S	7.686	12.697	5.003	15.849	11.662	12.804	10.143

Tab. 5.27 QCD Scale and PDF + α_S uncertainties [%] on the yields using the envelope method for VBFHH and various $(\kappa_\lambda, \kappa_{2V}, \kappa_V)$.

ggFH and VBFH QCD Scale and PDF + α_S Uncertainties [%]								
Production Modes	Sources	HM 1	HM 2	HM 3	LM 1	LM 2	LM 3	LM 4
ggFH	QCD Scale	8.892	8.780	8.963	4.975	4.625	6.368	7.476
	PDF + α_S	2.026	2.116	2.106	1.613	1.907	1.823	1.846
VBFH	QCD Scale	1.560	2.562	2.336	3.117	3.878	4.714	2.772
	PDF + α_S	3.608	4.575	3.729	3.025	3.778	3.675	4.072

Tab. 5.28 QCD Scale and PDF + α_S uncertainties on the yields for ggFH and VBFH production modes.

for ggFHH includes the contribution of the m_{top} uncertainty. The uncertainty on $\text{Br}(H \rightarrow \gamma\gamma)$ is applied to both HH and single- H processes, whereas the uncertainty from $\text{Br}(H \rightarrow b\bar{b})$ is considered only for ggFHH and VBFHH.

Uncertainties can also arise from different parton shower models, estimated by comparing the nominal yields with those from alternative MC samples generated using various parton shower models. The nominal MC samples for HH signal and single- H background are produced using

Uncertainty	σ_{ggFHH}	σ_{VBFHH}	σ_{ggFH}	σ_{VBFH}	σ_{WmH}	σ_{WpH}	$\sigma_{\text{q}\bar{\text{q}}\text{ZH}}$	σ_{ggZH}	$\sigma_{\text{t}\bar{\text{t}}\text{H}}$
Scale	+6% -23% (m_{top} included)	+0.03% -0.04%	+4.56% -6.72%	+0.4% -0.3%	+0.4% -0.6%	+0.5% -0.7%	+0.5% -0.6%	+25.1% -18.9%	+5.8% -9.2%
PDF + α_S	$\pm 3.0\%$	$\pm 2.1\%$	$\pm 3.2\%$	$\pm 2.1\%$	$\pm 2.0\%$	$\pm 1.8\%$	$\pm 1.9\%$	$\pm 2.4\%$	$\pm 3.6\%$

Branch Ratios	$Br(H \rightarrow \gamma\gamma)$	$Br(H \rightarrow b\bar{b})$
Uncertainty	+2.90% -2.84%	+1.70% -1.73%

Tab. 5.29 Scale and PDF + α_S uncertainties on the cross-section of double Higgs signal and dominant single Higgs backgrounds and the branching ratios uncertainties in the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis. The up and down values are included in the table. Credits: [LHC Higgs WG4 Group](#) and [CERN Yellow Report Page](#)

the PYTHIA 8 parton shower, while the alternative samples use the HERWIG 7 parton shower. Table 5.30 summarizes these uncertainties, covering typical ggFHH and VBFHH processes, as well as the main single Higgs processes in the $HH \rightarrow b\bar{b}\gamma\gamma$ analysis. The table includes only the significant uncertainties that are incorporated into the statistical model.

Systematic Uncertainties from Parton Shower on Yields [%]							
Production Modes	HM 1	HM 2	HM 3	LM 1	LM 2	LM 3	LM 4
SM ggFHH $\kappa_\lambda = 1$	2.119	-	-4.454	6.845	-	-	-
ggFHH $\kappa_\lambda = 10$	-	-	-8.260	-	-	-4.743	-7.973
SM VBFHH $\kappa_\lambda = 1$	-	-	-9.943	-	-	-	-
VBFHH $\kappa_\lambda = 10, \kappa_{2V} = 1, \kappa_V = 1$	-10.131	-	-5.940	-	-	-	-10.652
VBFHH $\kappa_\lambda = 1, \kappa_{2V} = 0, \kappa_V = 1$	7.269	-	-6.232	-	-	-15.516	-6.591
$qq \rightarrow ZH$	-	-	-	-	12.816	37.705	31.423
$t\bar{t}H$	-3.217	-	-	-2.690	-6.757	-	-

Tab. 5.30 Parton shower uncertainties on the yields for HH and single-Higgs boson production. "-" denotes contributions that are not significant and therefore ignored.

In the statistical model, the yield of each production mode at any set of $(\kappa_\lambda, \kappa_{2V}, \kappa_V)$ values is parameterized. The parameterization for ggFHH and VBFHH can introduce uncertainties in the yields. The κ_λ -reweighting method in Section 5.2.2.2 is used to evaluate the expected yield for ggFHH, while the linear combination method in Section 5.2.3.2 is applied to VBFHH. The uncertainties in ggFHH parameterization are determined by maximizing the relative differences between the yields of the generated samples and the parameterized samples obtained from the κ_λ -reweighting method. The parameterization uncertainties in VBFHH are derived from the relative difference between the expected yields from the linear combination method and the generated samples. If the statistical errors of these relative differences are smaller than the relative differences themselves, these uncertainties are considered as systematic uncertainties in the statistical model. All significant parameterization uncertainties are summarized in Table 5.31. These uncertainties are regarded as constant across all values of $(\kappa_\lambda, \kappa_{2V}, \kappa_V)$.

5.9.4 Implementation of Systematic Uncertainties in the Statistical Model

Systematic uncertainties on the observables are incorporated in the statistical model to constrain the couplings as NPs. Some unconstrained NPs are determined only from the data, while

Systematic Uncertainties from Parameterization on Yields [%]							
Production Modes	HM 1	HM 2	HM 3	LM 1	LM 2	LM 3	LM 4
ggFHH (κ_λ -reweighting)	-	-	4.284	-5.798	-7.545	7.716	-10.747
VBFHH (Linear Combination)	-7.437	14.010	15.230	19.395	-	22.941	-7.304

Tab. 5.31 Parameterization uncertainties on the yields for ggFHH and VBFHH. "-" indicates negligible contributions due to their lack of significance.

for other NPs the likelihood function includes a PDF that corresponds to auxiliary measurements of that quantity. Asymmetric uncertainties are considered when positive and negative variations are not equal. This scenario commonly arises when systematic effects impact the parameter in a non-symmetric manner. Examples include experimental systematic uncertainties, such as energy scale uncertainties that exert different influences above and below the nominal value, and theoretical uncertainties where model predictions exhibit asymmetric errors.

Most of the systematic uncertainties are treated using a Log-Normal PDF. In the case of uncertainties affecting the yields, the constraint is of the form:

$$N_c(\theta) = N_c^0 \cdot e^{[\log(1+\sigma)] \cdot \theta}, \quad (5.29)$$

where N_c^0 represents the nominal event yield and σ symbolizes the systematic uncertainty value. The value $\theta = 0$ indicates no shift due to the uncertainty. The values $\theta = \pm 1$ denote positive and negative shifts from the systematic uncertainty. Asymmetric systematic uncertainties ($\sigma_+ \neq \sigma_-$) are managed using the FlexibleInterpVar class from the HistFactory package [144]. The PDF can only take positive values and is suitable for uncertainties that affect the scale of the parameter rather than its central value. For instance, uncertainties from luminosity, cross-section and acceptance efficiency are constrained using the Log-Normal PDF. In cases where multiple uncertainties affect the same observable, several log-normal PDFs are multiplied together.

A Gaussian PDF is utilized when the uncertainties are symmetric and align closely with a normal distribution. This method, however, proves inadequate for uncertainties affecting quantities constrained to positive values. For a Gaussian PDF the constraint takes the form:

$$N_c(\theta) = N_c^0 \cdot (1 + \sigma \cdot \theta) \quad (5.30)$$

The Gaussian PDF is employed for instance to model the spurious signal uncertainty.

5.10 Results and Conclusions

After obtaining the expected yields, signal and background models, and pre-fit systematic uncertainties, the workspace incorporates them into a statistical model (likelihood functions) that can be constructed. Section 5.5 and Section 5.6 both present the blinded results for the event categorization strategy and the model for the multiple classification respectively. The section describes the unblinded results of the baseline analysis, including both statistical and systematic uncertainties.

5.10.1 Unblinded Results

The fits to the diphoton invariant mass distributions in the seven categories in data are shown in Figure 5.31. Both background-only and signal+background fits are performed. No significant excess is observed in the data under the background-only expectation. The best-fit value of the signal strength obtained from the signal plus background fit is $\hat{\mu}_{\text{HH}} = -1.72_{-0.00}^{+1.97}$. The negative $\hat{\mu}_{\text{HH}}$ is mainly due to a deficit of event around the $m_{\gamma\gamma}$ peak in Figure 5.31 (g), which represents that the number of observed events in the signal region is less than the number of expected events from the signal plus background. Considering the unconstrained μ_{HH} and constrained NPs, the signal strength might be negative to avoid the worse pulled NPs.

Upper limits on the signal strength and cross-section are evaluated at 95% CL from the Asimov dataset generated under the background-only hypothesis ($\mu_{\text{HH}} = 0$). The observed (expected) upper limits of μ_{HH} are 4.0 (5.0) times the SM predictions, encompassing both ggFHH and VBFHH production modes. For $\mu_{\text{HH}}^{\text{VBF}}$, the upper limits are 100 (131) times the SM predictions. The corresponding cross-sections are summarized in Table 5.32.

Upper Limits of μ , σ and Constraints of κ_λ , κ_{2V}						
Types	μ_{HH}	σ_{HH} [fb]	$\mu_{\text{HH}}^{\text{VBF}}$	σ_{VBF} [fb]	κ_λ	κ_{2V}
Expected	5.03	164.88	131.17	226.40	[-2.04, 7.25]	[-1.10, 3.30]
Observed	3.96	129.81	99.81	172.27	[-1.52, 6.93]	[-0.66, 2.86]

Tab. 5.32 Expected and observed values of the upper limits on the signal strength (μ_{HH} , $\mu_{\text{HH}}^{\text{VBF}}$) and cross-sections (σ_{HH} , σ_{VBF}). The κ_λ and κ_{2V} are constrained from the upper limits and the allowed ranges are given in brackets. Note that for $\mu_{\text{HH}}^{\text{VBF}}$, only VBFHH is considered and SM ggFHH is not treated as a background. Full systematic uncertainties are taken into account.

The coupling modifiers (κ_λ and κ_{2V}) are constrained by combining the observed (expected) cross-section limits and the theoretical cross-section predictions. The upper limits scan of κ_λ and κ_{2V} are shown in Figure 5.32 (a) and (b), where all the other coupling modifiers are fixed to SM predictions. The crossing-points between the observed (expected) limits and the theoretical ones yield the allowed ranges of $\kappa_\lambda \in [-1.52, 6.93](-2.04, 7.25)$ and $\kappa_{2V} \in [-0.66, 2.86](-1.10, 3.30)$.

Another statistical interpretation of the data to constrain κ_λ and κ_{2V} is based on the profiled log-likelihood scan of $-2\ln(\Lambda(\mu, \theta))$ where the profile likelihood is expressed as a function of the coupling strength modifiers, as shown in Figure 5.33. The observed and expected best-fit values of κ_λ and κ_{2V} are obtained from minimizing the negative log-likelihood. The constraints at 68% and 95% confidence intervals are derived, where all other coupling modifiers are fixed to SM predictions and the NPs are floated. All the results are summarized in Table 5.33.

5.10.2 Constrains on κ_{2V} and κ_V

Apart from the constraints on κ_λ and κ_{2V} , the VBFHH mode can provide some sensitivity to κ_V . To better evaluate the impact on κ_V , single-Higgs boson processes, including production and decay modes, are incorporated into the statistical model through the NLO EW corrections

Best Fit Values with $\pm 1\sigma$ Errors or Constraints of POIs from Likelihood							
Types	Best-Fit Values $^{+1\sigma}_{-1\sigma}$			Constraints			
	$\hat{\mu}_{HH}$	κ_λ	κ_{2V}	κ_λ [68%]	κ_λ [95%]	κ_{2V} [68%]	κ_{2V} [95%]
Expected	$1.00^{+2.44}_{-1.66}$	$1.00^{+5.10}_{-2.20}$	$1.00^{+1.53}_{-1.33}$	[-1.19, 6.08]	[-2.84, 7.82]	[-0.32, 2.52]	[-1.11, 3.31]
Observed	$-1.72^{+1.97}_{-0.00}$	$3.02^{+2.21}_{-2.49}$	$1.10^{+0.83}_{-0.83}$	[0.55, 5.23]	[-1.44, 6.92]	[-0.28, 1.92]	[-0.48, 2.68]

Tab. 5.33 Observed and expected results of best-fit with $\pm 1\sigma$ errors for the signal strength and the coupling modifiers. The constraints of κ_λ and κ_{2V} at 68% and 95% CL are shown in brackets.

described in Section 1.2.3. Through impacting the yields of single Higgs boson production and the branch ratios of Higgs decaying to diphoton, the coupling modifier κ_V is implemented in the model. The likelihood scan for κ_V is depicted in Figure 5.34(a). The observed constraints on κ_V range from [-1.38, 1.49] using only HH data, and from [-0.65, 1.20] when both HH and single-Higgs boson data are included, at 95% CL. It is evident that single-Higgs boson measurements play a dominant role in constraining κ_V .

2D constraints on κ_{2V} and κ_V are derived from profiled likelihood scan, as shown in Figure 5.34(b-e). Figures (b) and (c) illustrate respectively the observed and expected likelihood scans using only searches for Higgs boson pairs, where the observed best-fit values are $\kappa_{2V} = 0$ and $\kappa_V = 0$ due to the lack of sensitivity when not incorporating single-Higgs data in the interpretation. Higgs-boson pair data provides more sensitivity to κ_{2V} than to κ_V , resulting in a narrower shape along κ_{2V} . Figures (d) and (e) present the observed and expected results from a joint interpretation of both HH searches and single-Higgs boson measurements, where the observed best-fit values are $\kappa_{2V} = -0.26$ and $\kappa_V = 0.21$. Including single Higgs data results in a more stringent constraint on κ_V compared to using HH data alone. While the measurement of κ_{2V} from searches for Higgs boson pairs is less sensitive than the measurement of κ_V from single Higgs, the combined data provide a more comprehensive constraint profile.

5.10.3 Impact of Systematic Uncertainties

The impact of the systematic uncertainties introduced in Section 5.9 on the expected upper limits μ_{HH} is evaluated and presented in Table 5.34. The three dominant systematic sources are the renormalization and factorization scales, photon energy resolution, and the branching ratios of Higgs boson decays. The pulls of the systematic uncertainties are assessed by the differences in the best-fit values of the POIs between the nominal and various systematic sources, divided by their pre-fit uncertainties. The systematic to be checked is fixed to its best-fit value, while others are allowed to float to derive the best-fit value of the POI. The generation of Asimov datasets involves two steps: profiling the NPs to the observed data to derive the best values for these NPs, and generating the Asimov datasets from the total probability density function at a given signal strength μ_{HH} value after unblinding. Two scenarios are considered to evaluate the impact of the systematic uncertainties: background-only ($\mu_{HH} = 0$) and signal+background ($\mu_{HH} = 1$). To obtain reliable pull results, the Asimov dataset under $\mu_{HH} = 1$ is generated to estimate the impact of systematic uncertainties on μ_{HH} . The pull results, including twenty significant systematic sources, are illustrated in Figure 5.35. No large pulls of the systematic

uncertainties are observed in data. The photon energy scale uncertainty has the largest impact on the signal strength, followed by the combined uncertainty of Scale and m_{top} scheme. The uncertainties are summarized in Table 5.34. When all systematic uncertainties are considered, the expected ggFHH upper limit on μ_{HH} decreases by 1.6% while 0.8% for $\mu_{\text{HH}}^{\text{VBF}}$. The expected constraints on κ_λ and κ_{2V} worsen by 1.5% and 1.6%, respectively.

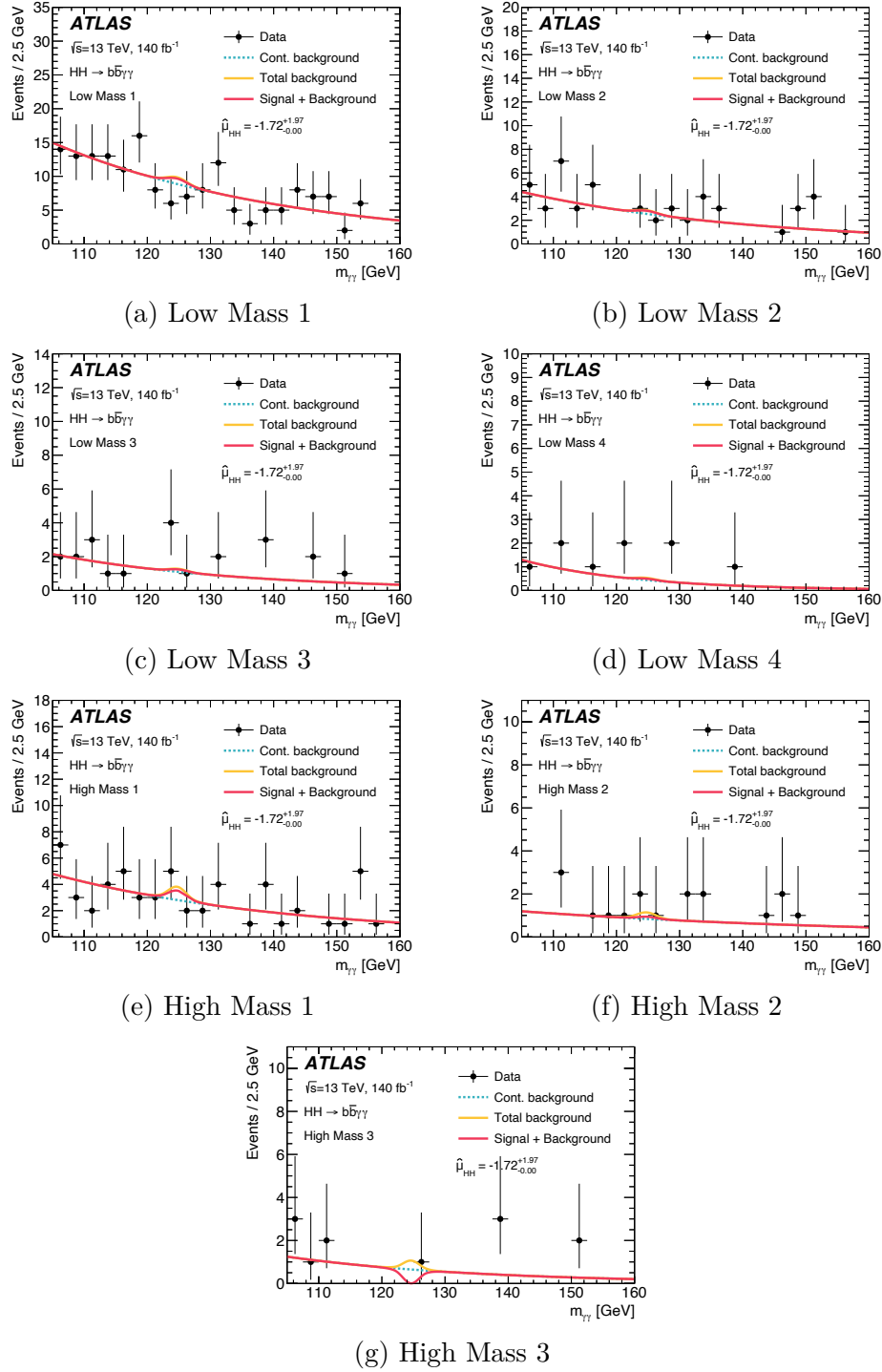


Fig. 5.31 Distributions of the diphoton invariant mass $m_{\gamma\gamma}$ for low (a-d) and high (e-g) mass regions. The best-fit value of $\hat{\mu}_{HH}$ is shown. The data events (black points with error bars) are fitted under the background-only hypothesis (yellow) and signal+background hypothesis (red). The peak close to 125 GeV is from the Higgs production. No significant excess is observed in the data under the background-only hypothesis.

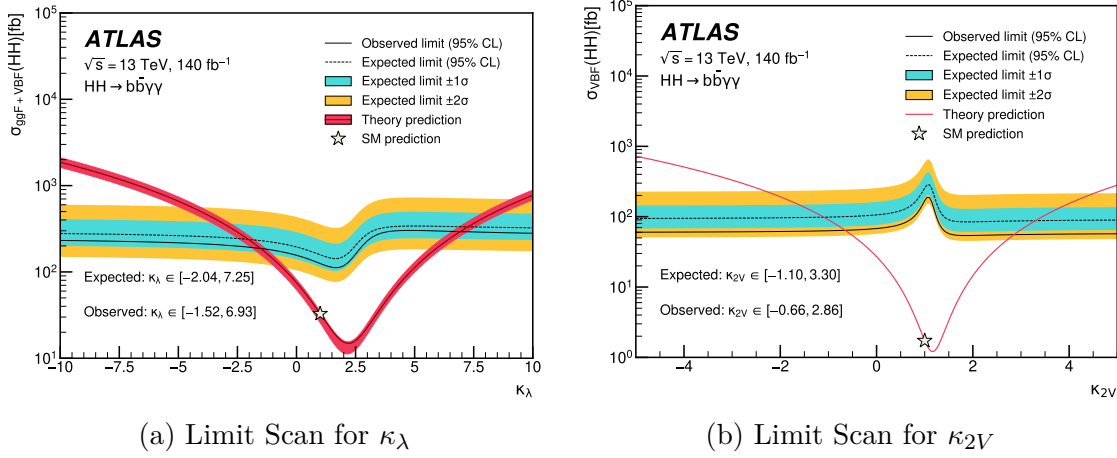


Fig. 5.32 Upper limits of the HH and VBFHH cross-section at 95% CL for (a) κ_λ and (b) κ_{2V} scans. The solid (dashed) line represents the observed (expected) upper limit. The expected error bands are shown with the $\pm 1\sigma$ (green) and $\pm 2\sigma$ (yellow). The red curve indicates the predicted cross-sections of ggFHH and VBFHH for κ_λ with the theoretical error band, only VBFHH for κ_{2V} . Theoretical error bands for κ_{2V} are not displayed, as the scale uncertainties (0.05%) are minimal [36]. Their intersections give the observed (expected) allowed intervals of κ_λ and κ_{2V} .

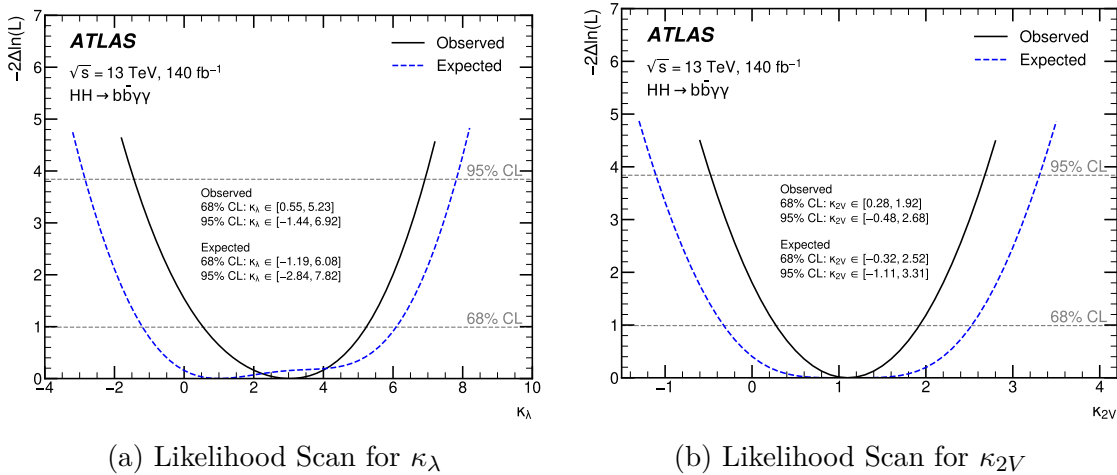
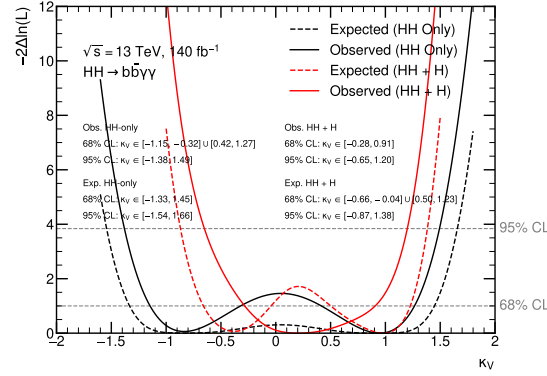
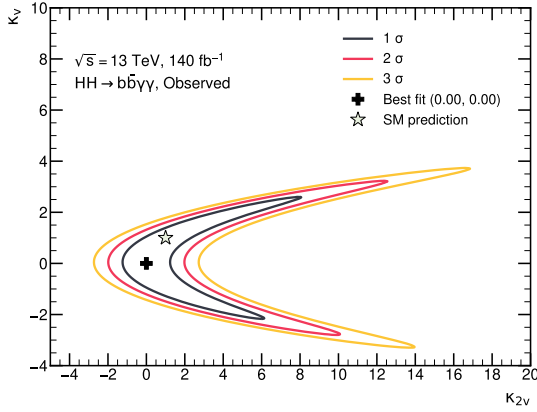
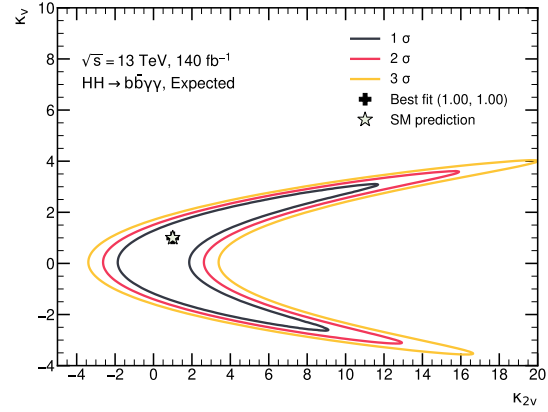


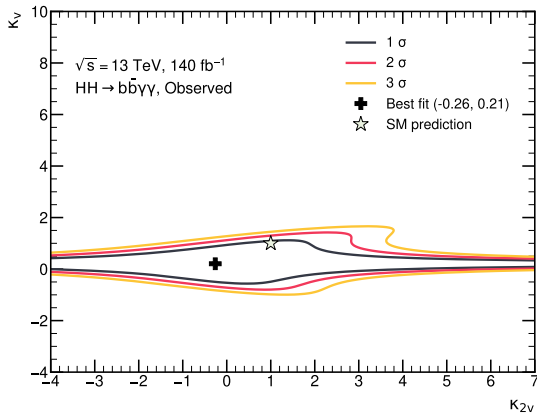
Fig. 5.33 Observed (solid curve) and expected (dashed curve) negative log-likelihood values for (a) κ_λ and (b) κ_{2V} . When evaluating the likelihood, all other coupling modifiers and μ_{HH} are fixed to SM predictions. The expected results are obtained from the hypothesis of SM HH production. The cross-points between the solid lines and dashed lines represent the 68% and 95% CL.

(a) Likelihood Scan for κ_V 

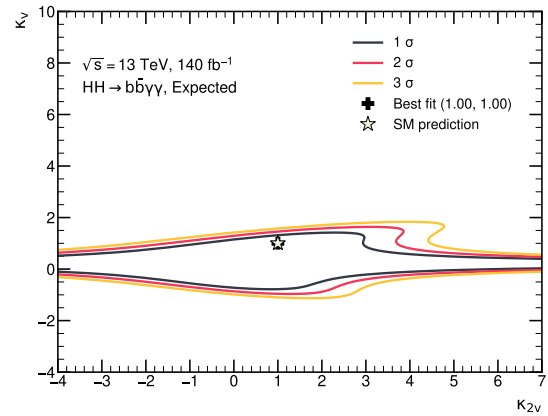
(b) Observed from only HH



(c) Expected from only HH



(d) Observed from HH and H with NLO



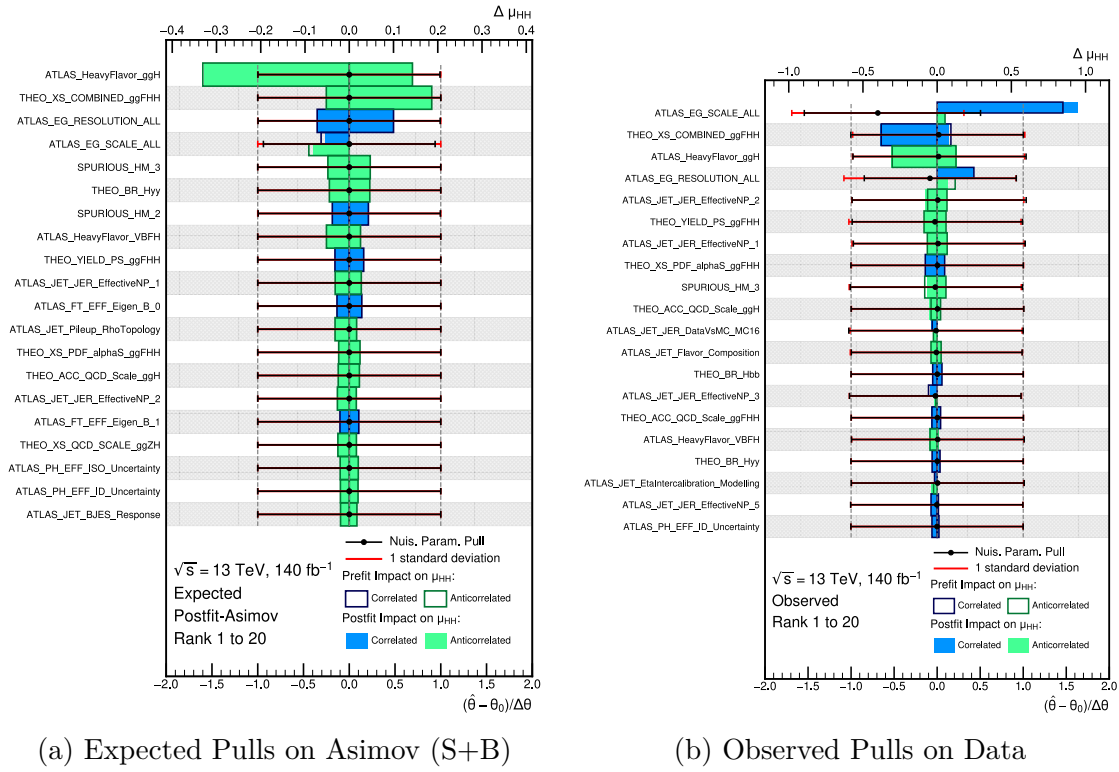
(e) Expected from HH and H with NLO

Fig. 5.34

Observed (solid curve) and expected (dashed curve) negative log-likelihood values for (a) κ_λ and (b) κ_{2V} . When evaluating the likelihood, all other coupling modifiers and μ_{HH} are fixed to SM predictions. The expected results are obtained from the hypothesis of SM HH production. The crossing-points between the solid lines and dashed lines represent the 68% and 95% CL.

Sources	Type	Observed		Expected	
		Upper Limit.	Difference w.r.t. full syst.	Upper Limit	Difference w.r.t. full syst.
Experimental					
Photon energy scale	Norm. + Shape	3.97	+0.29%	5.03	−0.13%
Photon energy resolution	Norm. + Shape	3.96	+0.11%	5.01	−0.43%
Jet energy scale and resolution	Normalization	3.96	+0.08%	5.03	−0.09%
Flavor tagging	Normalization	3.96	0.00%	5.03	−0.14%
Theoretical					
Factorization and renormalization scale	Normalization	3.81	−3.68%	4.79	−4.79%
PDF set and α_S value	Normalization	3.96	+0.04%	5.03	−0.11%
Parton showering model	Normalization	3.97	+0.19%	5.03	−0.15%
Heavy flavor content	Normalization	3.95	−0.20%	5.03	−0.24%
$BR(H \rightarrow \gamma\gamma, b\bar{b})$	Normalization	3.97	+0.16%	5.02	−0.05%
Background modeling (Spurious signal)	Normalization	3.97	+0.14%	5.03	−0.05%

Tab. 5.34 Breakdown of the significant systematic uncertainties and the impacts on the observed and expected upper limits on the signal strength μ_{HH} . Each systematic uncertainty is evaluated by the difference in the best-fit values between the full systematic model (nominal) and the model where the specific systematic is fixed to its best-fit value while others are allowed to float. These uncertainties impact the normalization (Norm) and shape of the chosen modeling function.



(a) Expected Pulls on Asimov (S+B)

(b) Observed Pulls on Data

Fig. 5.35 Pull plots of the significant systematic sources and their impacts on the signal strength μ_{HH} at the corresponding best-fit values are evaluated using the signal+background Asimov dataset ($\mu_{HH} = 1$) and the observed dataset. These plots illustrate the contributions and their influence on the final measurement of μ_{HH} .

5.10.4 Conclusions and Discussion

Understanding the shape of the Higgs field potential and the nature of spontaneous electroweak symmetry breaking necessitates an accurate measurement of the Higgs self-coupling modifier, κ_λ . This measurement is pivotal for probing possible new physics affecting the Higgs field self-interaction. The most direct approach for investigating the Higgs field self-interaction is through Higgs boson pair production at the LHC, primarily via ggFHH and VBFHH processes. Additionally, VBFHH serves as an excellent probe for the VVHH vertex interaction, κ_{2V} . Among all HH decay modes, the $b\bar{b}\gamma\gamma$ final state is one of the relatively most sensitive.

This chapter presents the results of a search of Higgs boson pair production in the two b -jets and diphoton final state, utilizing two analysis strategies: the baseline strategy used for the official ATLAS publication and an alternative strategy. Both strategies employ machine learning techniques to classify signal and background events, thereby enhancing the signal-to-background ratio. The blinded results from both strategies are consistent, while the unblinded results are derived from the baseline strategy.

The latest results in this channel at 95% CL are as follows. The observed (expected) upper limits of the signal strength μ_{HH} are 3.96 (5.03) times the SM predictions. The μ_{HH}^{VBF} upper limit is 100 (131) times the SM predictions. The Higgs self-coupling modifier is constrained

within the range $-1.44 < \kappa_\lambda < 6.92$ ($-2.84 < \kappa_\lambda < 7.82$). The VVHH vertex coupling modifier is constrained to the range $-0.48 < \kappa_{2V} < 2.68$ ($-1.11 < \kappa_{2V} < 3.31$). These results align with SM predictions, with no significant excess observed in the data under the background-only hypothesis. The dominant uncertainty arises from statistical limitations, with significant systematic uncertainties stemming from the renormalization and factorization scales, as well as photon energy resolution.

Machine learning techniques are highly effective in distinguishing signals from backgrounds, and further advancements in these techniques could enhance classification accuracy. Potential improvements include better performance in b -jet and photon object selection. As shown in Table 5.6 and described in Section 5.4.4, a substantial yield loss occurs due to b -jet selection inefficiencies, highlighting the need for enhancements in this area to improve the signal-to-background ratio. Additionally, improvements in photon energy resolution might be achieved through refined calibration and reconstruction algorithms. Increasing the dataset size is the most effective strategy to enhance the sensitivity of the search for Higgs boson pair production in this channel, with data-taking in Run-3 currently in progress. The targeted integrated luminosity will more than double that of Run-2, while the future high-luminosity phase of the LHC will bring a further tenfold increase in integrated luminosity, making the observation of HH production and constraining the Higgs boson self-interactions highly likely.

Higgs Boson Self-Coupling Constraints from Joint Single- and Di-Higgs Analyses

As shown in Chapter 1, the Higgs boson self-interaction vertex, with coupling λ_{HHH} , leads not only to Higgs boson pair production at leading order, but also to next-to-leading order electroweak corrections to single-Higgs boson production. For this reason, a joint interpretation of single- and di-Higgs boson analyses in terms of the Higgs boson self-coupling modifier κ_λ can increase the sensitivity with respect to interpretations based only on the latter. An additional benefit of a joint interpretation of single- and di-Higgs boson analyses is that the other coupling scale factors that affect Higgs boson pair production (κ_t , κ_V), and that were fixed to unity in the interpretation of the search for Higgs boson pairs, can be promoted to additional parameters of interest of the likelihood function (or freely floating nuisance parameters) and be constrained directly the data.

This chapter presents the constraints on the Higgs boson self-coupling obtained by a simultaneous interpretation of the main ATLAS single-Higgs boson measurements [28] and di-Higgs boson searches in the most significant final states, specifically $b\bar{b}\gamma\gamma$, $b\bar{b}b\bar{b}$, and $b\bar{b}\tau^+\tau^-$. All measurements were performed with the full ATLAS Run 2 dataset. The chapter is organized as follows. Section 6.1 explains the statistical model used to interpret the results of single- and di-Higgs boson analyses and their combination, based on the profiled likelihood approach explained in the previous chapter. The constraints on the Higgs boson self-coupling from the combined analysis of single-Higgs boson measurements are summarized in Section 6.2, while those obtained from the combination of the searches for Higgs boson pair production are given in Section 6.3. The joint interpretation of single-Higgs and di-Higgs boson analyses is performed in the following sections: possible overlaps between the phase spaces selected by the different analyses are investigated in Section 6.4; the statistical model for the correlation between systematic uncertainties in different analyses is studied in Section 6.5; and the final results are given

in Section 6.6.

6.1 Statistical Model

The statistical interpretation uses the profiled likelihood approach, where the likelihood function is built from the product of the individual likelihood functions for each of the input channels. Coupling modifiers are implemented as POIs, while systematic uncertainties are incorporated as nuisance parameters of model. To gain deeper insights into the potential physics implications of the analyzed data in terms of couplings constraints, Asimov datasets are generated using various sets of POIs. The fundamental concepts of the statistical model are elaborated in Section 5.3. However, the dedicated parameterization, the treatment of the systematic uncertainties and the generation of the Asimov dataset for the combined analysis are discussed in the following sections.

6.1.1 Parameterization Procedures

The parameterization used to implement into the statistical model the dependence of single- and di-Higgs boson cross-sections and Higgs boson branching ratios on the coupling modifiers, including the Higgs boson self-coupling and its couplings to other particles, are presented in the following sections.

6.1.1.1 Parameterizations for Single-Higgs Boson Measurements

As detailed in Section 1.2.3, the Higgs boson self-coupling induces next-to-leading-order electroweak corrections to the production cross-sections and branching ratios of the Higgs boson, through Feynman diagrams such as those shown in Figure 1.12.

The dependence of the cross-section of each Higgs boson production mode on the Higgs boson self-coupling, as well as on the couplings to other particles such as those to the top quark (κ_t), bottom quark (κ_b), tau-lepton (κ_τ), W boson (κ_W) and W, Z bosons (κ_V) is implemented using Equation 1.31. Deviations of κ_λ from its SM prediction can influence the cross-section through a process-dependent and kinematic-dependent factor (C_1^i). Full NLO EW corrections of the Higgs production cross-sections are considered using the K_{EW} factor, which is the cross-section ratio of NLO to LO scenarios under the SM hypothesis. The cross-section modifier κ_i^2 for the leading-order cross-section of process i is expressed in terms of the Higgs boson coupling modifiers affecting that process, assuming that the Higgs boson couples only to SM particles. The dependence of the Higgs boson branching ratios on κ_λ and the other coupling modifiers is implemented using Equation 1.33. Deviations of κ_λ from its SM prediction can influence the branching ratios through a decay-dependent factor (C_1^f). The branching-ratio modifier κ_f^2 for the leading-order branching ratio of the decay to final state f is expressed in terms of the Higgs boson coupling modifiers affecting that decay, assuming that the Higgs boson couples only to SM particles. The coefficients (C_1^i and C_1^f) and electroweak correction factors (K_{EW}) derived inclusively over the full phase space are given in Table 6.1. Additional sets of values for the coefficients and EW factors are obtained differentially for various Higgs processes [157], in regions of phase space used for the measurements of “simplified template cross-sections”. Those measurements provide more constraining power than inclusive ones. In addition, the impact of

the self-coupling on the analysis efficiency times acceptance within the various regions is found to be negligible for single-Higgs processes and thus it does not need to be included in the statistical model.

Higgs Production Modes						
Channels	$ggFH$	$VBFH$	ZH	WH	$t\bar{t}H$	$tHqb$
$C_1^i \times 100$	0.66	0.63	1.19	1.03	3.52	0.91
K_{EW}	1.049	0.932	0.947	0.93	1.014	0.95
Higgs Decays Modes						
Channels	$\gamma\gamma$	WW	ZZ	$Z\gamma$	gg	ff
$C_1^f \times 100$	0.49	0.73	0.82	0.72	0.66	0.00

Tab. 6.1 The C_1^i coefficients and K_{EW} factors extracted from the Higgs production modes under $\sqrt{s} = 13$ TeV. The C_1^f coefficients for different Higgs decay modes are derived. The "gg" represents two gluons and "ff" symbolizes two fermions. [158]

The decay modes $Z\gamma$ and gg can influence the total width of the Higgs boson and thus the various branching ratios, but they are not measured with significant precision ($Z\gamma$) or at all (gg). Their effect is considered in the analysis of decay modes by resolving the loop diagrams in terms of couplings to the particles running inside the loops. The same approach is applied to production processes such as ggF and ggZH and to the Higgs boson decay to two photons ($\gamma\gamma$). The decomposed parameterization of these loop diagrams [157] is thus the following:

$$\begin{aligned}
\kappa_{ggF}^2 &= 1.042\kappa_t^2 + 0.002\kappa_b^2 - 0.040\kappa_t\kappa_b - 0.005\kappa_t\kappa_c + 0.0005\kappa_b\kappa_c + 0.00002\kappa_c^2 \\
\kappa_{ggZH}^2 &= 2.456\kappa_Z^2 + 0.456\kappa_t^2 - 1.903\kappa_Z\kappa_t - 0.011\kappa_Z\kappa_b + 0.003\kappa_t\kappa_b \\
\kappa_{\gamma\gamma}^2 &= 1.589\kappa_W^2 + 0.072\kappa_t^2 - 0.674\kappa_W\kappa_t + 0.009\kappa_W\kappa_\tau + 0.008\kappa_W\kappa_b - 0.002\kappa_t\kappa_b - 0.002\kappa_t\kappa_\tau \\
\kappa_{Z\gamma}^2 &= 1.118\kappa_W^2 - 0.125\kappa_W\kappa_t + 0.004\kappa_t^2 + 0.003\kappa_W\kappa_b \\
\kappa_{gg}^2 &= 1.111\kappa_t^2 + 0.012\kappa_b^2 - 0.1\kappa_t\kappa_b
\end{aligned} \tag{6.1}$$

6.1.1.2 Parameterizations for Higgs Boson Pair Searches

As shown in the ggFHH Feynman diagrams in Figure 1.14, two couplings (κ_λ and κ_t) directly modify the cross-section of ggFHH. Consequently, the cross-section of ggFHH can be parameterized as a function of κ_λ and κ_t , as in Equation 5.2. The ratio $\kappa_\lambda / \kappa_t$ influences the kinematic distributions and signal acceptance of the ggFHH process, affecting how Higgs boson pairs are produced and detected. In contrast, the κ_t^4 factor solely scales the total cross-section, determining the overall frequency of the process without altering its kinematic characteristics. The κ_λ -reweighting technique is employed to generate additional basis samples, determining the linear coefficients of the cross-section function. This analytic function in Equation 5.6 is subsequently integrated into the statistical model for the ggFHH parameterization. The κ_λ -reweighting and the linear combination procedures for ggFHH are comprehensively detailed in Section 5.2.2.2.

The second largest Higgs boson pair production mechanism is the VBFHH mode. The LO Feynman diagrams are displayed in Figure 1.15. The cross-section is involved with κ_λ (HHH

vertex), κ_{2V} (VVHH vertex) and κ_V (VVH vertex) in Equation 5.8. These coupling modifiers are integrated into the statistical model using the linear analytic function in Equation 5.9 for the VBFHH parameterization. The parameterization procedure of the linear combination method for VBFHH is described in Section 5.2.3.2.

6.1.2 Systematic Uncertainties

Systematic uncertainties are incorporated in the model as described in the previous chapters. In the case of uncertainties correlated among different analyses, the same nuisance parameters are used and a single constraint term is included in the likelihood function. The study of the correlation scheme for the systematic uncertainties is described later in section 6.5.

6.1.3 Asimov Dataset Generation

The expected results are derived from fitting the generated Asimov dataset. Typically, this dataset is produced using a PDF profiled to data, with signal yields fixed to SM predictions. However, the Asimov dataset generated by this approach before profiling NPs fails to capture the correlation between signal yields and signal uncertainties. This can lead to discrepancies between the fitted results of the signal theory systematic, making the Asimov dataset less representative of the real data. Furthermore, certain background NPs that correlate with signal yields may contribute to these inconsistencies.

Therefore, the solution is that both the signal yields and the NPs are firstly profiled to the data to obtain the best values for the parameters. The discrepancies between the Asimov dataset and the real data are overcome by floating the signal yields and NPs. The Asimov dataset in the combined analysis is then generated with the signal yields fixed to SM predicted values, while the NPs remain at their profiled values. The global observables are maintained at these profiled values during the fitting of the Asimov dataset, ensuring consistency and accuracy.

In the combined analysis, the generic kappa model (κ_λ , κ_V , κ_t , κ_b , κ_τ) is used to generate the Asimov dataset, allowing these parameters to float and be profiled to the data. Although signal yields are profiled to the data, small differences can still emerge between Asimov datasets for various measurements due to variations in signal parameterization and theory uncertainty implementations. These differences are justified to ensure alignment with SM predictions. To maintain consistency and reliability, the combined workspace for single and double Higgs production generates specific Asimov datasets for each measurement, ensuring they align well with SM expectations.

6.2 Results from Single Higgs Combination

Single Higgs combination includes dominant decay channels of the single Higgs boson as listed in Table 6.2. The expected and observed likelihood scan results for κ_λ are listed in Figure 6.1 (a) and (b), respectively, with constraints at 68% and 95% CL. The best-fit values are obtained by floating all NPs and other POIs, then maximizing the likelihood for both the Asimov dataset and the collected data. The observed (expected) best-fit values of κ_λ are $2.497^{+4.595}_{-3.941}$ ($0.963^{+7.048}_{-3.816}$). The 68% and 95% CL one-dimensional confidence intervals for κ_λ are $[-1.4, 7.1]$ ($[-2.8, 8.0]$) and $[-4.0, 10.3]$ ($[-5.2, 11.5]$), respectively, as summarized in Table 6.3. Two-dimensional confidence

regions for κ_λ and κ_t are depicted in Figure 6.2, with κ_λ and κ_t floated as POIs while the other coupling modifiers are fixed to their corresponding SM predictions. The single Higgs shows significantly tighter constraints on the Higgs-top quark coupling modifier κ_t (5–10% level) than Higgs self-coupling κ_λ (500–1000% level), as κ_t affects single-Higgs production and decay at leading order via gluon-gluon fusion, $t\bar{t}H$ production and decays to diphoton. The results are consistent with the SM predictions.

Analysis Channels	Integrated Luminosity [fb^{-1}]	References
$H \rightarrow \gamma\gamma$	139	[159]
$H \rightarrow ZZ^* \rightarrow 4\ell$	139	[160]
$H \rightarrow \tau^+\tau^-$	139	[161]
$ggFH/VBFH \rightarrow WW^* \rightarrow e\nu\mu\nu$	139	[162]
$VH \rightarrow b\bar{b}$	139	[163]
$VBFH \rightarrow b\bar{b}$	126	[164]
$t\bar{t}H \rightarrow b\bar{b}$	139	[165]

Tab. 6.2 Analysis channels and their integrated luminosities used in the combination. Results for individual channel are referenced. All dominant production modes of the single Higgs boson are included in the first three channels.

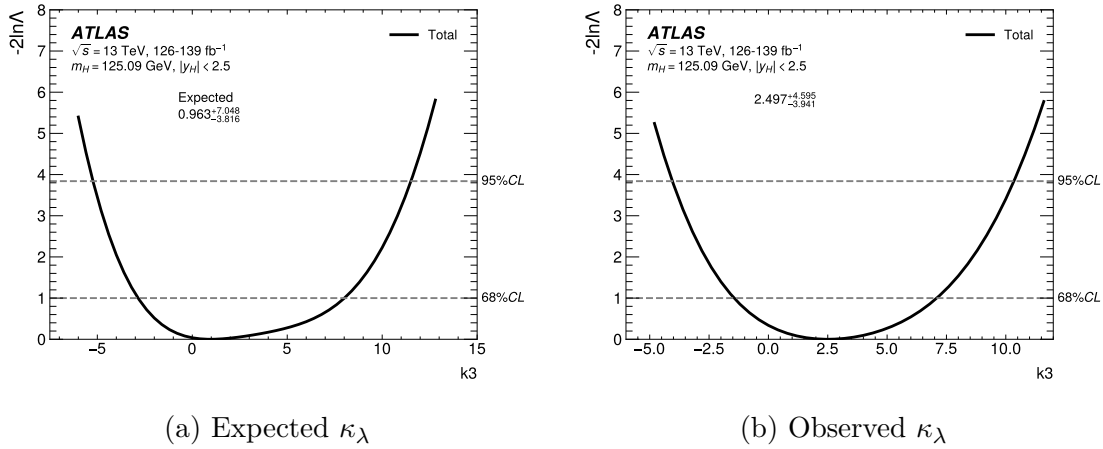


Fig. 6.1 Expected (a) and observed (b) results for the likelihood scan of κ_λ from single Higgs combination, fitted respectively to the Asimov dataset and the collected data. The κ_λ as the only POI is floated, with all other coupling modifiers fixed to their corresponding SM values. The relevant best-fit values are displayed. The constraints are given at 68% and 95% CL.

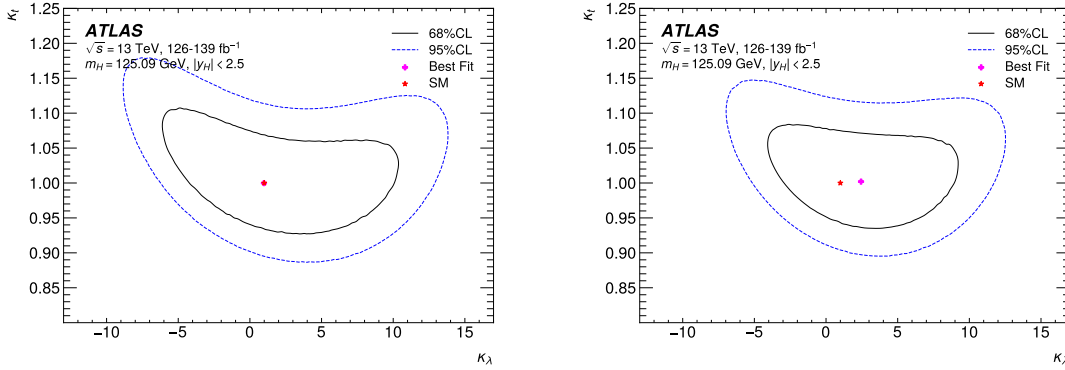
6.3 Results from Di-Higgs Analyses

As a trade-off between the branching ratios of the decays of Higgs boson pairs shown in Figure 1.16, possibility to reconstruct and identify the final state, and signal-over-background

Dataset	Best-Fit Values $^{+1\sigma}_{-1\sigma}$	Interval [68% CL]	Interval [95% CL]
Expected	$0.963^{+7.048}_{-3.816}$	$-2.8 < \kappa_\lambda < 8.0$	$-5.2 < \kappa_\lambda < 11.5$
Observed	$2.497^{+4.595}_{-3.941}$	$-1.4 < \kappa_\lambda < 7.1$	$-4.0 < \kappa_\lambda < 10.3$

Tab. 6.3

Expected and observed results of the best-fit, 68% and 95% CL intervals for the likelihood scan of κ_λ from single Higgs combination. The corresponding values are obtained from fitting respectively the Asimov dataset and the collected data. The κ_λ as the only POI is floated, with all other coupling modifiers fixed to their corresponding SM values.

(a) Expected κ_λ vs κ_t (b) Observed κ_λ vs κ_t **Fig. 6.2**

Expected (a) and observed (b) results for the constraints of κ_λ and κ_t from single Higgs combination, fitted respectively to the Asimov dataset and the collected data. The κ_λ and κ_t as the POIs are floated, with all other coupling modifiers fixed to their corresponding SM values. The SM prediction is shown as a red star. The values of best-fit (magenta plus), 68% (black solid curve) and 95% (blue dashed curve) CL intervals are displayed.

ratio, the most sensitive channels to search for Higgs boson pair production are the $b\bar{b}\gamma\gamma$, $b\bar{b}b\bar{b}$, and $b\bar{b}\tau^+\tau^-$ final states. These channels are combined to constrain the cross-section upper limit and to measure the couplings (κ_λ and κ_{2V}), as published in [28, 166, 167]. The results of individual channels are briefly presented, followed by the combined outcomes in the subsequent section.

6.3.1 Results from Individual Channels

$HH \rightarrow b\bar{b}\gamma\gamma$: The $b\bar{b}\gamma\gamma$ channel is distinguished by its high sensitivity for di-Higgs production. The final state with two photons offers a distinct and clean signature, characterized by excellent photon resolution. The diphoton invariant mass peak ($m_{\gamma\gamma}$) around 125 GeV serves as an effective discriminator against background processes, significantly mitigating contributions from non-resonant backgrounds. Although the branching ratio for this channel is relatively small, approximately 0.26%, resulting in a lower event yield compared to other decay channels, the clean signature and effective background suppression enhance the signal-to-background ra-

tio.

The analysis, as detailed in Reference [130], utilized the full ATLAS Run-2 dataset, totaling 139 fb^{-1} . Events were selected with two tight and isolated leading or sub-leading photons with $p_T/m_{\gamma\gamma} > 0.35$ (0.25) and exactly two b-jets with 77% working point selection of DL1r tagger. To maintain sensitivity, events were divided into low and high mass regions based on $m_{b\bar{b}\gamma\gamma}^*$, which differentiates between SM-like and BSM-like signals. Each mass region was further classified into loose and tight categories according to the BDT score, resulting in four distinct categories. BDT thresholds were optimized to maximize the significance for both SM and BSM signals.

Statistical model PDFs were derived by fitting analytic functions to the $m_{\gamma\gamma}$ spectrum. Signal modeling was performed by fitting the $m_{\gamma\gamma}$ distribution of simulated events post-selection using a DSCB function, as shown in Figure 5.8 (a). The continuum background was modeled by fitting an exponential function to the $m_{\gamma\gamma}$ spectrum from data sidebands.

The channel demonstrated the highest sensitivity in the low mass region for setting the cross-section upper limit and mainly constraining the Higgs boson self-coupling. The derived 95% CL upper limit on the di-Higgs production cross-section, from both the background-only Asimov dataset and the observed data, is 130 fb (observed) and 180 fb (expected). The observed (expected) upper limit on the signal strength μ_{HH} is 4.2 (5.7) times the SM prediction. The Higgs boson self-coupling κ_λ is constrained to the range $[-1.5, 6.7]$ ($[-2.4, 7.7]$) at 95% CL for the observed (expected) results.

$HH \rightarrow b\bar{b}b\bar{b}$: The $HH \rightarrow b\bar{b}b\bar{b}$ channel has the largest branching ratio (34%). Moreover, the final state with four b-jets provides a rich kinematic environment, allowing the use of advanced techniques like MVA to distinguish signal from background. However, the dominant backgrounds, such as QCD multijet and $t\bar{t}$ production, are significant and challenging to suppress due to their large cross-sections and the presence of multiple b-jets. Reconstructing four b-jets accurately is difficult due to jet energy resolution and possible overlaps, especially in high pile-up conditions typical in the LHC environment.

As described in Reference [166], the results are derived from 126 fb^{-1} of Run-2 pp collision data collected in 2016–2018. A complex selection and classification strategy is employed to optimize signal detection and minimize background interference. Jets are categorized into central jets ($|\eta| < 2.5$) and forward jets ($|\eta| \geq 2.5$), enhancing the acceptance for jets originating from the VBF production mode. To qualify for further analysis, events must satisfy specific trigger requirements and include at least four central jets, with a minimum of four jets being b-tagged to ensure the identification of b-quark jets, indicative of Higgs boson decays. Subsequent to this selection, events are classified into ggF and VBF production channels, with additional criteria applied to prioritize the identification of VBF events over ggF events.

The signal region (SR) is defined using a dedicated discriminating variable given by:

$$X_{HH} = \sqrt{\left(\frac{m_{H1} - 124\text{GeV}}{0.1m_{H1}}\right)^2 + \left(\frac{m_{H2} - 117\text{GeV}}{0.1m_{H2}}\right)^2} \quad (6.2)$$

where X_{HH} determines a specific contour in the (m_{H1}, m_{H2}) mass plane for the two reconstructed Higgs boson candidates. The center of the contour is approximately at $m_{H1} = 124\text{GeV}$ and $m_{H2} = 117\text{GeV}$. The backgrounds are estimated in control regions (CR) in the (m_{H1}, m_{H2})

mass plane outside from the SR, and then extrapolated to the SR. The results are determined from a profiled-likelihood fit to the distribution of the the invariant mass of the HH system (m_{HH}). To further refine the analysis, additional variables like X_{HH} and $|\Delta\eta_{HH}|$ are applied to categorize events.

The analysis of the data yielded an upper limit of 165 fb on the HH cross-section at 95% CL, with the expected limit at 241 fb. This indicates that the observed (expected) signal strength μ_{HH} is less than 5.4 (8.1). The Higgs boson self-coupling modifier κ_λ was constrained to be within the range $[-3.9, 11.1]$ at 95% CL, quite close to the expected range $[-4.6, 10.8]$. The observed (expected) one-dimensional confidence interval for the coupling modifier of the VVHH vertex, κ_{2V} , at 95% CL, was $[-0.03, 2.11]$ ($[-0.05, 2.12]$).

$HH \rightarrow b\bar{b}\tau^+\tau^-$: Both $H \rightarrow b\bar{b}$ and $H \rightarrow \tau^+\tau^-$ have relatively high branching ratios, leading to a combined branching ratio 7.3% for the $HH \rightarrow b\bar{b}\tau^+\tau^-$ decay. This allows a good balance between yield and background suppression. The presence of b -jets and τ -leptons provides a distinctive final state that can be effectively discriminated from many background processes. The τ -leptons can be identified with good efficiency and purity, allowing for effective background suppression. The final state kinematics involving b -jets and τ -leptons offer a rich environment for applying multivariate techniques to enhance signal discrimination.

The analysis, detailed in Reference [167], leverages the entire Run 2 dataset, amounting to 139 fb^{-1} of pp collisions. The study focuses on selecting events featuring two b -jets and two τ -leptons, aimed at defining signal regions for both fully-hadronic ($\tau_{\text{had}}\tau_{\text{had}}$) and semi-leptonic ($\tau_{\text{lep}}\tau_{\text{had}}$) channels, corresponding to various τ decay modes. In the semi-leptonic channel, events are further split into sub-channels based on the triggering mechanism: the single lepton trigger (SLT) and the lepton tau trigger (LTT). The SLT sub-channel requires one electron or muon and one hadronic τ with opposite charges, while the LTT requires a pair consisting of a lepton and a hadronic τ with opposite charges. The fully-hadronic channel selects events to pass both single and di-hadronic τ triggers, featuring two hadronic τ s with opposite charges. Additionally, both channels require the inclusion of exactly two b -jets, identified using the DL1r tagger at a 77% working point. Dominant background sources include $t\bar{t}$ and Z +heavy flavor production processes.

After event selection, separate multivariate classifiers to separate signal from background were trained and assessed for $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_{\text{lep}}\tau_{\text{had}}$ (SLT), and $\tau_{\text{lep}}\tau_{\text{had}}$ (LTT) regions using Monte Carlo samples. The classifier score distributions were fitted, with data from a Z +heavy flavor control region constraining the corresponding background normalization. The analysis yielded an observed (expected) upper limit on the Higgs boson pair production cross-section of 135 fb (114 fb) at a 95% CL. The corresponding upper limit on the HH signal strength μ_{HH} is 4.7 (3.9). The observed (expected) one-dimensional confidence interval for κ_λ at 95% CL was $[-2.4, 9.2]$ ($[-2.0, 9.0]$).

6.3.2 Results from the Combination

The aforementioned results of the individual channels are combined to yield tighter constraints on the signal strength μ_{HH} and the coupling modifiers κ_λ and κ_{2V} . The observed and expected upper limits on the signal strength for HH production for the individual channels and the combined channel are displayed in Figure 6.3. The observed and expected HH cross-section

upper limits from the combination are respectively 78.48 and 94.83 fb at 95% CL, where the theory uncertainties from the scale and m_{top} are included in the prediction appearing in the denominator of μ_{HH} . The results indicate that no significant excess is observed in data under the background-only hypothesis.

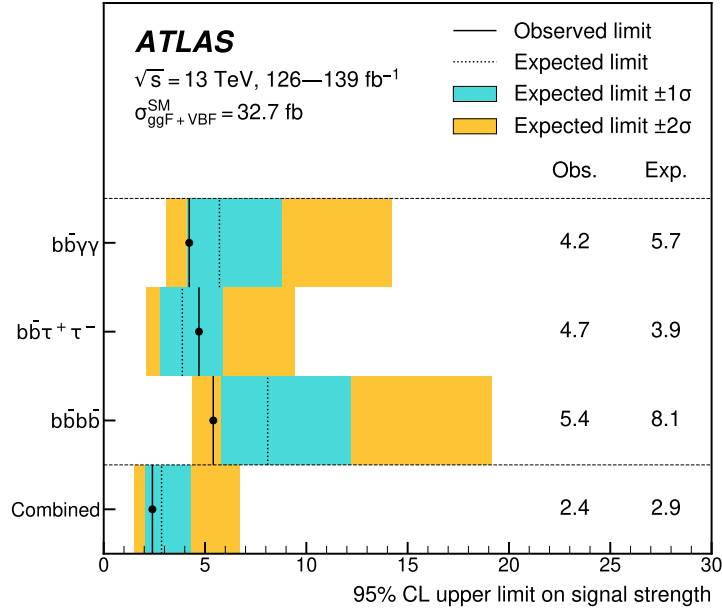


Fig. 6.3 Signal strength upper limit at 95% CL for individual di-Higgs channel and their combination. The expected limits (dashed line) with the corresponding $\pm 1\sigma$ (turquoise band) and $\pm 2\sigma$ (yellow band) error bands are obtained from background-only Asimov dataset with all NPs profiled to the observed data. The observed limits (solid line) are displayed.

The coupling modifiers κ_λ and κ_{2V} are constrained by the upper limits of the corresponding HH cross-sections at 95% CL, from the intersections of the expected limit curves and the theoretical predictions, as shown in Figure 6.4 (a) and (b) respectively. The results are summarized in Table 6.4.

Channels	κ_λ		κ_{2V}	
	Expected	Observed	Expected	Observed
$b\bar{b}\gamma\gamma$	$-2.34 < \kappa_\lambda < 7.62$	$-1.53 < \kappa_\lambda < 6.66$	$-1.52 < \kappa_{2V} < 3.70$	$-1.05 < \kappa_{2V} < 3.21$
$b\bar{b}b\bar{b}$	$-4.52 < \kappa_\lambda < 10.99$	$-3.81 < \kappa_\lambda < 11.32$	$-0.048 < \kappa_{2V} < 2.12$	$-0.033 < \kappa_{2V} < 2.11$
$b\bar{b}\tau^+\tau^-$	$-1.98 < \kappa_\lambda < 9.08$	$-2.42 < \kappa_\lambda < 9.34$	$-0.53 < \kappa_{2V} < 2.66$	$-0.57 < \kappa_{2V} < 2.70$
Combined	$-0.97 < \kappa_\lambda < 7.08$	$-0.58 < \kappa_\lambda < 6.65$	$0.024 < \kappa_{2V} < 2.06$	$0.073 < \kappa_{2V} < 2.03$

Tab. 6.4 Expected and observed allowed intervals of κ_λ and κ_{2V} from the upper limits, derived from the intersections of the expected limit curves and the theoretical limit curves in Figure 6.4.

Profile likelihood-ratio scans for κ_λ and κ_{2V} are performed to determine the expected and observed constraints at 68% and 95% CL. The individual and combined results are displayed

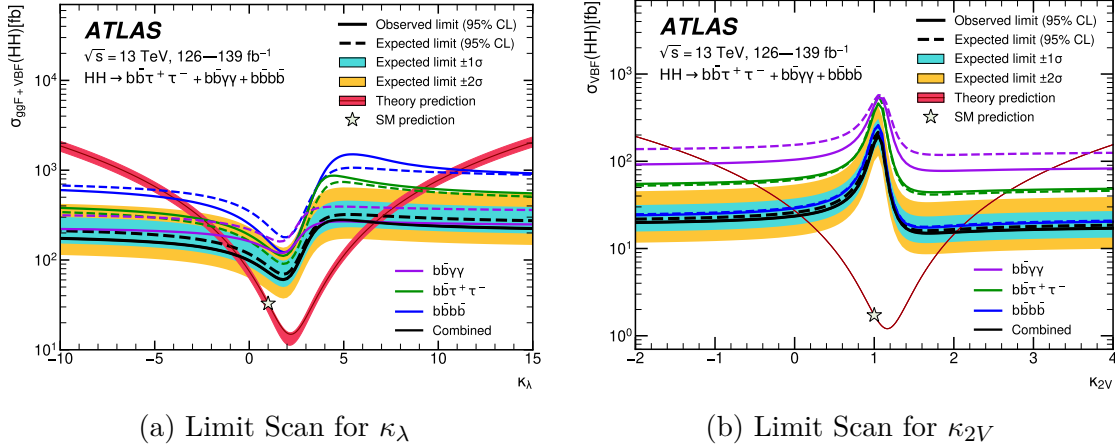


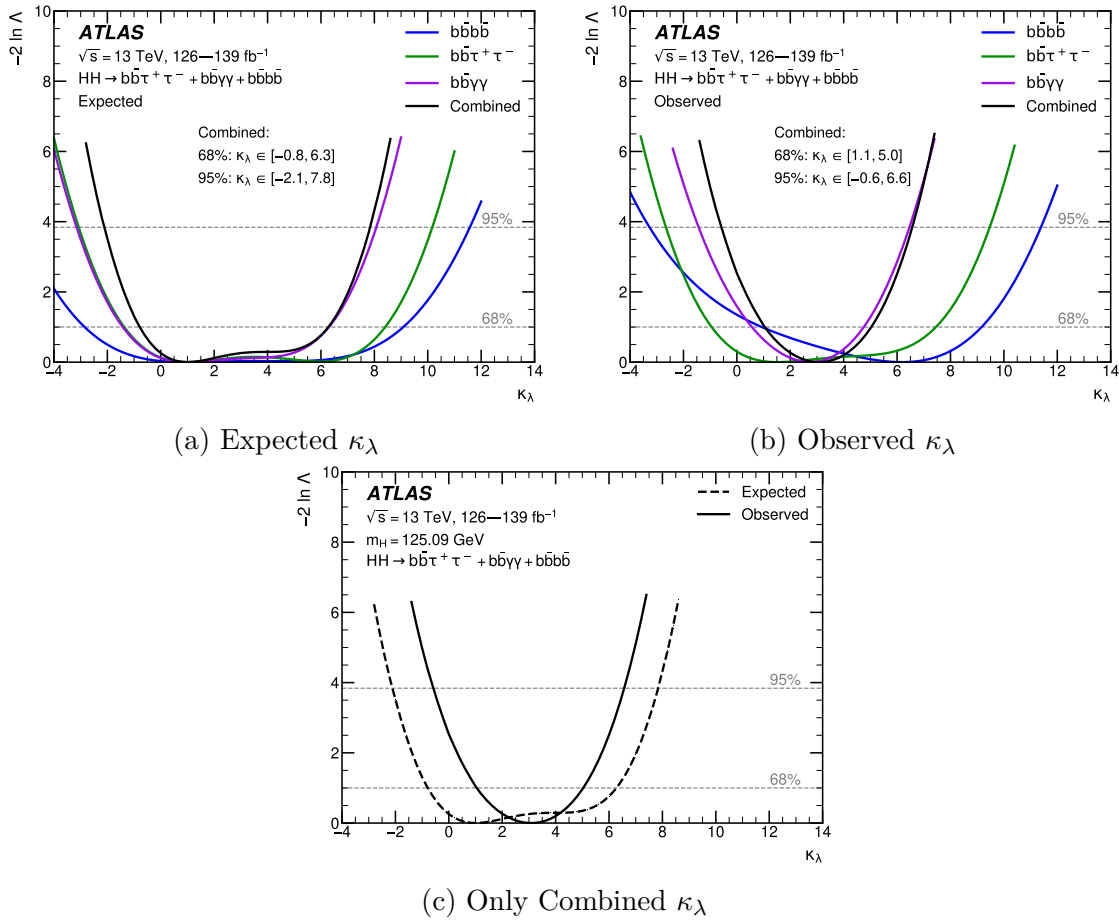
Fig. 6.4 Expected (dashed lines) and observed (solid lines) upper limits scan of κ_λ (a) and κ_{2V} (b) at 95% CL for individual (colored lines) and combined (black line) channels. The expected limits are fitted to the background-only Asimov dataset with all other NPs profiled to the observed data while the observed limits are from the collected data. The theoretical prediction with its uncertainties at each value is exhibited as red lines. The star marker denotes the SM prediction.

in Figure 6.5 and Figure 6.6. Two local minima for the expected profiled likelihood ratio as a function of κ_λ are observed due to the interference effects between various Feynman diagrams contributing to HH production. All other coupling modifiers are fixed to their corresponding SM values. The expected and observed constraints are derived from the likelihood scan results at 68% and 95% CL. The results are summarized in Table 6.5 and Table 6.6.

Constraints on κ_λ at Best-Fit, 68% and 95% CL				
Channels	Datasets	Best-Fit Values $^{+1\sigma}_{-1\sigma}$	Intervals [68% CL]	Intervals [95% CL]
$b\bar{b}\gamma\gamma$	Exp.	$1.0^{+5.3}_{-2.4}$	$-1.42 < \kappa_\lambda < 6.3$	$-3.22 < \kappa_\lambda < 8.14$
	Obs.	$2.8^{+2.0}_{-2.2}$	$0.57 < \kappa_\lambda < 4.76$	$-1.51 < \kappa_\lambda < 6.54$
$b\bar{b}b\bar{b}$	Exp.	$1.0^{+8.1}_{-3.9}$	$-2.85 < \kappa_\lambda < 9.09$	$-5.28 < \kappa_\lambda < 11.68$
	Obs.	$6.0^{+3.0}_{-5.2}$	$0.94 < \kappa_\lambda < 9.17$	$-3.39 < \kappa_\lambda < 11.48$
$b\bar{b}\tau^+\tau^-$	Exp.	$1.0^{+7.4}_{-2.4}$	$-1.36 < \kappa_\lambda < 8.41$	$-3.13 < \kappa_\lambda < 10.24$
	Obs.	$1.5^{+5.9}_{-2.5}$	$-0.94 < \kappa_\lambda < 7.46$	$-2.72 < \kappa_\lambda < 9.55$
Combined	Exp.	$1.0^{+5.3}_{-1.8}$	$-0.78 < \kappa_\lambda < 6.28$	$-2.11 < \kappa_\lambda < 7.84$
	Obs.	$3.1^{+1.9}_{-2.0}$	$1.05 < \kappa_\lambda < 5.04$	$-0.57 < \kappa_\lambda < 6.57$

Tab. 6.5 Best-fit values, expected and observed allowed intervals of κ_λ from the likelihood scans at 68% and 95% CL for each individual channel and combination.

Two-dimensional likelihood-ratio scans are performed for $(\kappa_\lambda$ and $\kappa_t)$ and $(\kappa_V$ and $\kappa_{2V})$. The expected and observed results are derived from the Asimov dataset and the collected data at $\pm 1\sigma$, $\pm 2\sigma$ and $\pm 3\sigma$, where the coupling modifiers in question are floated and others are fixed to the SM values. Best-fit values are also obtained for the expected and observed results. The

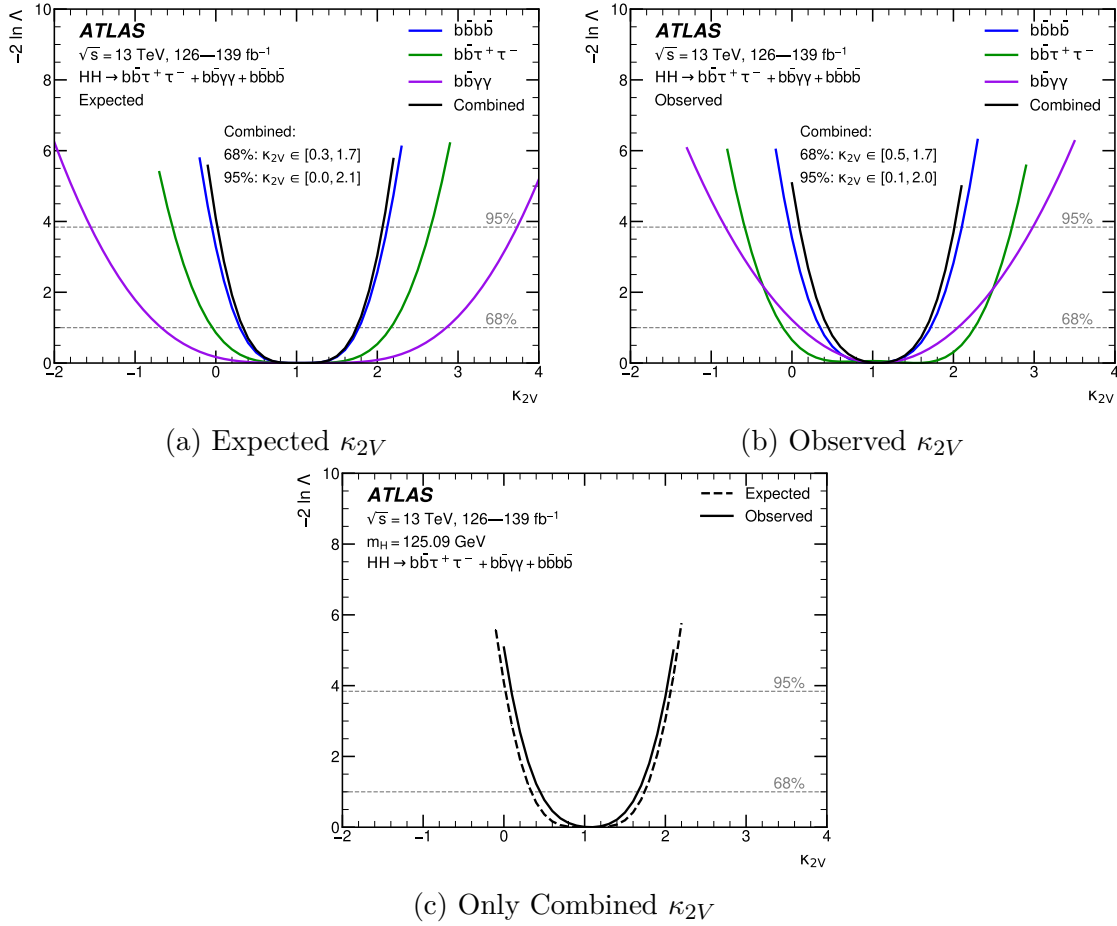
**Fig. 6.5**

Expected (a) and observed (b) results for the likelihood-ratio scans of κ_λ from di-Higgs individual channels and their combination. Expected vs observed scans for the combination (c). The expected results are fitted to the background-only Asimov dataset. The κ_λ is the only POI, with all other coupling modifiers fixed to their corresponding SM values. The allowed ranges are derived at 68% and 95% CL. The combined constraints are listed in the plots.

2D likelihood scan results are plotted in Figure 6.7 (a-b) for κ_λ vs κ_t and (c-d) for κ_V vs κ_{2V} . The observed best-fit value of $(\kappa_\lambda, \kappa_t)$ is (1.22, 0.13). The HH combination provides more stringent constraints on κ_λ than single-Higgs but much looser constraints on κ_t . In particular, the sensitivity of the experimental data to κ_t decreases at higher values. The best-fit value of (κ_V, κ_{2V}) is observed to be (0.33, 0.06). The HH combination provides more stringent constraints on κ_{2V} than on κ_V .

6.4 Investigation of Overlapping Events

Overlap occurs when the selections defining different analysis categories are not orthogonal, leading to the same event being selected by both categories. This duplication results in the event being included in the statistical interpretations of both analyses, introducing potential

**Fig. 6.6**

Expected (a) and observed (b) results for the likelihood-ratio scans of κ_{2V} from di-Higgs individual channels and their combination. Expected vs observed scans for the combination (c). The expected results are fitted to the background-only Asimov dataset. The κ_{2V} is the only POI, with all other coupling modifiers fixed to their corresponding SM values. The allowed ranges are derived at 68% and 95% CL. The combined constraints are listed in the plots.

biases and inaccuracies since the model, built as the product of the likelihood functions of each category, assumes that the samples are completely orthogonal. To maintain the robustness and precision of statistical interpretations, the analyses selection criteria are chosen to yield signal regions that are as orthogonal as possible. However, it might be possible that control regions of a given analysis overlap partially with signal regions of another analysis. Also, single-Higgs ttH measurements and di-Higgs searches have complex selections targeting similar final states and their selections might not be fully independent despite the efforts put in it.

The possible overlap of events between the various analysis channels in single and double Higgs analyses was investigated by checking, in data and in simulated single-Higgs and di-Higgs signal samples, whether events with the same unique identifier (based on a sequential event number within a given run, characterized by its run number) pass more than one category selection. These checks are performed across all regions defined by the input analyses, including

Constraints on κ_{2V} at Best-Fit, 68% and 95% CL				
Channels	Datasets	Best-Fit Values $^{+1\sigma}_{-1\sigma}$	68% CL	95% CL
$b\bar{b}\gamma\gamma$	Exp.	$1.0^{+1.9}_{-1.7}$	$-0.67 < \kappa_{2V} < 2.86$	$-1.58 < \kappa_{2V} < 3.77$
	Obs.	$1.1^{+1.0}_{-1.0}$	$0.11 < \kappa_{2V} < 2.06$	$-0.86 < \kappa_{2V} < 3.03$
$b\bar{b}b\bar{b}$	Exp.	$1.0^{+0.7}_{-0.7}$	$0.30 < \kappa_{2V} < 1.78$	$-0.06 < \kappa_{2V} < 2.14$
	Obs.	$1.0^{+0.7}_{-0.7}$	$0.36 < \kappa_{2V} < 1.72$	$-0.04 < \kappa_{2V} < 2.12$
$b\bar{b}\tau^+\tau^-$	Exp.	$1.0^{+1.2}_{-1.0}$	$-0.04 < \kappa_{2V} < 2.17$	$-0.55 < \kappa_{2V} < 2.68$
	Obs.	$1.5^{+0.7}_{-1.7}$	$-0.11 < \kappa_{2V} < 2.27$	$-0.60 < \kappa_{2V} < 2.75$
Combined	Exp.	$1.0^{+0.7}_{-0.7}$	$0.35 < \kappa_{2V} < 1.75$	$0.03 < \kappa_{2V} < 2.07$
	Obs.	$1.1^{+0.6}_{-0.6}$	$0.45 < \kappa_{2V} < 1.67$	$0.10 < \kappa_{2V} < 2.02$

Tab. 6.6 Best-fit values, expected and observed allowed intervals of κ_{2V} from the likelihood scans at 68% and 95% CL for each individual channel and combination. The expected results are fitted to the background-only Asimov dataset and the observed from the collected data.

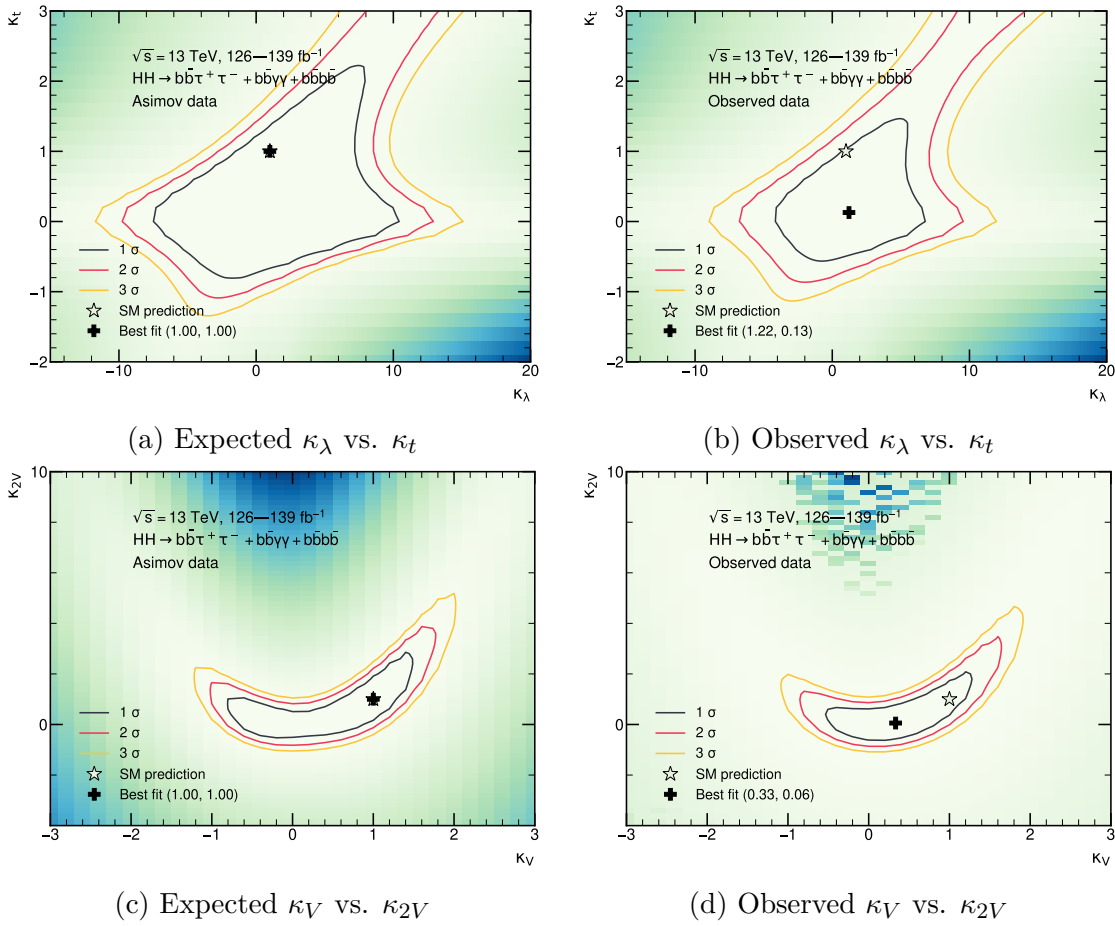
control and validation regions (CR or VR), with a specific focus on overlaps within the signal regions (SR), as SR versus SR overlaps present the most significant challenge.

Overlap between single-Higgs analyses is found to be negligible. Overlaps between di-Higgs analyses are also very small, significantly less than 0.1%, and their impact on the result has been found to be negligible comparing the fit results including or removing duplicate events in the analysis. Overlaps between di-Higgs analyses and single-Higgs analyses are also generally small, below 1%, with the notable exception of the $HH \rightarrow b\bar{b}\tau^+\tau^-$ and $H \rightarrow \tau\tau$ analyses, where an overlap at the level of 4% is observed in the HH signal regions due to the $t\bar{t}H$ categories of the single-Higgs analysis. For this reason, the $t\bar{t}H$ categories of the $H \rightarrow \tau\tau$ analysis were removed from the combination.

6.5 Systematic Uncertainties Correlations Studies

The systematic uncertainties are integrated into the statistical model through the NPs. Single-Higgs and di-Higgs analyses share 90 common sources of systematic uncertainties summarized in Table 6.7, which are incorporated into the workspace. Different correlation schemes for these shared NPs are investigated to properly account for their correlations and investigate the impact on the statistical models in terms of simplification versus flexibility. The study of NP correlations is crucial for accurate measurements, consistency checks, and optimized constraints on systematic uncertainties, ultimately leading to more reliable and sensitive physics results.

Three schemes for the correlation of NPs are investigated: *Simple-Scheme*, *Advanced-Scheme*, and *Fully-Correlated*. These correlation schemes are detailed in Table 6.7, which summarizes the systematic uncertainties related to both experimental and theoretical sources. In the table, a "1" denotes that the NP is correlated among the different analysis, which indicates that the same NP name is considered in the statistical model, while an empty cell means that uncorrelated NPs, with different names, are implemented in the statistical model. The performance of the

**Fig. 6.7**

Two-dimensional likelihood-ratio scans of κ_λ vs κ_t (a-b) and κ_V vs κ_{2V} (c-d) at $\pm 1\sigma$, $\pm 2\sigma$, and $\pm 3\sigma$ from diHiggs combination. The expected results are fitted to the background-only Asimov dataset under all NPs profiled to the observed data and only two modifiers in question are floated. The negative log-likelihood values are shown in the z-axis. The best-fit values are marked with a black cross while the star denotes the SM prediction.

correlation schemes is evaluated by the best-fit value and the allowed constraints on the coupling modifier κ_λ .

In the Fully-Correlated scheme all common NPs are correlated between the various analyses.

The Simple-Scheme contains 9 correlated NPs corresponding to a few selected uncertainties in luminosity, Higgs boson mass, Higgs boson branching ratio, photon resolution, electron identification, muon trigger systematic uncertainty, JER and JES. This scheme was proposed on the basis of the 50 highest-ranked NPs based on their impacts on κ_λ in di-Higgs analyses, as illustrated in Figure 6.8. Among these NPs, eleven NPs are related to sources of uncertainties that affect also single-Higgs analyses. However, two of them, related to flavour tagging, are considered as decorrelated since different flavour tagging algorithms or working points are applied by different analyses or different categories. The remaining 9 NPs are considered as correlated in the *Simple-Scheme*.

Common Systematic Terms Between Single Higgs and diHiggs Combinations							
Nuisance Parameter Name in Workspaces	Correlation Schemes			Nuisance Parameter Name in Workspaces	Correlation Schemes		
	Simple	Advanced	Fully-Corr.		Simple	Advanced	Fully-Corr.
ATLAS_LUMI_Run2	1	1	1	ATLAS_JER_DataVSMC_Rel21			
ATLAS_MSS_lchMass	1	1	1	ATLAS_JER_EffectiveNP_10_Rel21		1	1
ATLAS_PW_DATSF_Rel21				ATLAS_JER_EffectiveNP_11_Rel21		1	1
ATLAS_PH_EFF_ID_Uncertainty		1	1	ATLAS_JER_EffectiveNP_12restTerm_Rel21	1		1
ATLAS_PH_EFF_Iso_Uncertainty		1	1	ATLAS_JER_EffectiveNP_1_Rel21			1
ATLAS_PH_EFF_TRIGGER_Uncertainty		1	1	ATLAS_JER_EffectiveNP_2_Rel21			1
ATLAS_MET_SoftTrk_ResoPara_Rel21			1	ATLAS_JER_EffectiveNP_3_Rel21			1
ATLAS_MET_SoftTrk_ResoPerp_Rel21			1	ATLAS_JER_EffectiveNP_4_Rel21			1
ATLAS_MET_SoftTrk_Scale_Rel21			1	ATLAS_JER_EffectiveNP_5_Rel21			1
TheorySig_BR_HiggsDecayWidthTHU_WW		1	1	ATLAS_JER_EffectiveNP_6_Rel21	1		1
TheorySig_BR_HiggsDecayWidthTHU_hbb		1	1	ATLAS_JER_EffectiveNP_7_Rel21		1	1
TheorySig_BR_HiggsDecayWidthTHU_hgg		1	1	ATLAS_JER_EffectiveNP_8_Rel21			1
TheorySig_BR_HiggsDecayWidthTHU_huhtau		1	1	ATLAS_JER_EffectiveNP_9_Rel21			1
TheorySig_BR_HiggsDecayWidthTHU_hyy	1	1	1	ATLAS_JES_BJES_Response_Rel21			1
TheorySig_BR_param_mB		1	1	ATLAS_JES_EffectiveNP_Detector1		1	1
TheorySig_BR_param_mC		1	1	ATLAS_JES_EffectiveNP_Detector2		1	1
TheorySig_QCDalphaS		1	1	ATLAS_JES_EffectiveNP_Mixed1			1
ATLAS_EG_RESOLUTION_ALL	1	1	1	ATLAS_JES_EffectiveNP_Mixed2			1
ATLAS_EL_EFF_ID_TOTAL_INPCOR_PLUS_UNCOR	1	1	1	ATLAS_JES_EffectiveNP_Mixed3		1	1
ATLAS_EL_EFF_Iso_TOTAL_INPCOR_PLUS_UNCOR			1	ATLAS_JES_EffectiveNP_Modelling1			1
ATLAS_EL_EFF_RECO_TOTAL_INPCOR_PLUS_UNCOR		1	1	ATLAS_JES_EffectiveNP_Modelling2			1
ATLAS_EL_EFF_TRIG_TOTAL_INPCOR_PLUS_UNCOR		1	1	ATLAS_JES_EffectiveNP_Modelling3		1	1
ATLAS_MUON_EFF_ISO_STAT_Rel21		1	1	ATLAS_JES_EffectiveNP_Modelling4		1	1
ATLAS_MUON_EFF_ISO_SYS_Rel21			1	ATLAS_JES_EffectiveNP_Statistical1		1	1
ATLAS_MUON_EFF_RECO_STAT_LOWPt_Rel21		1	1	ATLAS_JES_EffectiveNP_Statistical2		1	1
ATLAS_MUON_EFF_TrigStatUncertainty_Rel21		1	1	ATLAS_JES_EffectiveNP_Statistical3		1	1
ATLAS_MUON_EFF_TrigSystUncertainty_Rel21	1	1	1	ATLAS_JES_EffectiveNP_Statistical4_PFlow		1	1
ATLAS_MUON_ID_Rel21		1	1	ATLAS_JES_EffectiveNP_Statistical5		1	1
ATLAS_MUON_MS_Rel21		1	1	ATLAS_JES_EffectiveNP_Statistical6		1	1
ATLAS_MUON_SAGITTA_RESBIAS_Rel21			1	ATLAS_JES_Etaintercalibration_Modelling_Rel21			1
ATLAS_MUON_SCALE_Rel21		1	1	ATLAS_JES_Etaintercalibration_NonClosure_2018data_Rel21		1	1
ATLAS_TAUS_TRUEELECTRON_EFF_ELEBDT_STAT_Rel21		1	1	ATLAS_JES_Etaintercalibration_NonClosure_highE_Rel21			1
ATLAS_TAUS_TRUEELECTRON_EFF_ELEBDT_SYST_Rel21		1	1	ATLAS_JES_Etaintercalibration_NonClosure_negEta_Rel21		1	1
ATLAS_TAUS_TRUEELECTRON_EFF_ELEOLR_TOTAL_Rel21		1	1	ATLAS_JES_Etaintercalibration_NonClosure_posEta_Rel21		1	1
ATLAS_TAUS_TRUEHADTAU_EFF_RECO_TOTAL_Rel21			1	ATLAS_JES_Etaintercalibration_TotalStat_Rel21		1	1
ATLAS_TAUS_TRUEHADTAU_EFF_RNNID_1PRONGSTATSYSTPTGE40_Rel21		1	1	ATLAS_JES_Flavor_Comp_Rel21			1
ATLAS_TAUS_TRUEHADTAU_EFF_RNNID_HIGHPT_Rel21		1	1	ATLAS_JES_Flavor_Resp_Rel21			1
ATLAS_TAUS_TRUEHADTAU_EFF_RNNID_SYST_Rel21			1	ATLAS_JES_PU_OffsetMu_Rel21			1
ATLAS_TAUS_TRUEHADTAU_EFF_TRIGGER_STATDATA161718_Rel21		1	1	ATLAS_JES_PU_OffsetNPV_Rel21		1	1
ATLAS_TAUS_TRUEHADTAU_EFF_TRIGGER_STATDATA2018_Rel21		1	1	ATLAS_JES_PU_PtTerm_Rel21			1
ATLAS_TAUS_TRUEHADTAU_EFF_TRIGGER_SYSTMU161718_Rel21			1	ATLAS_JES_PU_Rho_Rel21	1	1	1
ATLAS_TAUS_TRUEHADTAU_SME_TES_INSTITUEXP_Rel21		1	1	ATLAS_JES_PunchThrough_Rel21		1	1
ATLAS_TAUS_TRUEHADTAU_SME_TES_INSTITFIT_Rel21		1	1	ATLAS_JES_SingleParticle_HighPt_Rel21		1	1
ATLAS_TAUS_TRUEHADTAU_SME_TES_MODEL_CLOSURE_Rel21		1	1	ATLAS_JES_JVT_Rel21		1	1
ATLAS_TAUS_TRUEHADTAU_SME_TES_PHYSICSLIST_Rel21		1	1	ATLAS_JES_JVT_Rel21			1

Tab. 6.7 Summary of all common 90 NPs between single Higgs and diHiggs analyses. Three correlation schemes (Simple-Scheme, Advanced-Scheme, and Fully-Correlated) are explained. The value "1" denotes the NP is correlated which indicates that the same NP name is considered in the statistical model, and the empty cell for the uncorrelated NPs. Most NPs in Simple-Scheme are included in Advanced-Scheme except for the highlighted bold ones.

The Advanced-Scheme is designed by comparing the pulls and errors of NPs from the *Non-Correlated* and *Fully-Correlated* schemes, where the errors are calculated from the Hessian matrix. To mitigate any potential issues caused by strongly constrained or pulled NPs, a standard criterion adopted for ATLAS single-Higgs analyses combinations is applied to all common NPs. Specifically, NPs with pull > 0.5 and error < 0.7 in either the *Non-Correlated* or *Fully-Correlated* schemes will be uncorrelated within the *Advanced-Scheme*. The comparison of the pulls and errors of the common NPs in each correlation scheme are illustrated in Figure 6.10. The fitted values with their uncertainties are derived from Hesse matrix calculations. As a consequence, 31 NPs are considered as uncorrelated and 59 NPs correlated in the *Advanced-Scheme*.

The negative log-likelihood results for κ_λ across all correlation schemes are illustrated in Figure 6.11. The label "Simple-2" indicates that the two NPs highlighted in Table 6.7, related to the JER systematics, are uncorrelated in the Simple-Scheme. Best-fit values are obtained under different schemes, with allowed intervals determined at 68% and 95% confidence levels. The Fully-Correlated scheme yields the most stringent interval for κ_λ , whereas the Advanced-Scheme offers the least stringent interval. To streamline the statistical model and reduce parameters,

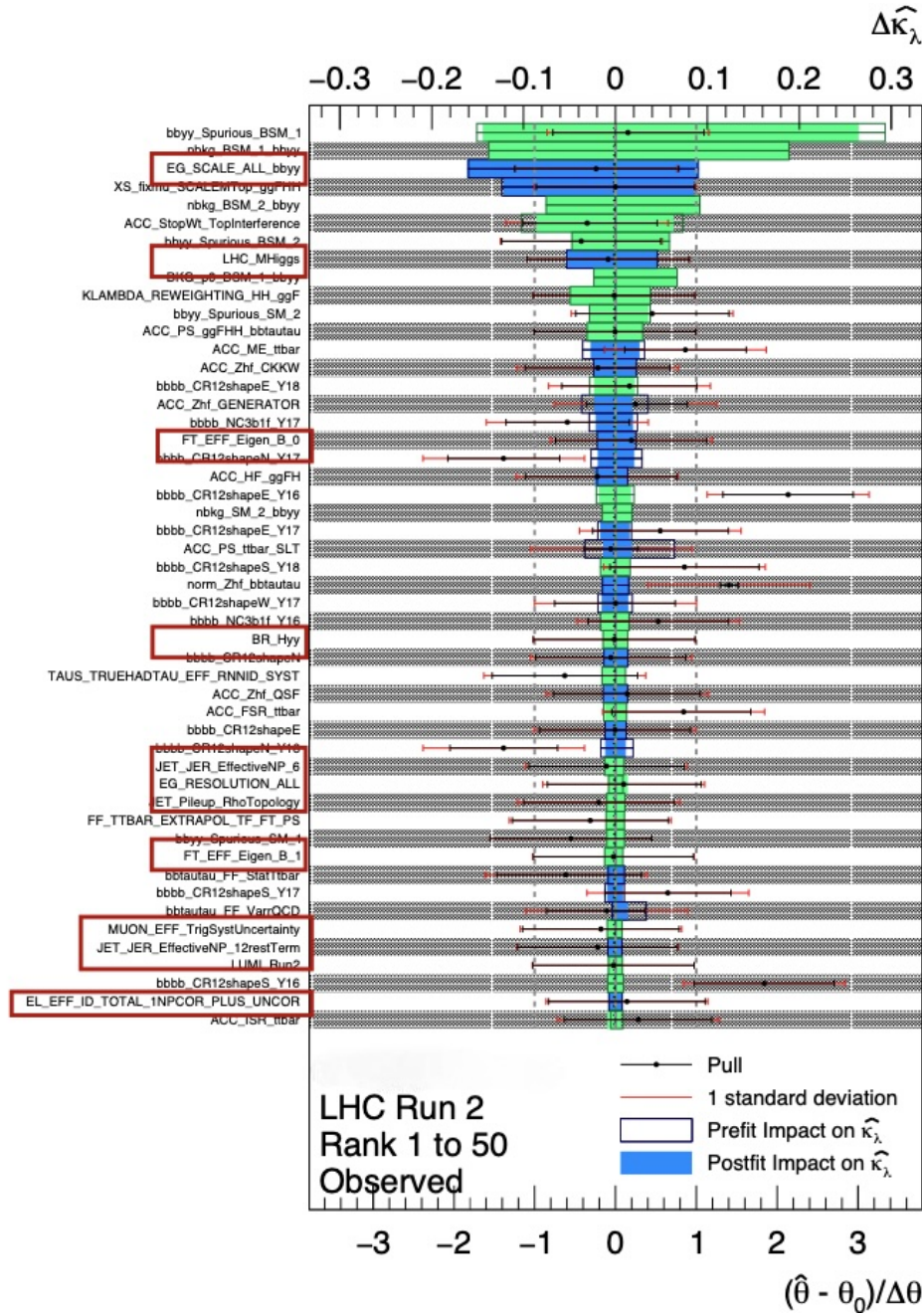
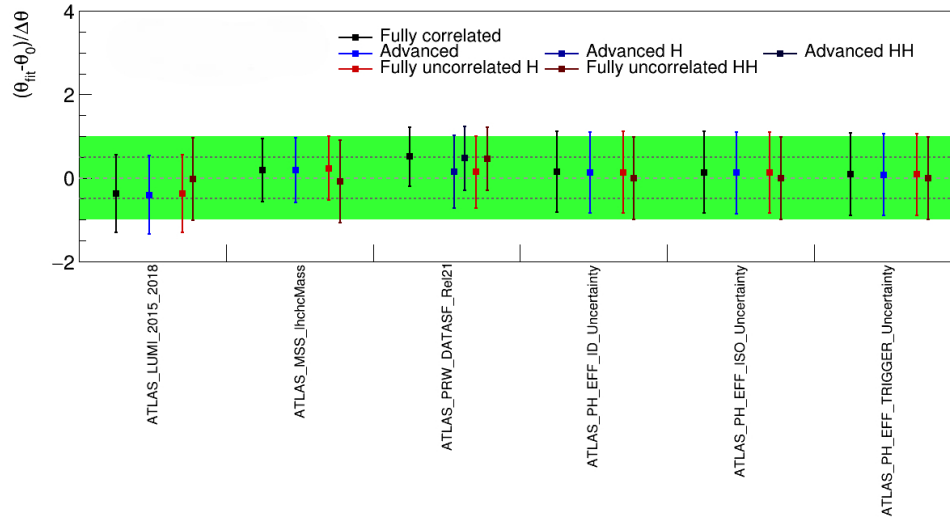


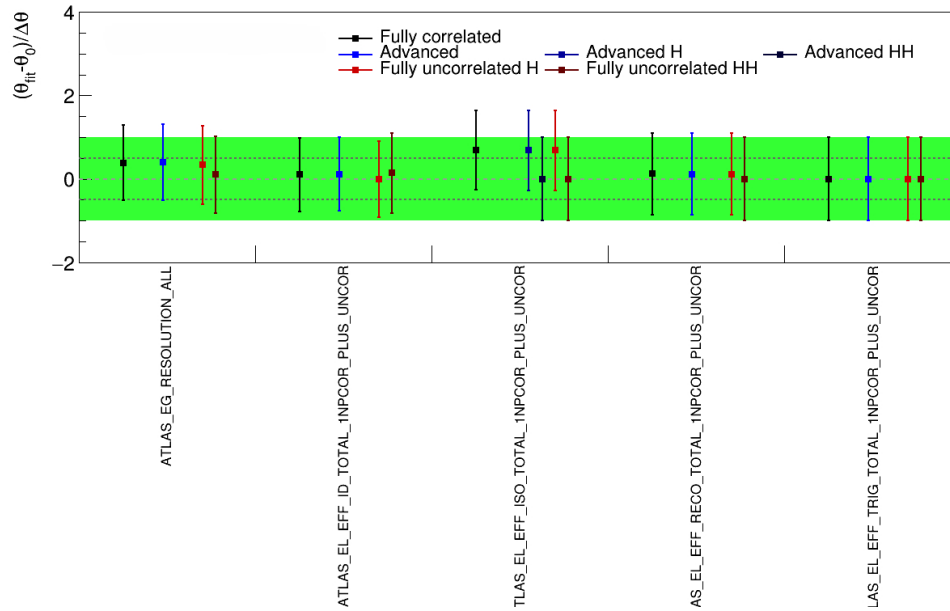
Fig. 6.8

Impact of NPs on the Higgs self-coupling modifier $\Delta\kappa_\lambda$ for the di-Higgs combination, sorted by their post-fit impact. The plot displays the top 50 NPs ranked by their influence, showing both pre-fit (blue) and post-fit (green) impacts, as well as the pull (black points) and their corresponding 1 standard deviation uncertainties (red lines). Eleven NPs highlighted in red boxes indicate NPs that are common with single-Higgs boson analyses.

while accounting for impacts on NPs from single Higgs and diHiggs analyses, the Advanced-Scheme is selected as the final correlation scheme to derive the fitted results for κ_λ .



(a) Common and Photon-related Uncertainties



(b) Electron Uncertainties

Fig. 6.9

Pulls of the common nuisance parameters in different correlation schemes of the systematic uncertainties (common, photon, and electron sources) from the observed data. Fully-Uncorrelated H (HH) indicate only single (double) Higgs model, while the Advanced H and HH cases are uncorrelated in each individual model. The Fully-Correlated scheme is also displayed for comparison.

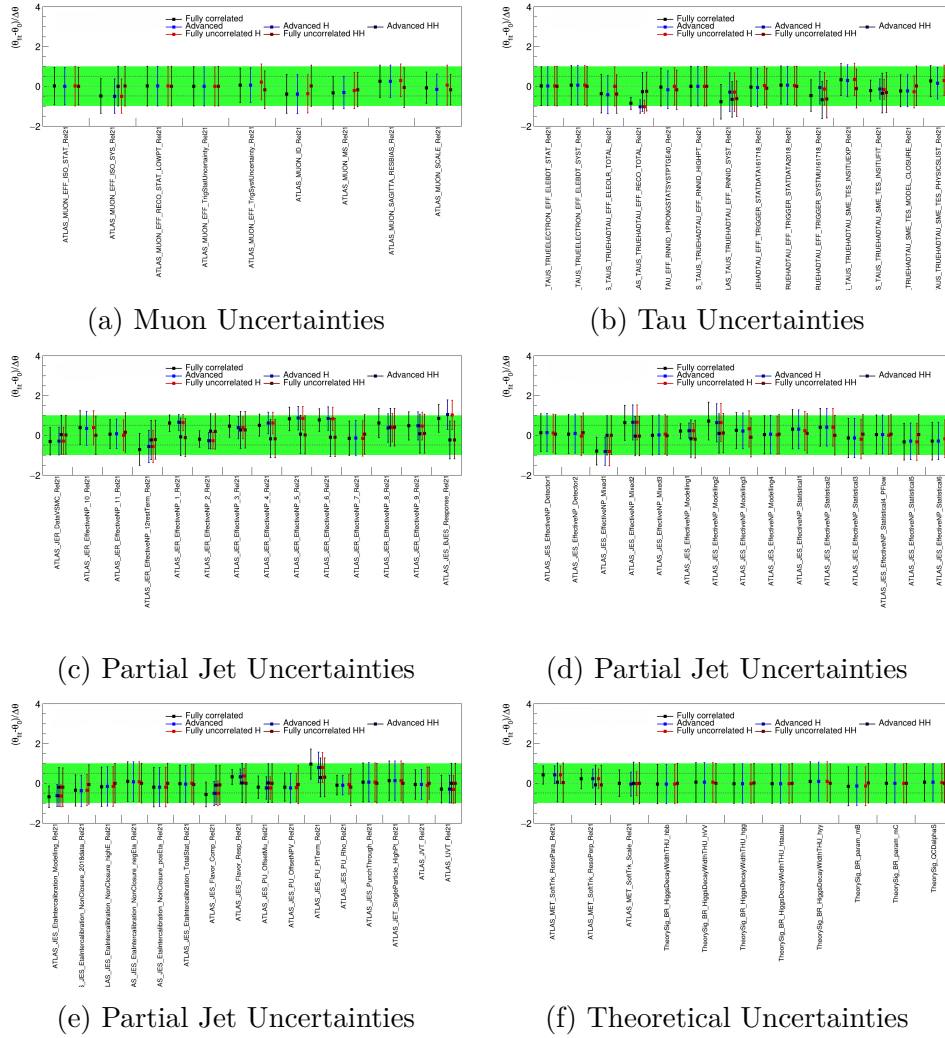


Fig. 6.10 Pulls of the common nuisance parameters in different correlation schemes of various systematic uncertainties from the observed data. Fully-Uncorrelated H (HH) indicate only single (double) Higgs model, while the Advanced H and HH cases are uncorrelated in each individual model. The Fully-Correlated scheme is also displayed for comparison.

6.6 Results

The expected and observed negative log-likelihood scans for κ_λ are shown in Figure 6.12 (a) and (b). Four curves are shown: three illustrate the scans for κ_λ when all other POIs (κ_t , κ_b , κ_τ , and κ_V) are fixed to one (labeled “ κ_λ only” in the figures), and one illustrates a scenario in which all POIs are profiled. The modifier κ_{2V} is fixed to its SM value due to the absence of a complete parameterization accounting for this modifier from single Higgs NLO EW corrections. However, a theoretical investigation [168] suggests the feasibility of parameterizing κ_{2V} , even though the contribution from single Higgs processes remains minimal. The expected constraints are derived from the Asimov dataset.

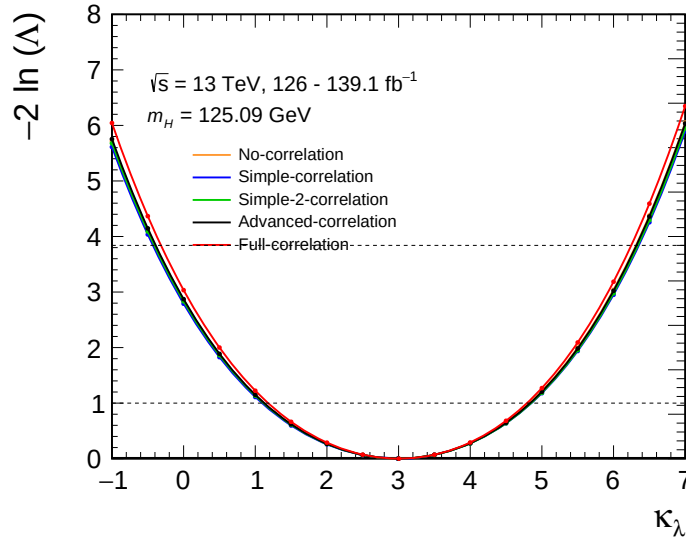


Fig. 6.11 Comparison of the negative log-likelihood scans for κ_λ from the observed data using various correlation schemes for the common nuisance parameters: Non-Correlated (orange), Simple-Scheme (blue and green), Advanced-Scheme (black), and Fully-Correlated (red). The 68% and 95% CL are displayed as the allowed intervals. The best constraints are from the Fully-Correlated scheme while the Advanced-Scheme with the impacts on NPs included and less NPs is selected as the final correlation scheme.

Comparison of Correlation Schemes for κ_λ		
Correlation Schemes	Best-Fit Values $^{+1\sigma}_{-1\sigma}$	Allowed Intervals [95% CL]
Non-Correlated	$2.992^{+1.836}_{-1.872}$	$-0.398 < \kappa_\lambda < 6.313$
Simple-2	$2.997^{+1.853}_{-1.885}$	$-0.409 < \kappa_\lambda < 6.341$
Simple-Scheme	$3.000^{+1.854}_{-1.907}$	$-0.429 < \kappa_\lambda < 6.353$
Advanced-Scheme	$2.997^{+1.839}_{-1.873}$	$-0.390 < \kappa_\lambda < 6.320$
Fully-Correlated	$3.005^{+1.788}_{-1.826}$	$-0.317 < \kappa_\lambda < 6.248$

Tab. 6.8 Comparison of best-fit values with $\pm 1\sigma$ error included and allowed intervals at 95% CL for κ_λ from different correlation schemes. The label "Simple-2" indicates that the two NPs highlighted in Table 6.7, related to the JER systematics, are uncorrelated in the Simple-Scheme. To reduce NPs and accounting for impacts on NPs from single Higgs and diHiggs analyses, the Advanced-Scheme is selected as the final correlation scheme.

The constraints on κ_λ from distinct scenarios are summarized in Tables 6.9 and 6.10, where the observed and expected values and the best-fit values are shown.

Overall, these results show that the observed data is consistent with SM predictions within the current level of uncertainty. At 95% CL, the observed (expected under the SM hypothesis) constraints for the combination are $-0.4 < \kappa_\lambda < 6.3$ ($-1.9 < \kappa_\lambda < 7.6$) when the other coupling

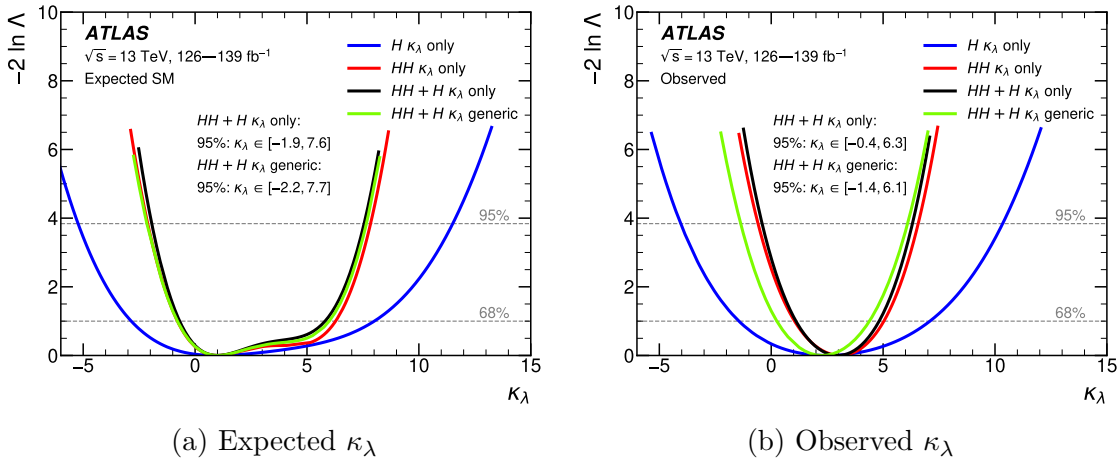


Fig. 6.12 Expected (a) and observed (b) negative log-likelihood results for the κ_λ from single-Higgs (blue), di-Higgs (red) and their combination (black) analyses. All other coupling modifiers are fixed to the SM predictions. The results from the generic Asimov dataset (green) with only κ_{2V} fixed to unity and other coupling multipliers profiled to the data for the combination is also shown. The shifted best-fit value of the generic model is caused by the correlations between the best-fit values of κ_λ and κ_b , κ_t , κ_τ . The constraints are displayed at 95% CL.

Combination Scenarios	Obs. 95% CL	Exp. 95% CL	Obs. Best-Fit $^{+1\sigma}_{-1\sigma}$
<i>HH</i> combination	$-0.6 < \kappa_\lambda < 6.6$	$-2.1 < \kappa_\lambda < 7.8$	$\kappa_\lambda = 3.1^{+1.9}_{-2.0}$
<i>Single-H</i> combination	$-4.0 < \kappa_\lambda < 10.3$	$-5.2 < \kappa_\lambda < 11.5$	$\kappa_\lambda = 2.5^{+4.6}_{-3.9}$
<i>HH+H</i> combination	$-0.4 < \kappa_\lambda < 6.3$	$-1.9 < \kappa_\lambda < 7.6$	$\kappa_\lambda = 3.0^{+1.8}_{-1.9}$
<i>HH+H</i> combination, κ_t floating	$-0.4 < \kappa_\lambda < 6.3$	$-1.9 < \kappa_\lambda < 7.6$	$\kappa_\lambda = 3.0^{+1.8}_{-1.9}$
<i>HH+H</i> combination, κ_t , κ_V , κ_b , κ_τ floating	$-1.4 < \kappa_\lambda < 6.1$	$-2.2 < \kappa_\lambda < 7.7$	$\kappa_\lambda = 2.3^{+2.1}_{-2.0}$

Tab. 6.9 Summary of expected and observed values for κ_λ under different combination assumptions. The constraints are given as 95% CL for both observed (Obs.) and expected (Exp.) results. The table also includes the best-fit values of κ_λ with their respective $\pm 1\sigma$ uncertainties. Different assumptions are considered: the di-Higgs (HH) combination, single-Higgs (Single-H) combination, combined di-Higgs and single-Higgs (HH+H), and generic model. Both κ_λ and other coupling modifiers are floated in HH combination.

modifiers are fixed to one, primarily driven by the di-Higgs analysis. The best-fit value of κ_λ is $3.0^{+1.8}_{-1.9}$. The “two-minima-like structure” seen in the expected likelihood scan arises from the quadratic relationship between the observed signal yields on κ_λ . The observed scan appears more parabolic because the best-fit lies near the point where the predicted diHiggs cross-section in Figure 6.4 (a) approaches its lowest value.

When the other coupling modifiers are profiled, the observed (expected) allowed range at for κ_λ at 95% CL is $-1.4 < \kappa_\lambda < 6.1$ ($-2.2 < \kappa_\lambda < 7.7$). As expected, the generic model provides looser constraints on κ_λ compared to the model with only κ_λ floating due to the larger number of degrees of freedom allowed to float in the fit. However, the effect is rather small. In addition

Asimov Models	Fixed or Profiled Coupling $^{+1\sigma}_{-1\sigma}$				Types	κ_λ	
	κ_t	κ_b	κ_τ	κ_V		Best-Fit $^{+1\sigma}_{-1\sigma}$	Constraints [95% CL]
κ_λ, κ -fixed	1.0	1.0	1.0	1.0	Exp.	$1.0^{+4.8}_{-1.7}$	$-1.9 < \kappa_\lambda < 7.5$
					Obs.	$3.0^{+1.8}_{-1.9}$	$-0.4 < \kappa_\lambda < 6.3$
κ_λ, κ_t -profiled	$1.0^{+0.05}_{-0.04}$	1.0	1.0	1.0	Exp.	$1.0^{+4.8}_{-1.7}$	$-1.9 < \kappa_\lambda < 7.6$
	$1.0^{+0.05}_{-0.04}$				Obs.	$3.0^{+1.8}_{-1.9}$	$-0.4 < \kappa_\lambda < 6.3$
Generic, κ -profiled	$1.0^{+0.07}_{-0.07}$	$1.0^{+0.12}_{-0.12}$	$1.0^{+0.08}_{-0.08}$	$1.0^{+0.05}_{-0.05}$	Exp.	$1.0^{+5.0}_{-1.8}$	$-2.1 < \kappa_\lambda < 7.6$
	$0.93^{+0.07}_{-0.06}$	$0.90^{+0.12}_{-0.11}$	$0.93^{+0.08}_{-0.07}$	$1.0^{+0.05}_{-0.05}$	Obs.	$2.3^{+2.1}_{-2.0}$	$-1.3 < \kappa_\lambda < 6.1$

Tab. 6.10 Summary of the expected and observed constraints at 95% CL and best-fit values with $\pm 1\sigma$ uncertainties for κ_λ under three different coupling assumptions. All other coupling modifiers are fixed to their SM values (κ -fixed), only κ_t is profiled to the data (κ_t -profiled) and all modifiers are profiled to the data (κ -profiled).

to contributing sensitivity to κ_λ , the single-Higgs analysis allows for more relaxed assumptions regarding other Higgs coupling modifiers. The Higgs-top coupling κ_t is especially crucial for the interpretation of di-Higgs data in terms of κ_λ , since the amplitude for HH production is proportional to $\kappa_t \kappa_\lambda$. Due to the stringent constraints on κ_t from single-Higgs measurements, fits with κ_t fixed to the SM value or profiled to the data yield similar constraints on κ_λ , as soon as single-Higgs data are included, as presented in Table 6.10. Fixing the other couplings to unity or profiling them has little impact in this case.

Two-dimensional constraints on κ_λ vs κ_t are also derived from the combined $H+HH$ analysis, after fixing all other coupling modifiers to their SM predictions. These results are illustrated in Figure 6.13.

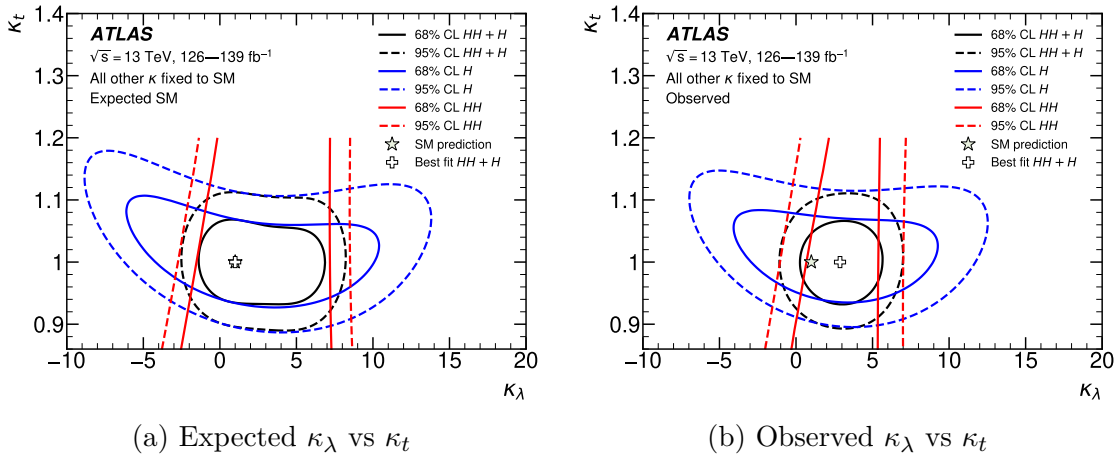


Fig. 6.13 Expected (a) and observed (b) constraints on $(\kappa_\lambda, \kappa_t)$ from single Higgs (blue), di-Higgs (red) and their combination (black) analyses. Two confidence levels are displayed at 68% (solid) and 95% CL (dashed). Only κ_t less than 1.2 from di-Higgs data is shown.

Two-dimensional constraints on κ_V vs κ_{2V} were also obtained from HH and $H+HH$ combinations, fixing all other coupling modifiers to their SM predictions. The expected and observed results are illustrated in Figure 6.14.

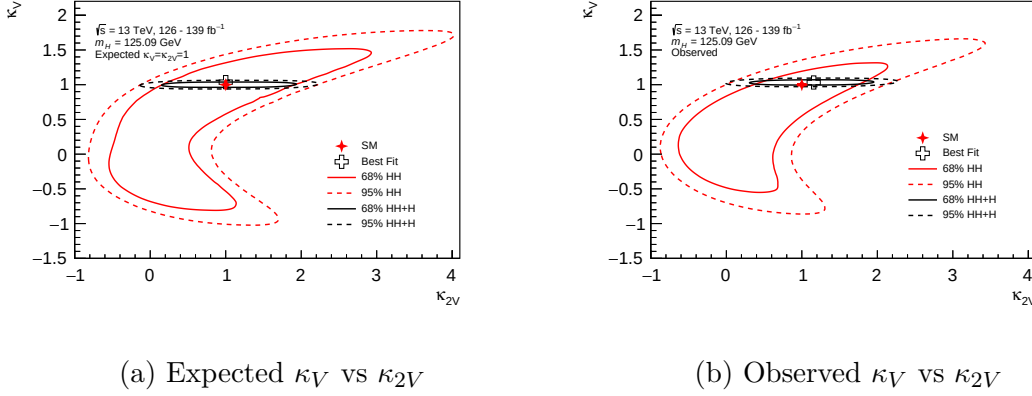


Fig. 6.14 Expected (a) and observed (b) constraints at 68% CL (solid) line and 95% CL (dashed) line on (κ_V, κ_{2V}) from the HH combination (red) and HH+H combination (black) and all other couplings are fixed to the corresponding SM predictions.

6.7 Conclusion

The combination of three ATLAS di-Higgs analyses with full Run-2 data, targeting the most sensitive final states ($b\bar{b}\gamma\gamma$, $b\bar{b}\tau^+\tau^-$, $b\bar{b}b\bar{b}$), leads to an observed (expected) upper limit on the HH signal strength of 2.4 (2.9) at 95% CL. These processes constrain κ_λ to $-0.6 < \kappa_\lambda < 6.6$ and κ_{2V} to $0.1 < \kappa_{2V} < 2.0$ at 95% CL, when the other coupling modifiers are fixed to unity.

The combination of di-Higgs ATLAS analyses with single-Higgs ATLAS analyses of eight decay channels with full Run-2 data provides a slightly more stringent constraint on the Higgs boson self-coupling than di-Higgs analyses alone. The observed allowed range at 95% CL for κ_λ is $[-0.4, 6.3]$, while the expected range is $[-1.9, 7.6]$, with κ_t floating and the other coupling modifiers fixed to one. The biggest advantage of the combination with single-Higgs data is that the constraint on κ_λ is much less model dependent, as the other coupling modifiers do not need to be fixed to the SM: in the generic model case when also κ_τ , κ_b and κ_V are floated, the constraint on κ_λ is worsened only marginally, to $[-1.4, 6.1]$. The combination with single-Higgs data thus further sheds light on the Higgs boson self-coupling and improves the constraints provided by di-Higgs data.

Conclusions and Outlook

The chapter will discuss the conclusion and outlook of the research work presented in this thesis manuscript on the search for Higgs boson pair production and the measurement of the Higgs boson self-coupling.

7.1 Summary of Higgs Boson Self-Coupling Measurements

Since the discovery of the Higgs boson in 2012, significant progress has been made in understanding the nature of electroweak spontaneous symmetry breaking. The Higgs boson self-coupling is a fundamental parameter that characterizes the Higgs potential within the Higgs mechanism. There are two primary approaches to measuring the Higgs boson self-coupling: direct measurement through Higgs boson pair production and indirect measurement via single Higgs boson production and decay exploiting the effect of the Higgs boson self-coupling through NLO electroweak corrections. This thesis presents some of the latest ATLAS measurements of the Higgs boson self-coupling, with the most stringent constraint achieved through the combined analysis of both double and single Higgs boson production.

A direct measurement of the Higgs boson self-coupling has been performed searching for Higgs boson pair production in $HH \rightarrow b\bar{b}\gamma\gamma$, one of the most sensitive channels due to clean diphoton signature and low irreducible backgrounds. The analysis uses a multivariate event selection and classification strategy to classify the events into seven categories with enhanced signal-to-background ratio. An unbinned maximum likelihood fit to the diphoton invariant mass spectrum of the selected events in each category is performed to determine signal and background yields. The expected upper limit on the signal strength μ_{HH} (μ_{HH}^{VBF}) is 4.95 (132.27) at 95% CL, while the constraint on the coupling modifier κ_λ (κ_{2V}) is [-2.02, 7.13] ([-1.06, 3.27]), when only statistical uncertainties are included. An alternative analysis strategy with multi-classification and binary-classification was investigated as an attempt to further enhance the significance of the

search. Eight categories are defined in this alternative approach, and a similar fit is performed to interpret the selected events. The alternative strategy yields an expected upper limit on μ_{HH} (μ_{HH}^{VBF}) of 5.00 (106.39) at 95% CL and an expected constraint on the coupling modifier κ_λ (κ_{2V}) of $[-1.95, 6.93]$ ($[-1.02, 3.20]$), when only statistical uncertainties are considered. Compared to the baseline analysis, the alternative strategy provides a promising improvement in terms of sensitivity to the coupling modifiers and the VBFHH signal strength. Even though the final results are limited by the statistical uncertainty, the systematic uncertainties from experimental and theoretical sources are fully evaluated and implemented in the statistical model for the interpretation of the data with the baseline analysis strategy. No significant excesses are observed over the expected background. The observed (expected) upper limit on μ_{HH} is 3.96 (5.03) at 95% CL while that on μ_{HH}^{VBF} is 99.81 (131.17) at 95% CL. A negative log-likelihood scan is performed to extract the constraint on the Higgs boson self-coupling modifier and the VVHH vertex coupling modifier. The Higgs boson self-coupling modifier is constrained within the range $-1.44 < \kappa_\lambda < 6.92$ ($-2.84 < \kappa_\lambda < 7.82$) while the VVHH vertex coupling modifier is constrained to the range $-0.48 < \kappa_{2V} < 2.68$ ($-1.11 < \kappa_{2V} < 3.31$). The systematic uncertainties led to 1-2% decrease in the expected upper limit on signal strengths (μ_{HH} and μ_{HH}^{VBF}) and coupling modifiers (κ_λ and κ_{2V}). The systematic uncertainty sources with the largest impacts on these results are the renormalization and factorization scales, as well as photon energy resolution.

An indirect measurement of the Higgs boson self-coupling is derived from single Higgs boson production and decay by accounting for NLO electroweak corrections to the predicted Higgs boson production cross section and branching ratios in the statistical interpretation of the data. The combination of various ATLAS single-Higgs boson analyses offers some sensitivity to the Higgs boson self-coupling. A negative log-likelihood scan is performed to extract the constraint on the Higgs self-coupling modifier. From the combination of ATLAS single-Higgs boson measurements, the observed (expected) best-fit value of κ_λ is $2.50_{-3.94}^{+4.60}$ ($0.96_{-3.82}^{+7.05}$), while the 95% CL confidence interval is $-4.0 < \kappa_\lambda < 10.3$ ($-5.2 < \kappa_\lambda < 11.5$). In parallel, the three most sensitive ATLAS searches for boson pair production ($HH \rightarrow b\bar{b}\gamma\gamma$, $HH \rightarrow b\bar{b}b\bar{b}$, $HH \rightarrow b\bar{b}\tau^+\tau^-$) are combined to directly measure the Higgs self-coupling. The combination gives an observed (expected) upper limit of the signal strength μ_{HH} is 2.4 (2.9) at 95% CL. The best-fit value for κ_λ is $3.1_{-2.0}^{+1.9}$ ($1.0_{-1.8}^{+5.3}$) from the likelihood scan. The Higgs self-coupling modifier κ_λ is constrained within the range $-0.57 < \kappa_\lambda < 6.57$ ($-2.11 < \kappa_\lambda < 7.84$) at 95% CL. The VVHH vertex coupling modifier κ_{2V} is constrained to the range $0.1 < \kappa_{2V} < 2.0$ ($0 < \kappa_{2V} < 2.1$). These results are obtained fixing the other coupling modifiers of the Higgs boson to unity, as in the SM. Finally, single-Higgs boson and di-Higgs boson data are interpreted together in terms of the Higgs boson self-coupling. The impact of overlapping events among signal and control regions of different analyses are evaluated and found to be negligible. The different correlation schemes of systematic uncertainties between single-Higgs and di-Higgs analyses are investigated to obtain the final results. The joint analysis integrates the results from the dominant single Higgs boson analyses with those from the double Higgs boson combination through reediting the statistical workspaces. Distinct Asimov datasets are generated for the various scenarios. The observed (expected) constraint on κ_λ from the joint interpretation is $[-0.4, 6.3]$ ($[-1.9, 7.6]$) while the best-fit value is $3.0_{-1.9}^{+1.8}$, when the other Higgs boson coupling modifiers are fixed to one. The combination with single-Higgs analyses makes it possible to use the data to constrain

the Higgs boson couplings, and thus κ_λ can be floated while the other coupling modifiers are profiled. The allowed interval on κ_λ from this more generic model is $[-1.4, 6.1][[-2.2, 7.7]]$ with the best-fit value of $2.3^{+2.1}_{-2.0}$ at 95% CL from the likelihood scan.

The observed results from NLL for other significant decay channels are shown in Figure 6.5 (b). The $b\bar{b}\gamma\gamma$ and $b\bar{b}\tau^+\tau^-$ channels exhibit relatively narrow and symmetric profiles, with best-fit values near SM expectation of $\kappa_\lambda = 1$, indicating a stronger sensitivity to small deviations from the SM. In contrast, the $b\bar{b}b\bar{b}$ channel with heavy QCD backgrounds displays a broader curve with a minimum at significantly higher κ_λ , reflecting a weaker sensitivity and larger uncertainties in this channel, which allows for a wider range of self-coupling values. The combination of all channels provides the most stringent constraints, with a best-fit value around $\kappa_\lambda = 3.1$, excluding negative values at the 68% confidence level. This result points toward a potential enhancement in the Higgs self-coupling, deviating from the SM prediction, while simultaneously ruling out large negative values with high confidence. The combined analysis underscores the importance of multi-channel approaches in providing robust constraints on κ_λ , offering insights into potential new physics in the Higgs sector. The best-fit and constraints on κ_λ are summarized in Table 6.5.

The CMS experiment has also conducted a search for Higgs boson pair production in the $b\bar{b}\gamma\gamma$ channel [169], and has constrained the Higgs self-coupling parameter κ_λ through the combination of single and double Higgs boson analyses [170]. The results of these analyses are displayed in Figure 7.1 (a) and (b), respectively. In the $b\bar{b}\gamma\gamma$ channel, CMS places an observed (expected) constraint on κ_λ of $-3.3 < \kappa_\lambda < 8.5$ ($-2.5 < \kappa_\lambda < 8.2$) at 95% CL. The expected sensitivity is consistent with the ATLAS experiment, while large discrepancy is observed in the observed constraints. Several factors contribute to this discrepancy, including statistical fluctuations, distinct analysis strategies, systematic uncertainties, etc. However, the combined CMS analysis, which incorporates both single and double Higgs production, constrains κ_λ to the range $-1.24 < \kappa_\lambda < 6.49$ at 95% CL, in good agreement with the combined result from ATLAS.

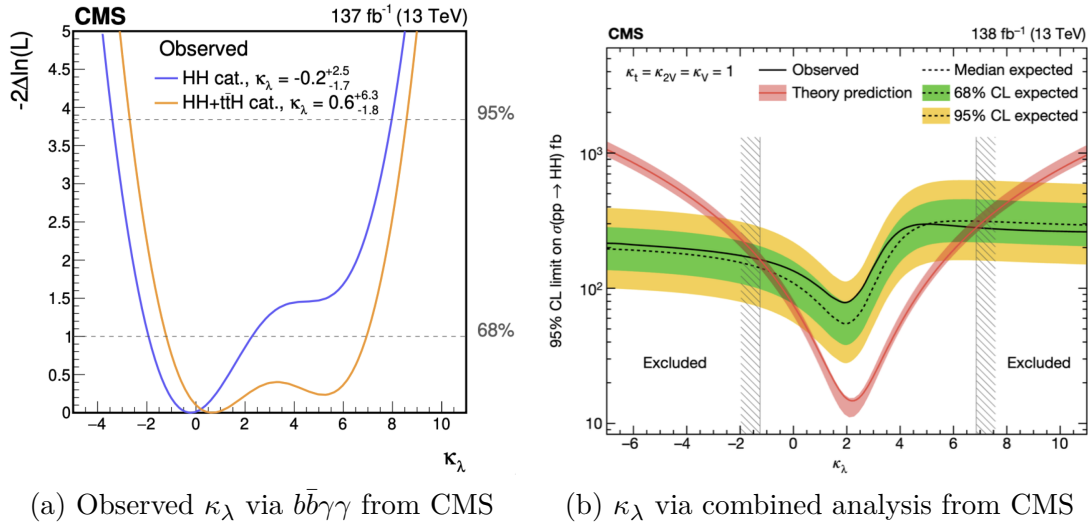


Fig. 7.1 Observed constraints on the Higgs self-coupling κ_λ from CMS via the $b\bar{b}\gamma\gamma$ [169] and combined analyses [170].

Finally, some studies related to the photon identification under the harsher pile-up envi-

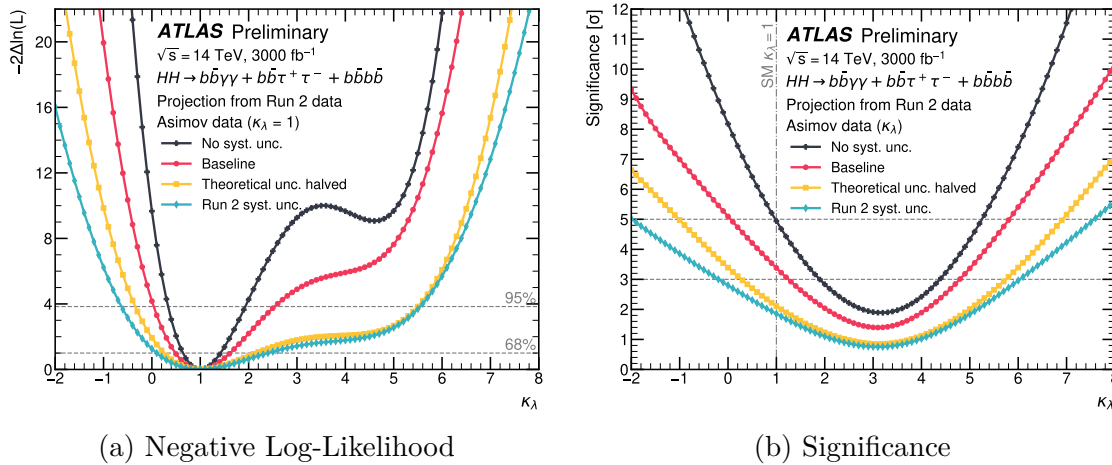
ronment at ATLAS experiment for the Run-3 of the LHC are presented. Prompt photons were identified using a cut-based method applied to nine shower shape variables. The increased pileup environment is expected to reduce the efficiency of prompt photon identification algorithm used in Run-2. To address this issue, an optimization was performed using a Genetic Algorithm implemented in the TMVA software toolkit to define μ -dependent requirements on the shower shape variables. The performance of the new criteria was evaluated as a function of pile-up and photon pseudorapidity and transverse momentum. The prompt photon identification efficiency was improved at high pile-up by 10-15% and remains stable across the full range of pile-up conditions, while the fake photon rejection rate experienced a reduction of up to 20-25%. The expected sensitivity of single (di-) Higgs boson measurements with $H \rightarrow \gamma\gamma$ decays and high pile-up data could thus be increased by about 9-13% (10-15%).

7.2 Future Prospects for Higgs Boson Self-Coupling Measurements

The quest to measure the Higgs boson self-coupling with high precision is pivotal in testing the electroweak spontaneous symmetry breaking (Higgs mechanism) and probing potential new physics scenarios. While current measurements provide only weak constraints, future advancements in collider technology and analysis methods promise significant improvements in this area.

The statistical uncertainty is the dominant source of the measurement, so the statistical power of these measurements is expected to increase with more data. The LHC Run-3 is ongoing since 2022, with an anticipated integrated luminosity of more than 200 fb^{-1} , more than doubling the size of the previous dataset. Furthermore, the HL-LHC, with an integrated luminosity of 3000 fb^{-1} , will drastically increase the statistical power available for Higgs boson physics, particularly in rare processes such as Higgs boson pair production. Figure 7.2 (a) and (b) illustrates the projected sensitivity to κ_λ at the HL-LHC for various Higgs boson pair production decay channels. The NLL plot shows that the HL-LHC has the potential to measure κ_λ with a high degree of precision, as indicated by the sharp minimum around the Standard Model value, $\kappa_\lambda = 1$. However, the width of the curves highlights the strong dependence of this precision on systematic uncertainties. The significance plot suggests that, under baseline assumptions (black line), the HL-LHC will likely constrain κ_λ within a range near the SM prediction, with a significance of approximately 2 to 3σ , contingent on the level of uncertainties. The red curve, which assumes no systematics, demonstrates that the sensitivity could be significantly higher in an idealized scenario, while the yellow curve (halved theoretical uncertainties) underscores the potential gains in precision that could be achieved through improvements in theoretical predictions. In summary, the HL-LHC is expected to measure κ_λ with moderate to strong significance, with the possibility of achieving greater precision if systematic uncertainties, particularly theoretical ones, are reduced.

Beyond the HL-LHC, several proposed future collider projects offer exciting prospects for the Higgs boson self-coupling measurements. The Future Circular Collider (FCC), which could reach proton-proton center-of-mass energies of up to 100 TeV, represents a significant step forward in energy reach and luminosity, potentially enabling percent-level precision in the Higgs boson self-coupling measurement. Proposed linear colliders such as the International Linear Collider (ILC) and the Compact Linear Collider (CLIC) promise to provide complementary measurements of

**Fig. 7.2**

Projections of the Higgs self-coupling (κ_λ) measurement at the HL-LHC. The plots show (a) the Negative Log-Likelihood ($-2\Delta\ln L$) and (b) the Significance as functions of κ_λ , based on Asimov data ($\kappa_\lambda = 1$) and projections for the HL-LHC with an integrated luminosity of 3000 fb^{-1} . The analysis [171] combines the $b\bar{b}\gamma\gamma$, $b\bar{b}\tau^+\tau^-$, and $b\bar{b}b\bar{b}$ decay channels. Different systematic uncertainties are compared: No systematic uncertainties (red), Baseline (black), Theoretical uncertainties halved (yellow), and Run 2 systematic uncertainties (cyan).

the Higgs boson self-coupling with precision at the 15-20% level through precise single and double Higgs boson production in a clean electron-positron collision environment. These facilities are expected to achieve high precision due to their clean experimental environments and the ability to tune collision energies.

The application of advanced analysis techniques, including machine learning for event classification, is expected to further enhance the sensitivity of these measurements, allowing for tighter constraints on the Higgs boson self-coupling parameter. The future of Higgs boson self-coupling measurements also lies in the combination of results from multiple channels. By integrating findings from Higgs boson pair production with those from single Higgs boson processes, particularly in rare decay channels, the overall constraint on the Higgs boson self-coupling can be significantly improved. Additionally, global fits that incorporate both direct measurements and indirect constraints from electroweak precision observables will be crucial in refining our understanding of the Higgs potential. These fits will help reduce uncertainties from assumptions on the other Higgs boson couplings and provide a more comprehensive picture of the Higgs sector.

Advances in theoretical and computational methods will also be essential in future Higgs boson self-coupling studies. Improved theoretical predictions, including higher-order corrections and more precise modeling of backgrounds, will help reduce the theoretical uncertainties that currently limit the interpretation of experimental data. The development of more sophisticated Monte Carlo event generators and advanced simulation tools will further enhance the accuracy of predictions for both signal and background processes, enabling more precise extractions of the Higgs self-coupling.

The larger dataset and various analysis improvements could bring ATLAS and CMS close

to the first evidence at more than three standard deviations for Higgs boson pair production by the end of Run-3, while the HL-LHC tenfold larger sample, improved detectors, and further progress in analysis techniques could lead to observation at more than five standard deviations, with constraints on the Higgs boson self-coupling at 50% level or better.

The potential discovery of deviations from SM predictions in Higgs boson self-coupling measurements would provide compelling evidence for new physics. As future experiments achieve greater precision, they will become increasingly sensitive to such deviations, offering insights into possible extensions of the SM, such as models with additional scalar fields or modified Higgs potentials. These measurements will also be interpreted in conjunction with other observables, such as Higgs boson couplings to fermions and vector bosons, providing a more holistic understanding of the Higgs sector and its role in the fundamental structure of the universe. In conclusion, the future of Higgs self-coupling measurements is promising, with substantial prospects for significant advancements in precision and sensitivity.

APPENDICES

The following appendices document additional research activities performed during my Ph.D. thesis. Additional materials related to the trigger studies and hardware design are recorded in Appendices. Appendix [A](#) describes work performed on glass resistive plate chamber (GRPC) gas detector for the ATLAS Muon Phase-II Upgrade project. The design of the fast timing readout electronics and the development of data acquisition system (DAQ) for a Semi-Digital Hadronic Calorimeter (SDHCAL) for the Circular Electron-Positron Collider (CEPC), performed within the CALICE Collaboration, are described in Appendix [B](#). Investigations and preliminary results for new ATLAS triggers studied to collect $H \rightarrow Z(\nu\nu)\gamma$ events and increase the sensitivity of the current searches for the rare Higgs boson decay to $Z\gamma$ are presented in Appendix [C](#).



Glass Resistive Plate Chamber

Since the resistive plate chamber was proposed in 1981 [172], lots of possible improvements like eco-friendly gas and various materials are investigated. This work focused on the structure optimization of the glass resistive plate chamber (GRPC). The GRPCs with different structure and size were simulated and fabricated in the clean rooms. The efficiency of the chamber was evaluated with a cosmic rays platform.

A.1 Introduction to Resistive Plate Chamber

Resistive Plate Chambers (RPCs) are gaseous detectors that have become indispensable in high-energy physics experiments, particularly in the detection of muons, neutrinos, and cosmic rays. Their prominence is attributable to their exceptional time resolution, straightforward construction, and cost-effectiveness. RPCs are integral components in experiments requiring precise timing measurements, such as those conducted at the LHC and other particle physics facilities. Additionally, their utility extends to fields like medical imaging, where precision timing is crucial.

A.1.1 Mechanism of Gas Detectors

RPCs operate on the fundamental principle of gas ionization within a confined chamber, leading to the detection of traversing charged particles. The typical RPC configuration consists of two parallel resistive plates, often fabricated from materials like bakelite or glass, separated by a narrow gap filled with a carefully selected gas mixture, commonly comprising Argon, Freon, and iso-butane. As a charged particle passes through the chamber, it ionizes the gas, generating electron-ion pairs.

The mechanisms of the resistive plate chamber are illustrated in Figure A.1 and described below:

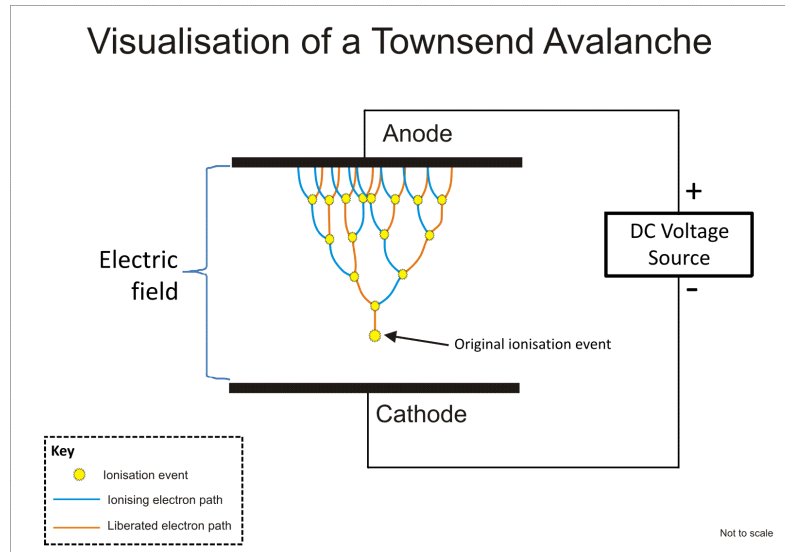


Fig. A.1 Visualization of the ionization avalanche process in gas detectors. The ionized electrons and ions are drifted along the resistive plates under the strong electric field generated by the high voltage. Credits: [Wikipedia](#)

- **Electric Field and Gas Ionization:** The resistive plates are subjected to a high voltage, establishing a strong electric field across the gas-filled gap. When a charged particle traverses this region, it ionizes the gas molecules along its trajectory, creating primary ionization clusters.
- **Avalanche Multiplication:** The initial ionization acts as a seed for an electron avalanche, driven by the strong electric field. The electrons generated in the ionization process are accelerated towards the anode, creating further ionization events through collisions with gas molecules. This leads to a rapid multiplication of charge carriers, culminating in a detectable avalanche of electrons moving towards the positive electrode, while ions migrate towards the negative electrode.
- **Signal Detection:** The avalanche-induced charge is collected by external readout electrodes, typically implemented as strips or pads, which are positioned adjacent to the resistive plates. The resulting signals are then processed by sophisticated data acquisition systems, enabling precise determination of both the position and the timing of the particle's passage through the detector.

RPCs offer time resolutions in the nanosecond range, making them highly suitable for applications requiring precise timing measurements. The relatively low cost of materials and construction for RPCs makes them an attractive option for large-scale detector arrays. RPCs are robust detectors capable of functioning reliably under a wide range of environmental conditions. Whereas, the rate capability of RPCs is limited by their design, which can pose constraints in environments with high particle flux. Over extended periods, the materials in RPCs may experience degradation, leading to a decline in performance. Ongoing research is focused on enhancing the longevity and reliability of RPCs through improved materials and design optimizations. The work investigated the single-gap glass resistive plate chamber in this thesis.

A.1.2 Glass Resistive Plate Chamber

The GRPC is an advanced variant of RPCs that utilizes glass for the resistive plates, offering distinct advantages in detector performance. These include enhanced mechanical stability, reduced aging effects, and improved resistance to environmental factors. The use of glass as the resistive material ensures consistent and reliable detector performance over extended operational periods.

The construction of GRPCs typically features two parallel glass plates separated by a gas-filled gap. A high voltage is applied across these plates, generating the electric field necessary for gas ionization. This ionization process produces electron avalanches, which are subsequently collected by external readout electrodes for signal processing. Figure A.2 illustrates the fundamental schematic of the GRPC. The single-gap GRPC is composed of two parallel glass plates, with an anode measuring 0.7 mm in thickness and a cathode measuring 1.1 mm. The central regions of the chamber are supported by cylindrical nylon spacers (8 mm diameter, 1.2 mm height), while the edges are reinforced by FR4 walls and sealed with epoxy AB glue. The external surfaces of the glass plates are coated with a thin layer of graphite (at the micrometer level) for high-voltage application. To prevent sparking and protect the readout electrodes, a 0.2 mm thick Mylar insulation film is placed on the exterior of both the anode and cathode. The readout copper strips, which collect the induced charges from the electron avalanches, are positioned close to the outer surface of these films and are integrated onto a supporting honeycomb panel. The gas inlet and outlet at the corners are connected to the chamber for maintaining the appropriate gas mixture. The GRPC is filled with a gas mixture comprising 94.7% $\text{C}_2\text{H}_2\text{F}_4$ (R314a, a refrigerant), 5% C_4H_{10} (isobutane), and 0.3% SF_6 (sulfur hexafluoride). R314a serves as the primary ionizing medium, providing excellent electron drift characteristics that contribute to the overall ionization efficiency. Isobutane acts as a quenching agent, absorbing excess energy from ionized electrons and preventing secondary discharges or sparking within the chamber. Sulfur hexafluoride, a highly electronegative gas with a strong affinity for free electrons, enhances the quenching process by capturing free electrons, thereby preventing unwanted secondary ionizations. This reduces noise in the detector and improves its timing resolution.

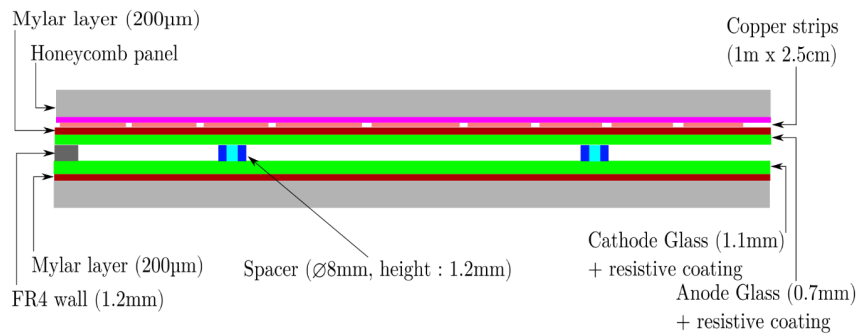


Fig. A.2 Schematic of a common Glass Resistive Plate Chamber (GRPC) with a gap of 1.2 mm.

A.2 Gas Flow Simulation

According to the structure description, the motivation for gas flow simulation is to reduce the dead zone through optimizing the assignment (number and position) of the spacers in the GRPC. The optimization of the numbers of inlet and outlet for the gas are taken into account. The target design is to obtain the similar detection efficiency under the common working high voltage while less dead zone.

First of all, various attempts of the GRPCs with different structure and size were simulated using the MultiPhysics Simulation Tools COMSOL [173]. The theorem governing gas flow in COMSOL MultiPhysics is based on the principles of fluid dynamics, primarily the Navier-Stokes equations, which describe the motion of gases and fluids. These equations, combined with the conservation laws of mass, momentum, and energy, form the foundation for gas flow simulation. The continuity equation ensures the conservation of mass, while the Navier-Stokes equations account for the conservation of momentum by balancing forces such as pressure, viscous effects, and external forces. Additionally, the energy conservation equation governs heat transfer and temperature variations within the flow. To fully describe the behavior of gases, an equation of state, such as the ideal gas law, relates pressure, temperature, and density. COMSOL solves these equations numerically, using finite element methods (FEM) to simulate gas flow behavior under various conditions, providing insights into complex fluid dynamics problems.

In these works, the critical evaluation of the performances for the gas flow simulation are the velocity and the pressure inside the chamber. Whereas the vorticity should be a better factor to evaluate the gas distribution inside the chamber, the future work will take the evaluation method. Some structure models of the GRPCs with a size of $20 \times 20 \text{ cm}^2$ and a gas gap of 1.2 mm are shown in Figure A.3, which are constructed from the software. The investigations primarily concentrate on the optimization of the inlet and outlet design, and the spacer shifts. Figure A.3 (a) depicts the normal design of the GRPC with one inlet and one outlet using FR4 wall building a space with $2.2 \times 0.7 \times 0.12 \text{ cm}^3$. While (b) and (c) display the same designs with two outlets and one inlet but distributed in different positions. The spacer shifts are exhibited in (d) and (e) under the designs (b) and (c) respectively, where the spacers are reduced and shifted to suppress the dead zone. The inlet and outlet of all the models utilize the plastic PPP tubes of inner diameter 0.8mm and outer diameter 1.2mm.

During the simulation, some initial conditions including the material, the flow speed, the pressure, the mesh, and the boundary conditions are set. Nitrogen gas is considered as the material and the mesh setting used extremely coarse due to the limit of computing sources. Additionally, the boundary condition for the inlet is the gas inflow speed set as 1 m/s and the pressure of the outlet boundary condition is set as atmospheric pressure (101.3 kPa). The primary evaluations are the velocity and the pressure, which are illustrated in Figure A.4 and Figure A.5, respectively.

In the Normal Design Figure A.4 (a), the maximum velocity reaches approximately 1.27 m/s, concentrated near the inlet and outlet, while the rest of the chamber experiences much lower velocities, approaching $5.62 \times 10^{-6} \text{ m/s}$ in the central region, indicating uneven flow distribution. The Outlet Design Figure A.4 (b) and Inlet Design Figure A.4(c) the maximum velocity is significantly lower, with peak values around 0.1 m/s, suggesting that these designs

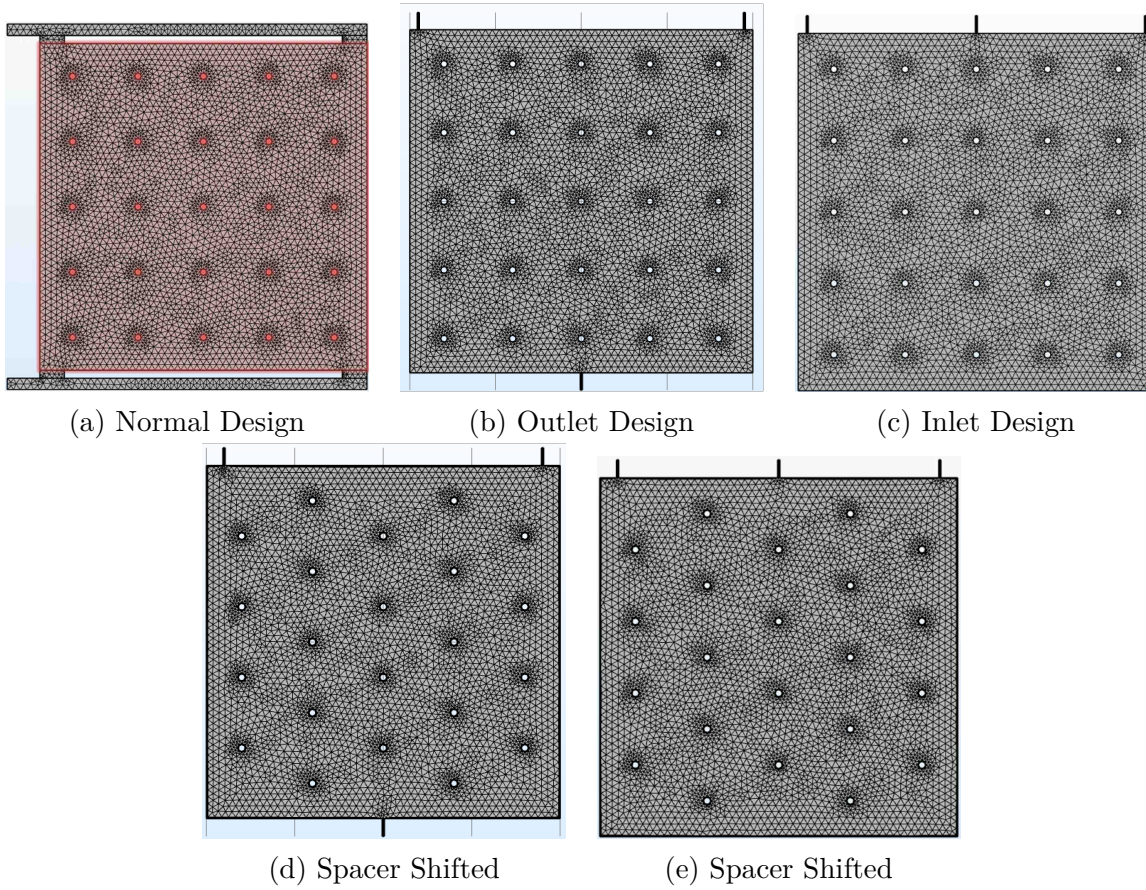
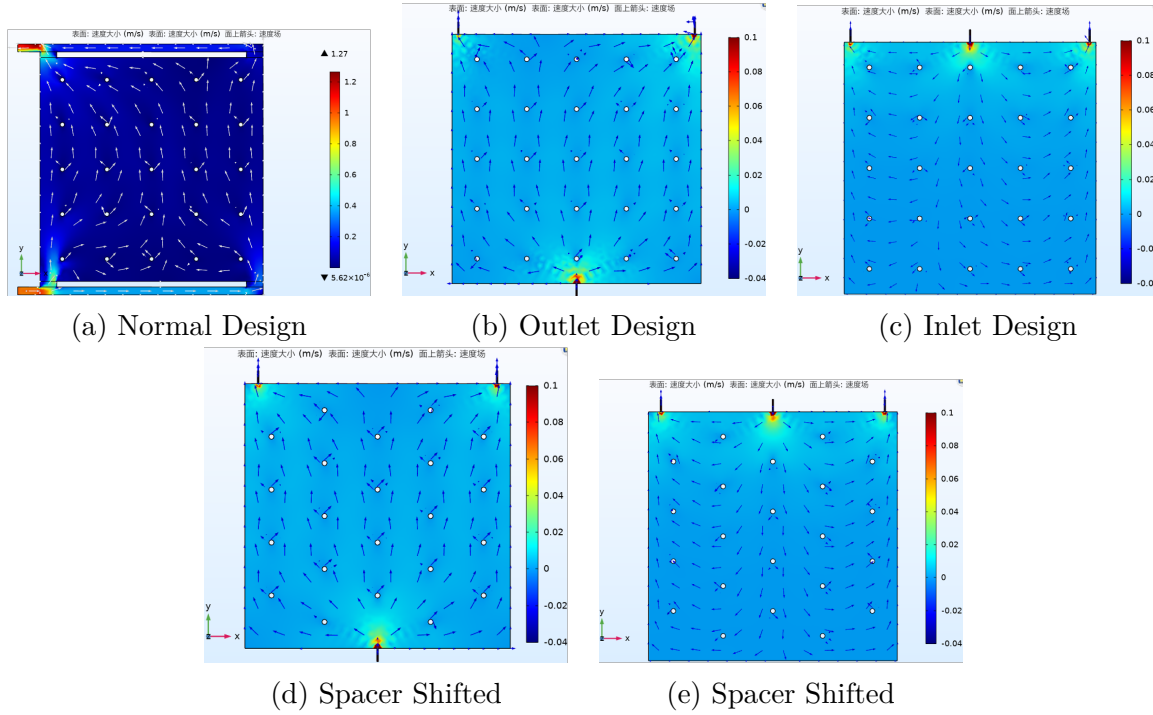


Fig. A.3 Models of various designs of the GRPCs with a size of $20 \times 20 \text{ cm}^2$ and a gas gap of 1.2 mm for the gas flow simulation in COMSOL. (a) Normal design with one inlet and one outlet, red shadowed region as the sensitive zone. (b) and (c) designs with two outlets and one inlet assigned in two sides or the same side of the chamber respectively. Under the designs (b) and (c), the spacers are reduced and shifted in (d) and (e) to suppress the dead zone.

result in a more balanced and slower flow throughout the chamber. In both designs, the flow is more uniformly distributed, and the velocity magnitude in the central region remains relatively constant around 0.04 m/s. For the Spacer Shifted Designs Figure A.4 (d and e), the velocity fields remain below 0.1 m/s in most areas, similar to the Outlet and Inlet Designs. The central regions experience velocities close to 0.04 m/s, but the flow direction is more affected by the spacers. This design shows slightly higher velocities near the boundaries, with peak values also near 0.1 m/s, maintaining a more consistent flow compared to the Normal Design. These numerical results highlight how design changes in the GRPCs affect gas flow, with each modification influencing flow uniformity and velocity distribution across the detector.

In the Normal Design Figure A.5 (a), the pressure ranges from $1.012998 \times 10^5 \text{ Pa}$ to $1.013252 \times 10^5 \text{ Pa}$, with the highest pressure near the inlet and outlet. The pressure is unevenly distributed across the chamber, and pressure gradients are visible, especially near the boundaries. In the Outlet Design Figure A.5 (b) and Inlet Design (c), the pressure distribution is more uniform,

**Fig. A.4**

Velocity field distribution in x-y plane for various GRPCs designs based on gas flow simulations performed in COMSOL. The velocity magnitude, represented by color, shows the flow behavior in meters per second (m/s), while the arrows indicate the direction of the gas flow.

with pressure values ranging from 1.012999×10^5 Pa to 1.013017×10^5 Pa in the Outlet Design and from 1.013004×10^5 Pa to 1.013056×10^5 Pa in the Inlet Design. These designs show smoother pressure fields across the GRPC chamber, indicating improved gas flow dynamics compared to the Normal Design. The Spacer Shifted Designs Figure A.5 (d and e) also exhibit uniform pressure distributions, with ranges from 1.012999×10^5 Pa to 1.013131×10^5 Pa in (d) and from 1.012999×10^5 Pa to 1.013077×10^5 Pa in (e). In both designs, the pressure variation is minimal across the chamber, showing that the spacer placement has a moderate effect on pressure uniformity. Overall, the design modifications improve the uniformity of the pressure distribution, with the Normal Design showing the most significant pressure variations and the other designs achieving more balanced flow conditions.

A.3 GRPC Fabrication Procedure

Under the help from USTC and Lyon group, we built the fabrication procedure for the GRPCs in the clean room. The whole fabrication process of the GRPC chamber involves several key steps to ensure its structural integrity and gas tightness. Initially, the walls and pipes are positioned carefully (Step 1) and then glued (Step 2). After securing the structure, a spacer position sketch is drawn on the surface to indicate where spacers will be placed (Step 3). The spacers are then carefully placed onto the glass (Step 4) and glued to ensure stability (Step 5).

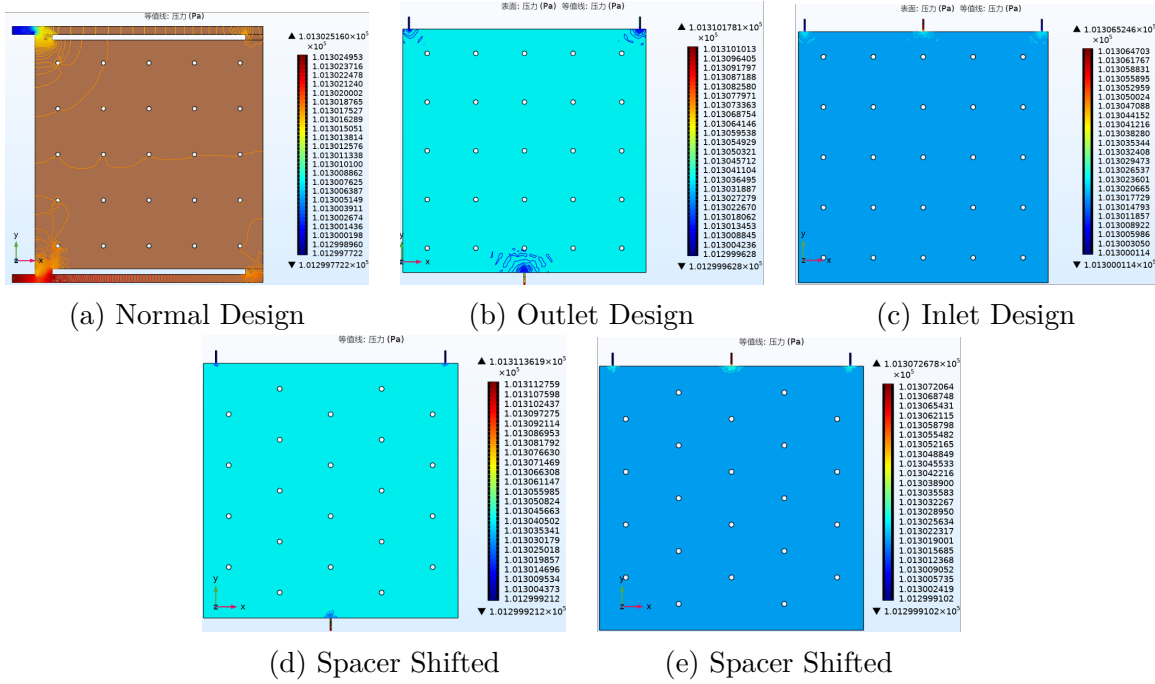


Fig. A.5 Pressure distribution in x-y plane for various GRPCs designs based on gas flow simulations performed in COMSOL. The pressure is measured in Pascals (Pa), and contour lines indicate areas of equal pressure.

A second glass is glued onto the walls to enclose the chamber (Step 6). The chamber is made gas-tight using silicone, and leak tests are performed to ensure proper sealing (Step 7). Finally, the exterior is finished with graphite coating and mylar fixing (Step 8) to enhance conductivity and protect the structure, completing the assembly. This sequence is crucial for achieving a high-quality, functional detector for particle physics experiments. The construction procedure of a small size chamber is elaborated in Figure A.6.

Followed the above procedure, the gas chamber with $35 \times 50 \text{ cm}^2$ and 1.2 mm gap as shown in Figure A.8 (a) for testing was constructed in the clean room. Besides, the conductive graphite coating is made by the silk screen printing method [174], which is illustrated in Figure A.7 (a) and (b). The graphite coating is formed by mixing two different products (PM404 84% and S6017 16%) and their fraction will drastically affect the resistivity. Stirring the mixture for 10 minutes is to ensure enough uniformity. The 300 mesh screen is used to print the graphite layer on the chamber. The graphite layer is dried under a lamp with a temperature 80-90 degrees Celsius for 2 hours in Figure A.7 (c). The surface resistivity uniformity of the graphite coating layer is evaluated using four-probe method [175]. Figure A.7 (d) and (e) show the resistivity distribution of two graphite layers, which indicates good uniformity with a mean value of $3.24 \text{ M}\Omega/\square$. The coated chamber will be protected by the APET mylar film with a thickness of 0.2 mm. Figure A.8 displays the gas chamber (a) in the clean room and physical GRPC (b) with a size of $35 \times 50 \times 0.12 \text{ cm}^2$.

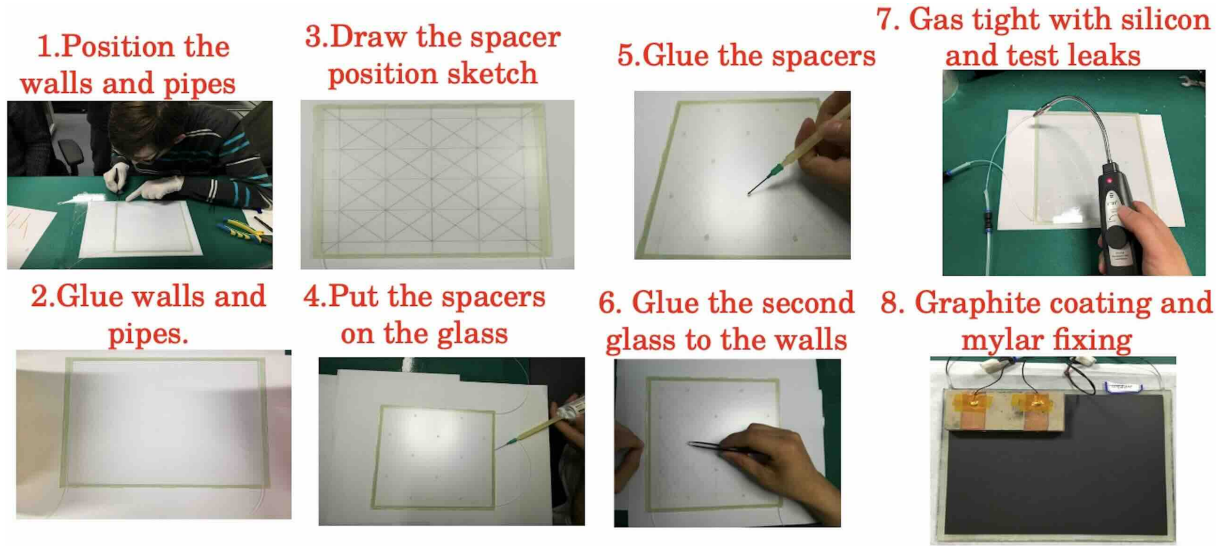


Fig. A.6 Step-by-step fabrication process of the chamber, illustrating the critical stages from positioning walls and pipes to graphite coating and final assembly.

A.4 Cosmic Ray Test Platform

As cosmic ray muons, with an approximate rate of $1/(\text{min} \cdot \text{cm}^2)$ and the mean energy of around 3-4 GeV at sea level [176], pass through the detector, ionized electrons and ions are drifted by a strong electric field. The 2 cm-wide readout strips generate induced charges, which are transmitted to the front-end board and amplified with a gain factor of 16. The schematic diagram illustrating the principle of the cosmic ray test is shown in Figure A.9. Four plastic scintillator detectors, each measuring $40 \times 20 \text{ cm}^2$, are positioned above and below the GRPC detector chamber to trigger cosmic rays. The signals from these scintillators are combined to provide a trigger for measuring detector efficiency. The data acquisition system is developed using CAEN V172 modules with a 5 GB/s digitization rate. The platform setup for the cosmic ray test in the crack is depicted in Figure A.10. The braid coppers are used to protect the electronics from the static charges.

Prior to data collection, the detectors undergo high voltage training, where the voltage is incrementally increased from 2 kV to 8 kV to ensure stable, efficient, and reliable long-term performance. This process is critical for conditioning the RPCs to operate effectively under the high electric fields required for precise particle detection. During the training, the detector materials, particularly the resistive plates and the gas mixture, are stabilized, minimizing the occurrence of electrical discharges, commonly referred to as *sparking*.

Figure A.12 (a) shows the current versus voltage curve for the GRPC chamber with dimensions of $35 \times 50 \times 0.12 \text{ cm}^2$. The current remains stable at around a few hundred nano-amperes (nA) throughout the voltage range, particularly between 6 kV and 8 kV, which is the standard operational range. However, once the voltage exceeds 8 kV, the chamber capacitor nears breakdown, resulting in a sharp increase in current.

The muon signal captured from the chamber is displayed on the oscilloscope in Figure A.11 (a), with corresponding data recorded by the DAQ system in Figure A.11 (b). The rising edge

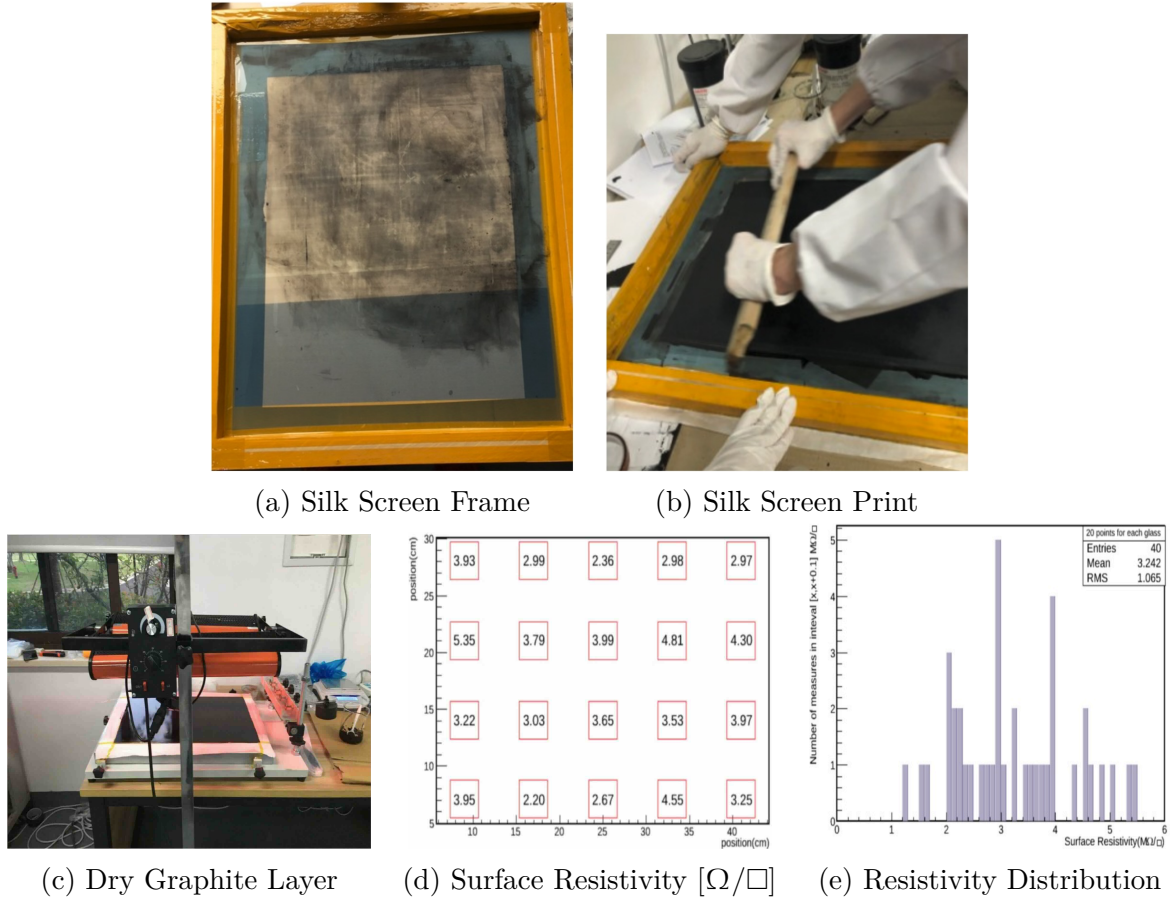


Fig. A.7 Process of making the conductive graphite coating of the chamber with the high voltage electrodes. The procedures are displayed in (a) and (b), while (c) expresses the dry process. The surface resistivity (d) for one side coating. The resistivity distribution (e) from two sides of the chamber.

is around a few nano-second and the amplitude is approximately 10 mV.

The efficiency (ϵ) is defined as the ratio of the number of muons passing both scintillators ($N_{\text{triggered}}$) divided by the total number of muons detected by a GRPC (N_{signal}). The detector efficiency as a function of high voltage is shown in Figure A.12 (b). The efficiency increases with the high voltage, and the plateau is reached at around 7kV where the efficiency is more than 95%. Based on the platform, further optimizations are investigated and published in Reference [177].

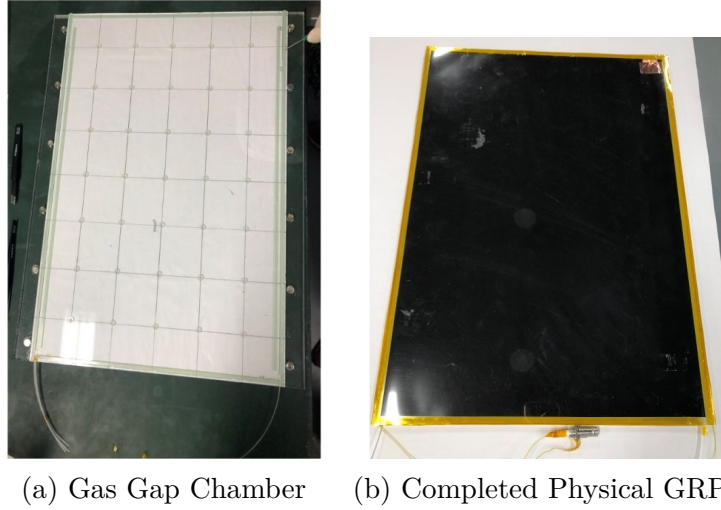


Fig. A.8 Gas Chamber (a) and Physical GRPC (b) with $35 \times 50 \text{ cm}^2$ constructed in the clean room and the high voltage electrodes are positioned in the chamber.

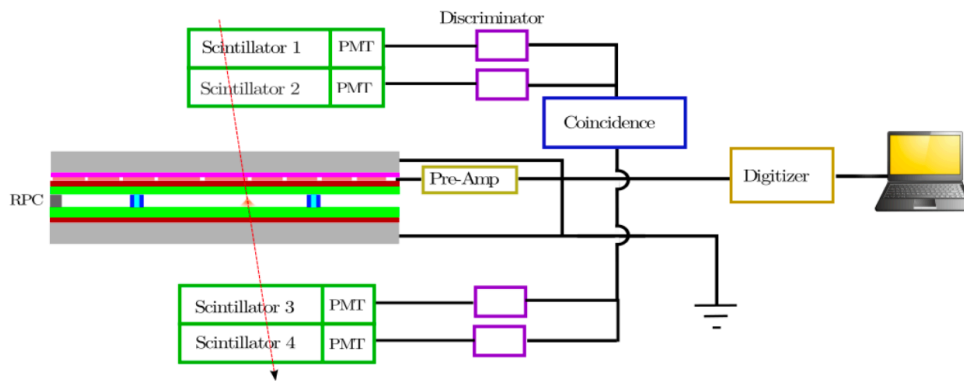


Fig. A.9 Principle of the measurement of the detection efficiency using the muons from the cosmic ray. Scintillators are considered as triggers to measure the detector efficiency.

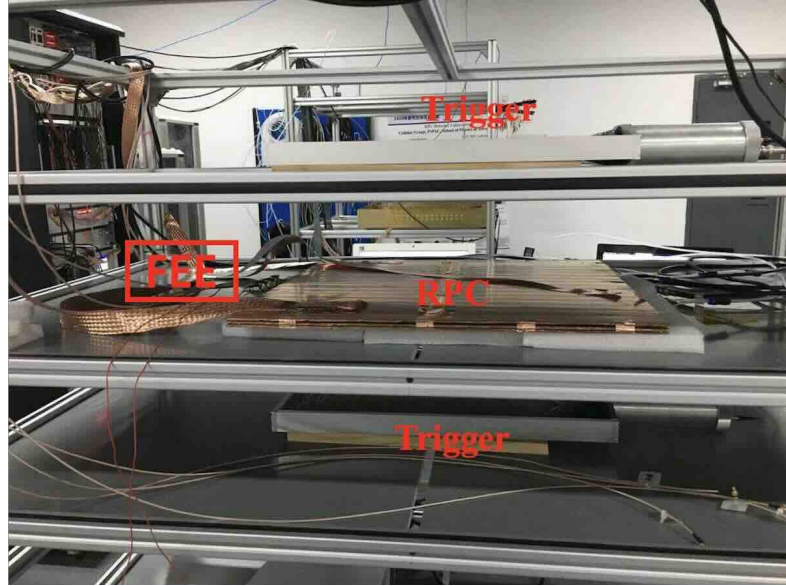
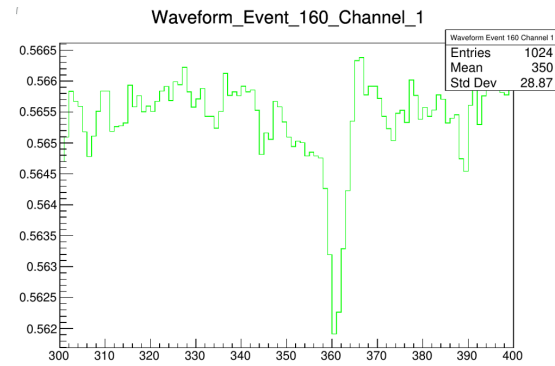


Fig. A.10 View of the cosmic ray test platform. Scintillators are placed on the top and bottom of the detector. The detector with the corresponding readout strips and electronics (FEE) is in the middle region, where the chamber is surrounded by the honeycomb readout panel. The braid copper connected to the underground is used to protect the electronics by transferring the static charges to the ground. Gas and high voltage on the right side of the platform are connected to the GRPC.

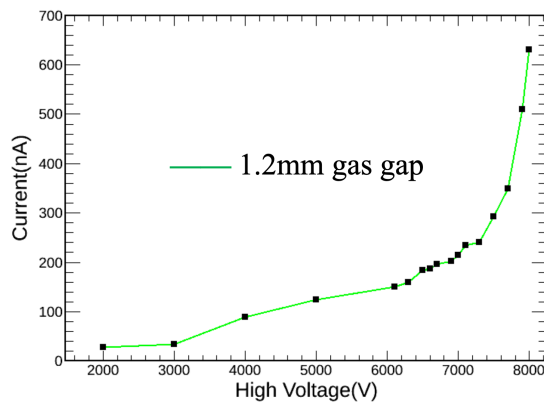


(a) Signal from Oscillator

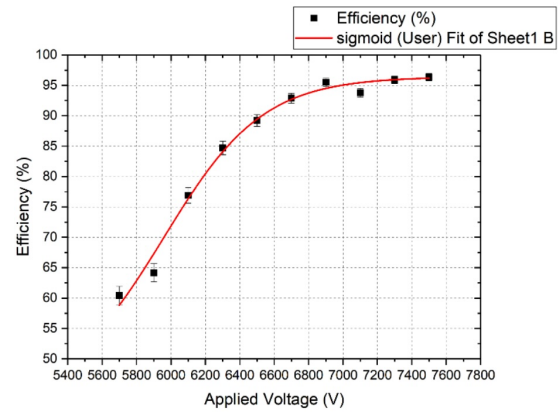


(b) Signal from DAQ System

Fig. A.11 Observed muon signal from the cosmic ray: (a) Oscilloscope waveform without the front-end board (FEB), showing the trigger signal from a scintillator (green) and the positive and negative signals from two readout panels (cyan and pink). (b) Digitized signal shown by the DAQ system from one channel of FEB.



(a) I vs V Curve



(b) Detector Efficiency.

Fig. A.12 Performance plots of the fabricated GRPC detector: (a) Current versus high voltage curve for the detector training. (b) Detector efficiency curve versus the high voltage from the cosmic ray test.

APPENDIX B

Fast Timing Electronics Readout System Design

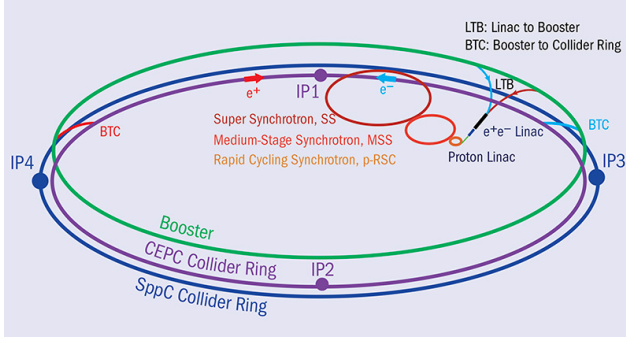
The Circular Electron Positron Collider (CEPC), a proposed high-energy particle collider to be built in China [178], aims to advance particle physics research. The Semi-Digital Hadronic Calorimeter (SDHCAL), originally designed for the International Linear Collider (ILC) and tested with beams at CERN [174], is a potential option for the CEPC detector. The SDHCAL offers excellent energy resolution and track reconstruction capabilities. Through Geant4 simulations, it has been shown that integrating timing information can further enhance SDHCAL performance. In this strategy, the single-gap GRPC will be replaced by a Multi-gap GRPC to improve timing resolution. As the original electronics are not compatible with this upgrade, new readout electronics based on PETIROC2B (an Application Specific Integrated Circuit, ASIC) have been developed to achieve fast time resolution. The design of these readout electronics, including the data acquisition system (DAQ), will be discussed in this chapter.

B.1 Introduction to CEPC and SDHCAL

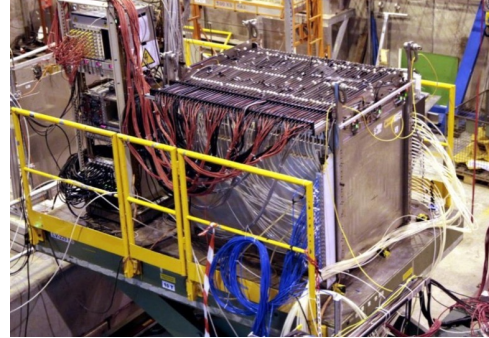
The CEPC in Figure B.1 (a), with a 100 km circumference, is designed to study the Higgs boson through electron-positron collisions at 240 GeV [178]. It aims to provide high-precision measurements of Higgs couplings, offering valuable insights into potential new physics beyond the standard model. The SDHCAL [174] in Figure B.1 (b) is a potential option of the hadronic calorimeters for the CEPC.

The SDHCAL is a type of hadronic calorimeter based on particle flow algorithm (PFA) [179] consisting of 48 active layers, each utilizing $1 \times 1 \text{ m}^2$ single-gap GRPCs as the sensitive medium, with overall dimensions of $1 \times 1 \times 1.3 \text{ m}^3$. Its primary feature is high granularity, enabling precise detection of energy deposits in small, distinct regions. This fine spatial resolution enhances particle energy measurement accuracy and improves the reconstruction of complex particle showers. The SDHCAL employs a semi-digital readout system, which differs from traditional analog

readout calorimeters by measuring energy deposits in discrete levels rather than continuously. Typically, three threshold levels (110 fC, 500 fC, 15000 fC) that means the induced charges by the hit are used to record energy deposits, providing improved energy resolution and reducing data size, thereby optimizing analysis efficiency. The readout system consists of 440,000 channels, with 144 HARDROC ASICs, each handling 64 channels. The SDHCAL demonstrates excellent reconstruction energy resolution, achieving 7.7% at 80 GeV [174, 180], and shows strong particle identification capabilities for hadrons [181].



(a) Overall of CEPC-SppC Layout



(b) Semi-Digital Hadronic Calorimeter

Fig. B.1 Layout of CEPC-SppC accelerator. Credits: IHEP. Image of semi-digital hadronic calorimeter designed by CALICE collaboration [174].

B.2 Motivation of Timing

Figure B.2 shows the time evolution of hadronic showers within the SDHCAL for two cases: one including neutrons (a) and one excluding neutrons (b). In both scenarios, the spatial and temporal progression of the shower is clearly observed. The presence of neutrons significantly increases the average distance from the shower axis and extends the overall shower duration, as indicated by the broader distribution in both spatial and temporal dimensions compared to the neutron-free case. Neutron interactions contribute to the production of secondary particles and scatter the shower development, resulting in a more widespread distribution in both distance and time. Consequently, timing information plays a crucial role in identifying delayed neutrons, which can enhance energy reconstruction accuracy in the detector.

Figure B.3 illustrates the impact of time resolution on the separation of hadronic showers within the SDHCAL. In plot (a), with a time resolution of 1 ns, the shower is distributed over multiple cells, resulting in a broader and less precise spatial representation. In contrast, plot (b), which features a finer 100 ps time resolution, shows a more confined and precise localization of the shower. The enhanced resolution significantly reduces the spread of energy deposits, improving the ability to distinguish between closely spaced showers. This refinement is essential for optimizing PFA, which depend on accurate reconstruction of individual particle showers in high granularity detectors like the SDHCAL.

To achieve better time measurements, single-gap GRPCs are replaced with multi-gap GRPCs (MGRPCs)[182], which offer significantly better time resolution, typically in the range of tens

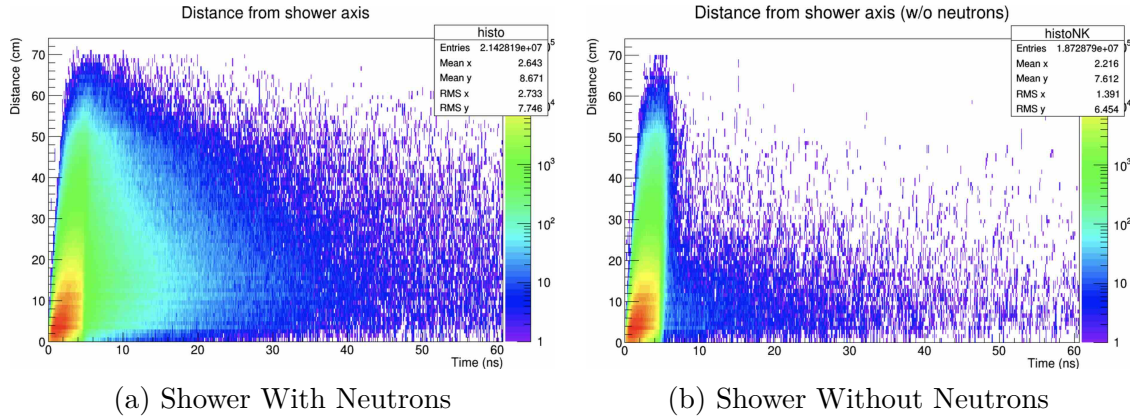


Fig. B.2 Time evolution of hadronic showers in the SDHCAL, comparing showers with (a) and without (b) neutron contributions. The x-axis represents time in nanoseconds, while the y-axis indicates the distance from the shower axis in centimeters. The color scale on the right depicts the number of entries in the histogram, with higher densities in red and lower densities in blue. The presence of neutrons cause a more diffuse and prolonged shower, as evidenced by the wider distribution in both time and distance in (a). Credits: CALICE SDHCAL group.

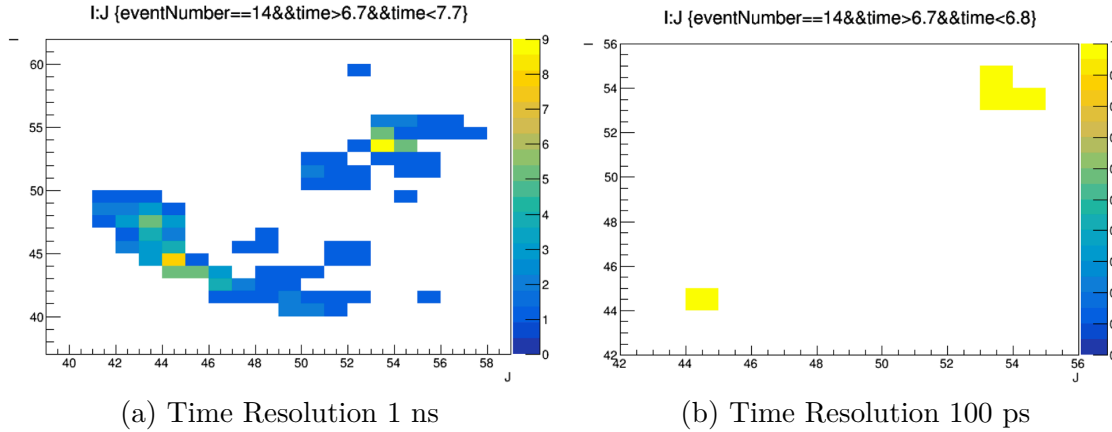


Fig. B.3 Comparison of hadronic shower profiles in the SDHCAL at different time resolutions: 1 ns (a) and 100 ps (b). The finer time resolution enhances the localization of energy deposits, reducing overlap between nearby showers and improving the accuracy of PFA. Credits: CALICE SDHCAL group.

of picoseconds[183]. The structure of the MGRPC is shown in Figure B.4 (a). To process the fast signals from the MGRPC, the PETIROC2B ASIC chip [184], displayed in Figure B.4 (b) and developed by the OMEGA company, is employed. This chip can achieve time resolutions better than 20 ps, and when combined with the MGRPC, the overall time resolution can reach below 50 ps. As a result, the corresponding readout electronics must be specifically designed to accommodate both the MGRPC and the PETIROC2B ASIC. Thanks to its high granularity and excellent time resolution, the SDHCAL will evolve into a five-dimensional (5D) imaging detector, offering precise measurements of position, energy, and time.

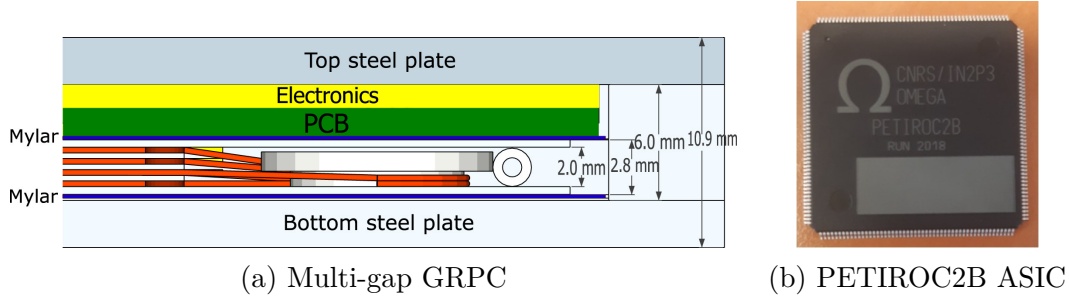


Fig. B.4 Structure of the multi-gap GRPC (a) [183] and the picture of PETIROC2B ASIC chip (b) [184].

B.3 Readout Board Design

The readout system comprises a front-end board (FEB) and a detector interface board (DIF). The FEB is designed using the PETIROC2B ASIC and positioned on the exterior of the MGRPC to read out the induced charge signals. The DIF board facilitates the connection between the FEB and the ZCU102 FPGA board, on which the data acquisition system is developed.

B.3.1 PETIROC2B ASIC Chip

The PETIROC2B front-end ASIC is designed using AMS $0.35\ \mu\text{m}$ SiGe technology [184] and comes in an LQFP 208 package with dimensions of $28 \times 28 \times 1.4\ \text{mm}$. The block diagram and chip layout, as shown in Figure B.5 (a) and (b), include both analog and digital components. This chip contains 32-channels, each of which integrates a preamplifier, a fast and low-jitter trigger, achieving precise measurements of both charge and time. These functionalities are configured through 648 shift registers (SR), also known as Slow Control parameters.

The charge measurement is based on the integration of the input signal from all channels, depicted in Figure B.5 (a). Upon detecting a signal, a variable time shaper conditions the pulse for optimal integration, ensuring that the charge is accurately measured over a controlled shaping time. The processed signal is subsequently digitized by a 10-bit analog-to-digital (ADC), converting the integrated analog charge into a precise digital value.

The time measurement utilizes both coarse and fine timing techniques for high-precision temporal resolution, illustrated in Figure B.6 (a). The coarse timing is handled by a 9-bit counter synchronized with a 40 MHz clock, providing a digital time stamp that records the arrival of an event. Fine timing is achieved via a Time-to-Amplitude Converter (TAC), which interpolates between clock pulses (25 nanoseconds), explained in Figure B.6 (b). The TAC generates an analog signal proportional to the time interval between the event trigger and the nearest clock edge. This signal is digitized by an ADC, yielding a fine time measurement with a jitter of approximately 18 ps RMS, ensuring exceptional temporal accuracy.

The ADC conversion and readout system for charge and time measurements is illustrated in Figure B.7 (a). The coarse time (9-bit) and hit signal (1-bit) from the Switch Capacitor Array (SCA) are encoded into 10-bit registers, while the fine time (10-bit) from the TAC and charge values (10-bit) are also respectively recorded in 10-bit registers using Wilkinson ADCs. The output data, encoded in Gray format, includes 960 bits of information for coarse time, hit, fine

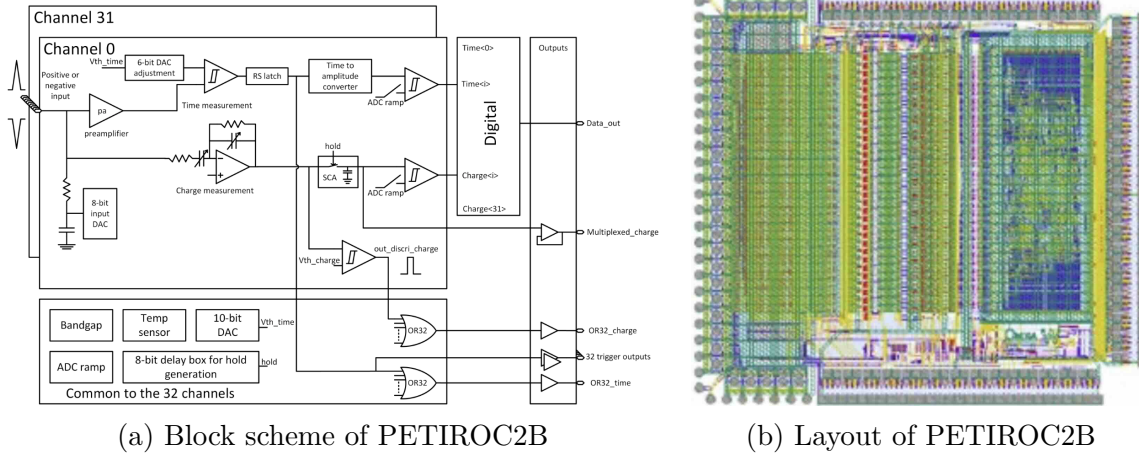


Fig. B.5 Block scheme (a) and layout (b) of PETIROC2B ASIC [184].

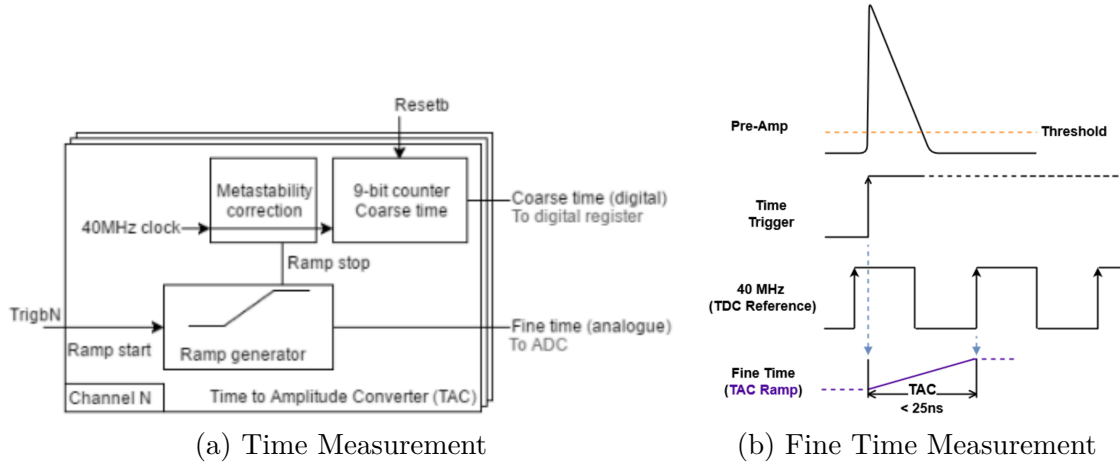


Fig. B.6 Theorem of time measurement (a) and fine time measurement (b) of PETIROC2B ASIC.

time, and charge, requiring approximately $12 \mu s$ for transmission. Figure B.7 (b) displays the memory address mapping of the encoded output data, which is transmitted to the computer via the DAQ system operating at 80 MHz. The acquired data can be further converted to the measurements following the formula:

$$T_{\text{Absolute Time}} = (T_{\text{Coarse Time}} + 1) \times (\text{clock } 40 \text{ MHz period}) - T_{\text{Fine Time}} \quad (\text{B.1})$$

where the coarse time and fine time are decoded from the readout data, with the fine time having a resolution of 37 ps per ADC unit. The coarse time is measured with a clock period of 25 ns, which is used by the counter for its calculations.

B.3.2 Front End Readout Board

Considering the dimension of SDHCAL, the front-end board should be the same size as the MGRPC ($1 \times 1 \text{ m}^2$). The project is divided into two phases that are the verification of the

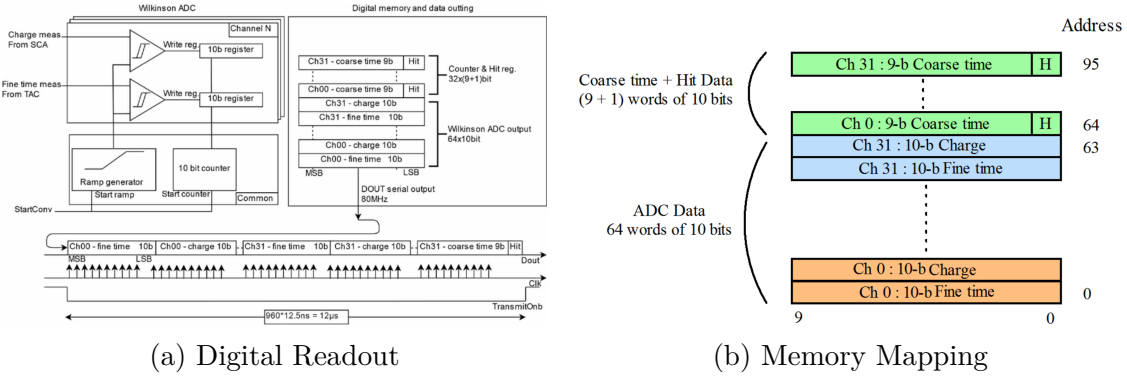


Fig. B.7 Schematic of the ADC conversion and readout system (a) and the memory address mapping (b) with 960 bits output of PETIROC2B ASIC.

function of PETIROC2B and the final design of the FEB for SDHCAL. The verification phase is conducted by designing a small front-end board ($19 \times 8 \text{ cm}^2$) with four PETIROC2B chips. The scheme of the verification platform is shown in Figure B.8, where the FEB and FPGA ZCU102 are connected through an adapted board (DIF). The DAQ system in PC communicates with FPGA ZCU102 through the Ethernet port.

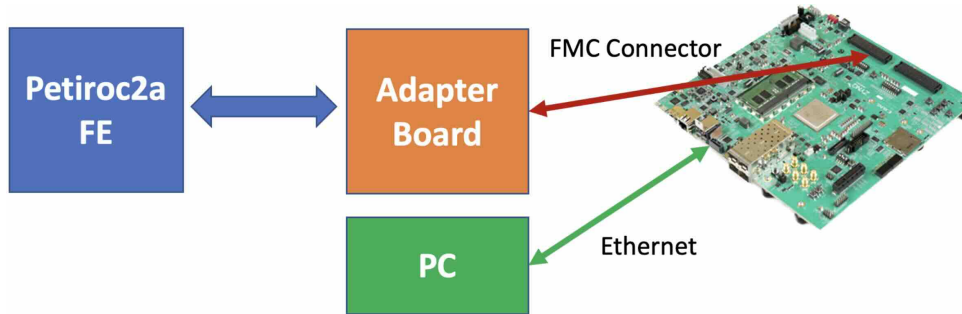


Fig. B.8 Verification platform of the PETIROC2B including FEB, adapted board (DIF) and ZCU102 for the DAQ system.

According to the guide of PETIROC2B, those critical signals from the chip must be connected to the DIF board through a connector with 2×30 pins, as shown in Figure B.9 (a). Some test points like the voltage thresholds of discriminated charge and the reference are accounted for several significant signals. The FEB integrates four PETIROC2B chips, one clock buffer (CDC1VD2104), two headers, and several SMA connectors for testing points.

Figure B.10 (a) illustrates that all PETIROC2B are simultaneously configured through a Serial Peripheral Interface (SPI) method (daisy-chain) to write 648-bits data to the corresponding shift registers. The clock buffer, configured with 40 MHz and 160 MHz inputs, is responsible for delivering synchronized clock signals at both frequencies to four chips, ensuring efficient timing and coordination across the system. The headers are connected to the DIF board to facilitate the transmission of voltage, clock signals, configuration data, and output data between the FEB and the DIF, ensuring seamless communication and power distribution. The power rail for the chips contains analog (VDD_3.3V) and digital (VDDD_3.3V) voltages, as displayed in Figure B.10

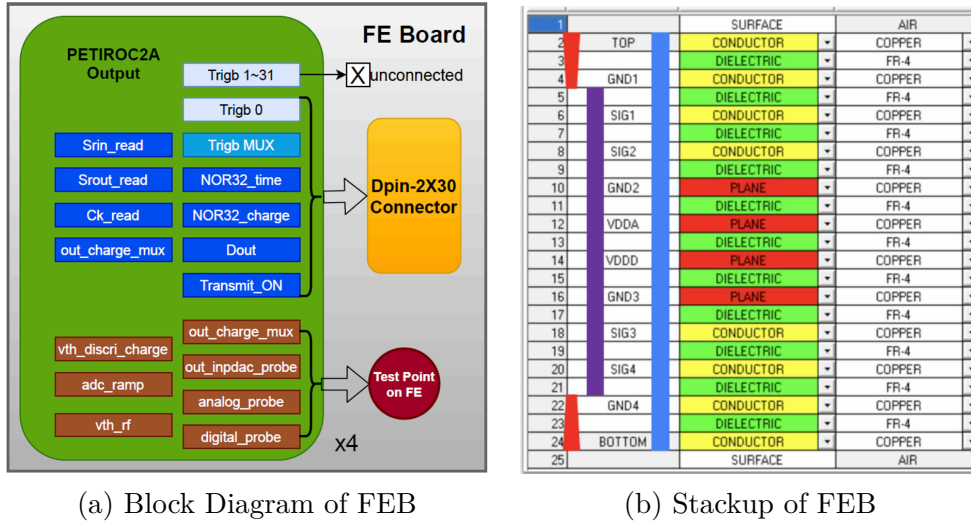


Fig. B.9 Logic (a) and design of stackup layer (b) for the FEB. Advance laser blinded vias for two layers close to the surface and mechanical buried vias for the middle layers are adopted.

(b). Considering the complexity of the wire nets, FEB adopts a PCB with 12 layer stackup (TOP, GND1, SIG1, SIG2, GND2, VDDA, VDDD, GND3, SIG3, SIG4, GND4, BOTTOM), as shown in Figure B.9 (b). The bottom layer contains 128 induction copper pads, each measuring $9.6 \times 9.6 \text{ mm}^2$, with a gap of 0.4 mm between adjacent pads. As illustrated in Figure B.9 (b), the two layers adjacent to the top and bottom employ laser-drilled via-in-pad technology (High Density Interconnection, HDI), represented by red trapezoids, with small holes approximately 0.1 mm in diameter. The remaining layers use buried vias, shown in purple, with a size of 0.3 mm, while mechanical support is provided by through vias, depicted in blue.

The FEB was designed using Cadence Allergo [185] for the schematics and PCBLayout Software for the layout design. The whole FEB PCB layout is shown in Figure B.11 (a) and the placement of the components on the top and bottom layers is displayed in Figure B.11 (b) and (c). The real pictures for the FEB are shown in Figure B.11 (d) and (e) with the devices welded.

B.3.3 Detector Interface Board

As discussed in the previous section, the detector interface board (DIF), also known as the Adapted Board, manages communication between the FEB via two headers and the FPGA via two FMC connectors, while also providing the necessary clock signals and voltage. The DIF card plays a critical role in facilitating communication and data transfer between the FEB and the FPGA, through two designated headers, and the ZCU102, which connects via two FMCs. Key features of the DIF card include voltage regulation, achieved through both Low Dropout (LDO) regulators (TPS79501) and a DC-DC converter (LTM4644), as well as precise clock management enabled by the jitter attenuator (Si5345). The card also incorporates four ADCs operating at a sampling rate of 5 MSPS. To minimize interference and optimize performance, the analog and digital power systems are distinctly separated. The schematic of the DIF board is presented in

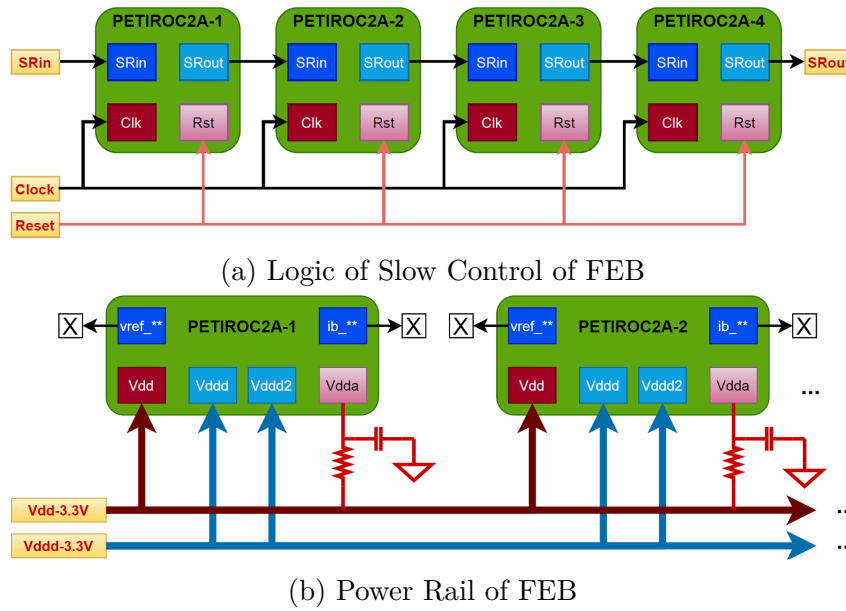


Fig. B.10 Designed Logic of Slow Control (a) containing data for shift registers, clock and reset signals. Power Rail (b) including analog and digital voltage levels of FEB.

Figure B.12 (a). The stack-up layer of the DIF board is illustrated in Figure B.12 (b), which consists of 8 layers to ensure proper signal integrity, grounding, and power distribution. The top and bottom layers are conductive copper planes used for signal routing. In between these layers are alternating power and ground planes, along with dielectric layers made of FR-4 material, providing insulation between the conductive layers. The stack-up typically includes multiple ground planes (GND1, GND2, GND3) to ensure low noise and stable signal returns, along with dedicated power planes for VCC and VDD. This structure helps in maintaining signal integrity, reducing electromagnetic interference (EMI), and ensuring proper power distribution across the board.

The power rail architecture, as depicted in Figure B.13 (a) is designed to provide stable and regulated power to various components of the system. At the core of this design is the LTM4644 DC-DC converter, which supplies up to 4A per channel, with a total of four independent channels. The converter delivers different voltage levels, including 3.3V (VH_3P3) and 2.5V (VDD_2P5), which are distributed to different subsystems, such as the PETIROC ASIC. The TPS79501 LDO regulators provide additional fine-tuned regulation to specific components, such as the jitter cleaner (Si5345) with a regulated 1.8V (VCC_1P8), and the PETIROC's analog and digital power lines, ensuring precise and stable operation. The power architecture separates analog and digital power supplies, such as VDDA_3P3 and VDDD_3P3, to minimize cross-domain noise, improving the performance and reliability of the system. This thoughtful distribution of power ensures each component operates under optimal conditions, enhancing overall system efficiency and stability.

The clock distribution system, as outlined in Figure B.13 (b), is orchestrated by the Si5345 jitter cleaner, which plays a pivotal role in maintaining precise and stable clock signals throughout the system. The jitter cleaner receives multiple input frequencies, such as 40 MHz from the

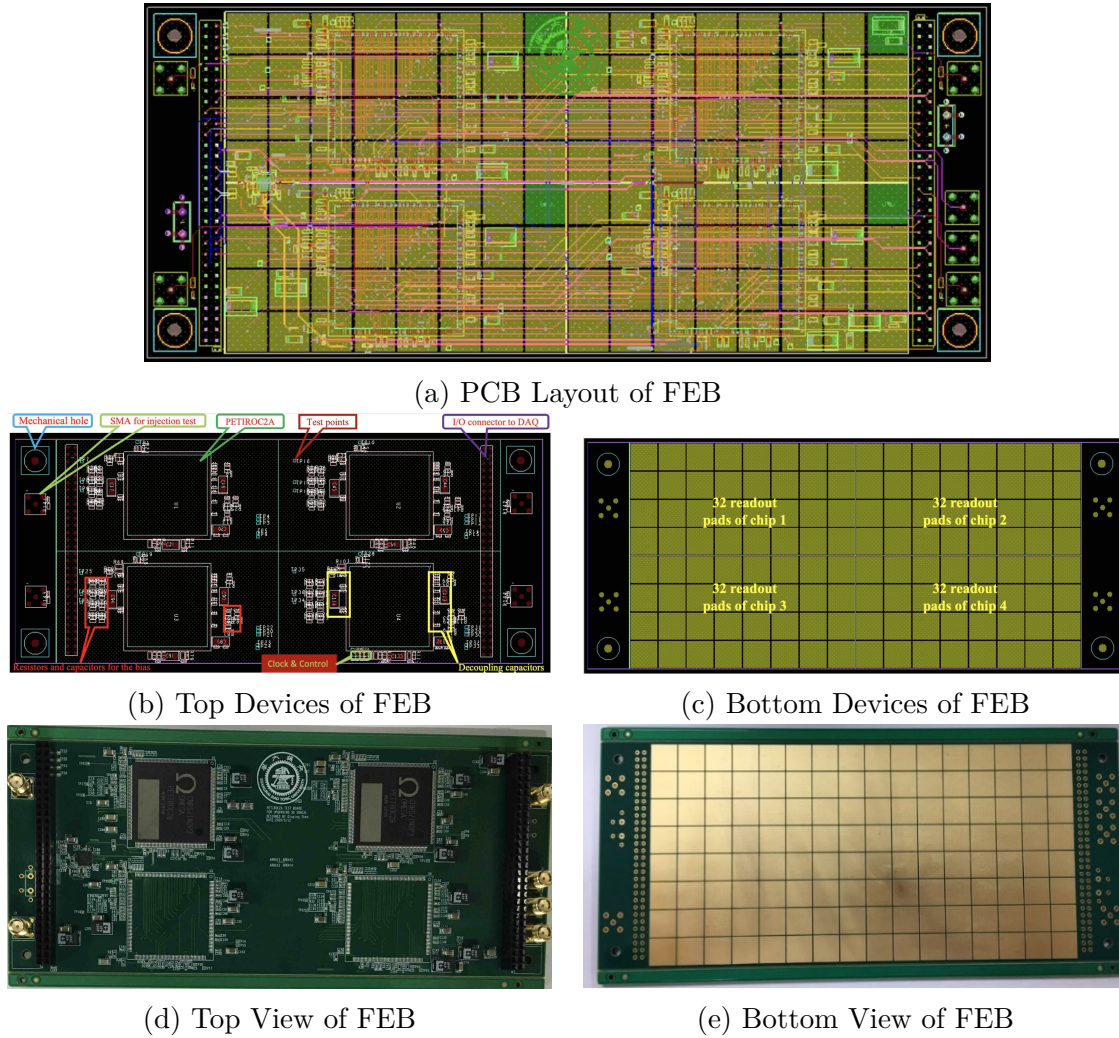
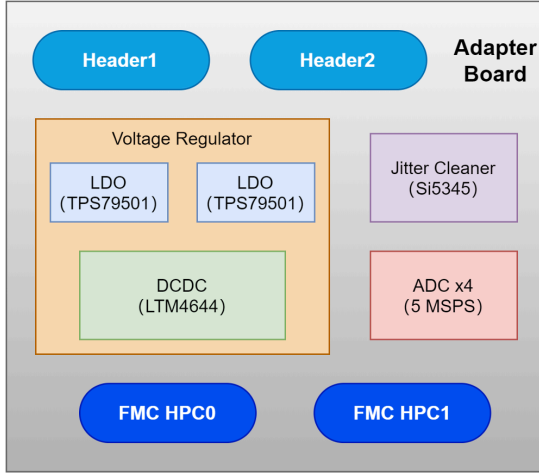


Fig. B.11 Layout (a-c) of FEB with four PETIROC2C chips. Real pictures of the top (d) and bottom (e) view of the FEB with four PETIROC2C chips while only two are welded for testing.

crystal oscillator, and outputs several key clock signals. These include a 160 MHz clock directed to the FEB that integrates four PETIROC ASICs, as well as a 100 MHz signal routed to the FMC HPC ports for interfacing with DAQ system. Additionally, 80 MHz clock signals are generated for the ADCs, which operate at 5 MSPS, and other connectors such as the SMA ports for testing on the oscilloscope. This clock architecture ensures that all components receive accurate and low-jitter signals, essential for high-performance operation, particularly in fast data acquisition and processing environments. The clear separation of frequencies and dedicated paths for different components further optimizes signal integrity, contributing to the system's overall reliability and efficiency.

The PCB layout of the DIF board in Figure B.14 (a) displays a clear arrangement of key components. The top view (b) and the back view (c) of the board highlight the precise placement of essential components.

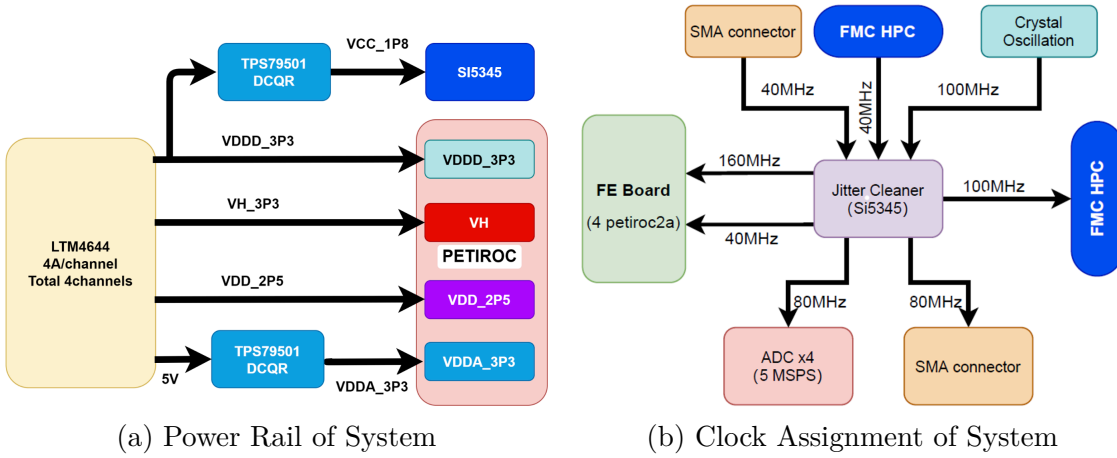


(a) Block Diagram

	Subclass Name	Type	Material
1		SURFACE	AIR
2	TOP	CONDUCTOR	COPPER
3		DIELECTRIC	FR-4
4	GND1	PLANE	COPPER
5		DIELECTRIC	FR-4
6	VCC	PLANE	COPPER
7		DIELECTRIC	FR-4
8	GND2	PLANE	COPPER
9		DIELECTRIC	FR-4
10	SIG	CONDUCTOR	COPPER
11		DIELECTRIC	FR-4
12	VDD	PLANE	COPPER
13		DIELECTRIC	FR-4
14	GND3	PLANE	COPPER
15		DIELECTRIC	FR-4
16	BOTTOM	CONDUCTOR	COPPER
17		SURFACE	AIR

(b) Stackup Layer

Fig. B.12 Schematic (a) of the DIF board containing voltage level translator, jitter attenuator, ADCs, headers, and FMCs. Stackup layer (b) of the DIF board with 8 layers



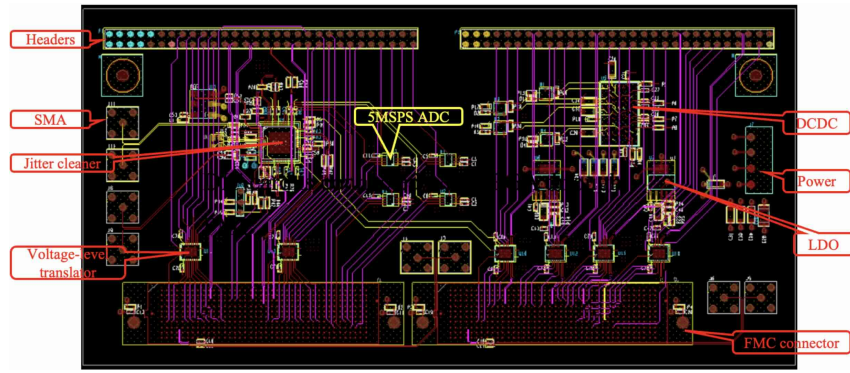
(a) Power Rail of System

(b) Clock Assignment of System

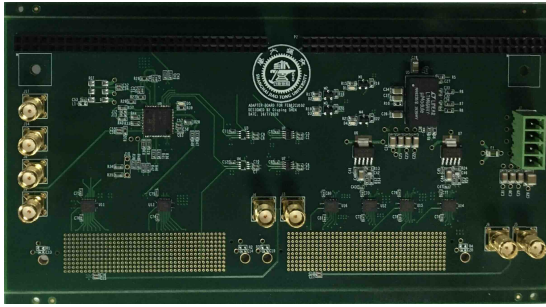
Fig. B.13 Power Rail and Clock Assignment of the DIF board.

B.4 Data Acquisition System Development

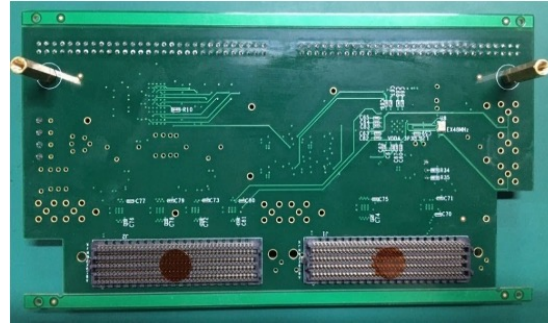
The DAQ system is designed using the Xilinx ZCU102 FPGA, which integrates both a Processing System (PS) and Programmable Logic (PL). This design enables efficient data communication and processing between the FPGA and the PC. The embedded design, implemented using Vitis on the PS side of the ZCU102, facilitates UART communication for direct interface, Ethernet communication for high-speed data transfer, and internal data transmission between the PS and PL using the AXI bus. The system architecture ensures reliable and flexible data handling, essential for real-time acquisition and processing tasks.



(a) Overview of PCB Layout



(b) Top View



(c) Bottom View

Fig. B.14 Design of DIF board: (a) Overview of PCB layout with devices and wires placed on the board. Real pictures of the top (b) and bottom (c) view of the DIF board with two FMCs are shown.

B.4.1 Xilinx FPGA Board ZCU102

The Xilinx UltraScale+ ZCU102 FPGA board [186] in Figure B.15 is a highly advanced development platform designed for applications requiring high performance, flexibility, and scalability. It features the ZYNQ UltraScale+ MPSoC, which combines a powerful quad-core ARM Cortex-A53 processor, dual-core ARM Cortex-R5 real-time processors, and an integrated FPGA fabric. This enables the ZCU102 to handle complex workloads with real-time processing and hardware acceleration. The board supports high-speed connectivity options like Gigabit Ethernet, PCIe, and DisplayPort, making it ideal for data-intensive applications such as embedded systems, machine learning, and signal processing. Additionally, the ZCU102 offers ample memory resources, including DDR4 and programmable logic, along with a robust software and hardware development environment, providing an all-in-one solution for prototyping and deploying cutting-edge systems. The development of DAQ system primarily adopted the PL and PS, Ethernet, UART, and JTAG interfaces for communication.

B.4.2 Embedded System Co-design with PL and PS

The procedure for the embedded system co-design with the ZCU102 involves the integration of the PS and PL within the Zynq UltraScale+ MPSoC architecture. The process starts by defining the hardware design in PL using tools like Vivado [187], where custom logic or IP



Fig. B.15 Commercial development kit of Xilinx FPGA board ZCU102.

blocks are implemented. The next step is to configure the PS, typically using an embedded Linux operating system or bare-metal software in Xilinx Vitis [187]. The software running on the PS communicates with the custom hardware in the PL via AXI interfaces, allowing seamless interaction. Once the hardware and software designs are completed, they are compiled and deployed on the ZCU102, where the system can be debugged and optimized through iterative testing.

Figure B.16 shows an overview of the DAQ system based on the ZCU102 Evaluation Board. The system architecture highlights the interaction between the PL and the PS within the FPGA. The Interface Board is connected to the PL, which communicates with the PS through an AXI interface. The PS is responsible for managing the communication with external systems, including a PC, via several interfaces: JTAG for debugging and configuration, Ethernet for high-speed data transfer, and UART for serial communication. The PC can control, monitor, and debug the system through these interfaces, ensuring seamless data flow and system management. The system leverages both the flexibility of the PL for hardware-specific tasks and the processing capabilities of the PS for software execution.

B.4.2.1 Firmware Development on PL

Figure B.17 (a) illustrates the flow of data and control between the PETIROC2B and the ZCU102 FPGA, with a focus on the interactions between the PL and the PS. The slow control data is transmitted to the PETIROC2B chip via the GPIO interface, allowing for peripheral device management. The data output from PETIROC2B is then handled by the FIFO (First-In, First-Out) buffer, which temporarily stores the incoming data. Afterward, the data is trans-

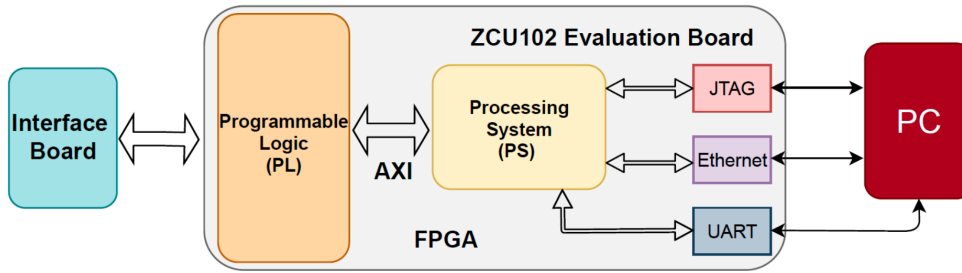
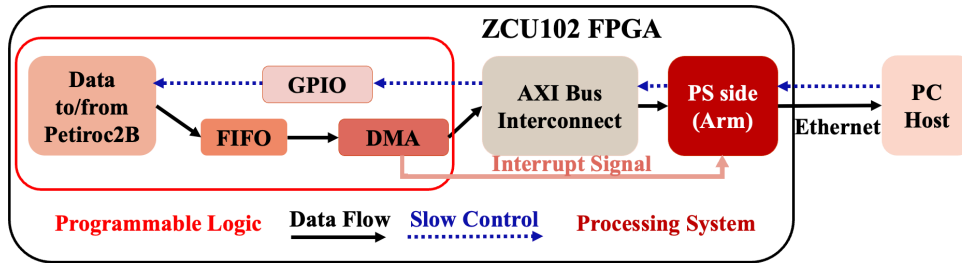
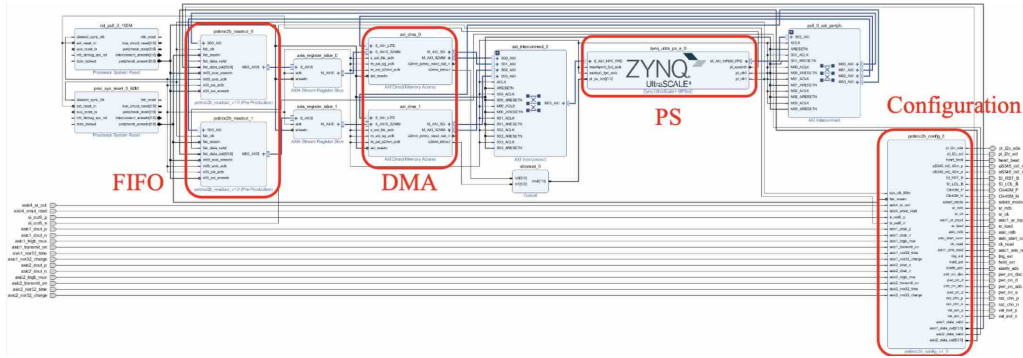


Fig. B.16 Development of the Data Acquisition System using PL and PS on FPGA ZCU102.

ferred to the Direct Memory Access (DMA) engine for efficient memory transactions. This processed data is then sent to the PS through the AXI bus interconnect. The AXI bus acts as the primary communication channel between the PL and PS, enabling seamless data transfer. Interrupt signals are generated as needed to notify the PS of data processing events, while the PS communicates with external systems, such as a PC host, through Ethernet, ensuring real-time monitoring and control of the system. This architecture provides a high-performance, low-latency solution for managing data flow and control within the FPGA design.



(a) Overview of Firmware for PL



(b) Visualization Design of Firmware on Vivado

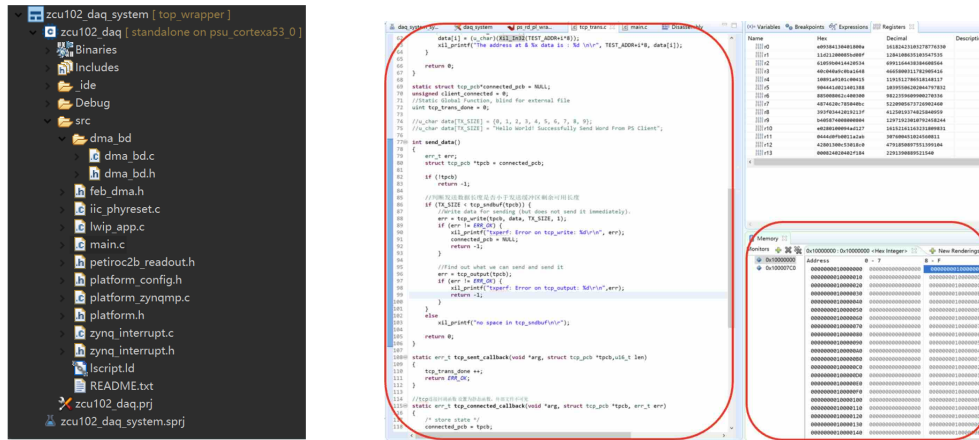
Fig. B.17 Design of firmware on PL: (a) Schematic of the logic flow including slow control and data transmission. (b) Visualized logic design using official IPs and custom IP.

The corresponding logic design, using VHDL (VHSIC Hardware Description Language) in Vivado software, is shown in Figure B.17 (b). Several official IPs, such as DMA, FIFO, Clock Wizard, and the AXI bus, are integrated into the design. Additionally, a custom IP named

“Configuration” is specifically defined to manage the configuration data of the PETIROC2B. The custom IP implements the Serial Peripheral Interface (SPI) mode for configuring the PETIROC2B and the Inter-Integrated Circuit (I²C) mode for configuring the Si5345. The 648-bit configuration data is divided into twenty 32-bit words and one 8-bit word, which are then transmitted directly to the chips for configuration. Several ports on the left and right sides are connected to the available pins of the ZCU102 FPGA via the FMC connectors. Once the firmware is developed and compiled, it can be deployed onto the ZCU102 FPGA via the JTAG interface for the software development on PS.

B.4.2.2 Software Development on PS

The software on the PS side of the ZCU102 is based on the processing system (PS) developed by Xilinx Vitis. The firmware programmed into the FPGA using Vivado can be automatically detected via JTAG by Vitis, which generates the corresponding software template for further development. The primary program utilizes C language to implement the control of DMA, the ethernet communication, and the interrupt signal. Figure B.18 (a) shows the structure of the preliminary software on the PS, while (b) exhibits the program on TCP ethernet communication and the data in the registers. The ethernet communicates with the PC host through the TCP protocol, allowing for high-speed data transfer.



(a) Top-level Software on Vitis

(b) Codes on Ethernet via TCP

Fig. B.18 Software development on PS: (a) Top-level Software on Vitis, (b) Codes on the ethernet via TCP.

B.5 Results from Signal Injection Test

To perform the signal injection test, the preliminary application on PC host was developed using the PyQt5 framework. The primary function contains the ethernet connection between the computer and the FPGA, configuring the slow control parameters and sending to the FPGA. In the Connection Window in Figure B.19 (a), users can configure network settings such as the IP address and port number for establishing a TCP connection between the computer and the FPGA. This section also provides options to send or receive data and allows the user to

export data files for further analysis. In the Main Window in Figure B.19 (b), users have detailed control over PETIROC2B settings, including parameters for masking discharge and timing channels, ADC ramp compensation, DAC configuration, and polarity adjustments. The 648-bit configuration data can also be transferred to the software via a text format in the connection window. These settings facilitate fine-tuning of the chip behavior, enabling efficient data acquisition and configuration management. The software provides a user-friendly way to interact with the hardware, supporting seamless communication for real-time data exchange and system configuration.

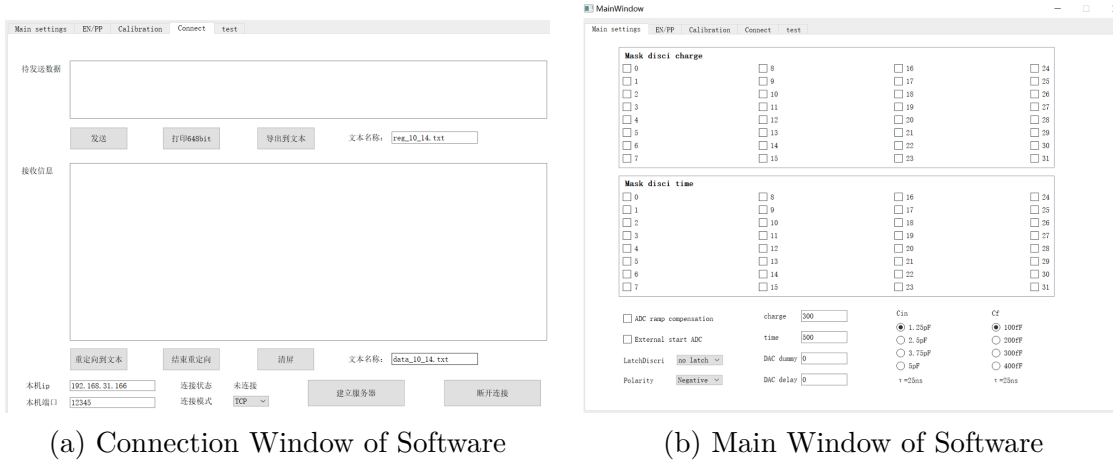


Fig. B.19 Software developed using PyQt5 running on the computer for the communication between the computer and the FPGA. The function contains the configuration of PETIROC2B, the data acquisition, and the simple data analysis.

Figure B.20 illustrates the setup for the PETIROC2B configuration test. A 648-bit data stream was transmitted via Ethernet from the host computer to the FPGA and FEB. The oscilloscope was utilized to assess data quality from the “SR_out” pin of PETIROC2B, specifically verifying bit accuracy and timing by capturing both the data and clock signals. Simultaneously, the data was monitored using the Integrated Logic Analyzer (ILA) in Vivado, as depicted in Figure B.21. In this figure, panel (a) shows the entire 648-bit data and clock signals, while panel (b) provides a more detailed view of the 32-bit data segments transmitted in each cycle. This step confirms that the data was correctly received by PETIROC2B from the FPGA.

The time trigger threshold is determined by two DACs: a 10-bit common DAC and a 6-bit channel-specific DAC, enabling precise adjustments for each channel. The 10-bit DAC provides a voltage range from 0.89 V to 1.89 V with a resolution of 0.92 mV per unit, while the 6-bit DAC fine-tunes the threshold with a range of 100 mV and 1.5 mV resolution per unit. The time threshold is calculated as:

$$T_{\text{threshold}} = 0.89V + (\text{DAC}_{10\text{-bit}} \times 0.92mV - \text{DAC}_{6\text{-bit}} \times 1.5mV) * 0.001. \quad (\text{B.2})$$

For the time threshold evaluation in Figure B.22 (a), a 10-bit DAC was employed to analyze the linearity between DAC values and the corresponding output voltage. The result demonstrates strong agreement between the designed FEB and the evaluation board. The linear fit for the FEB

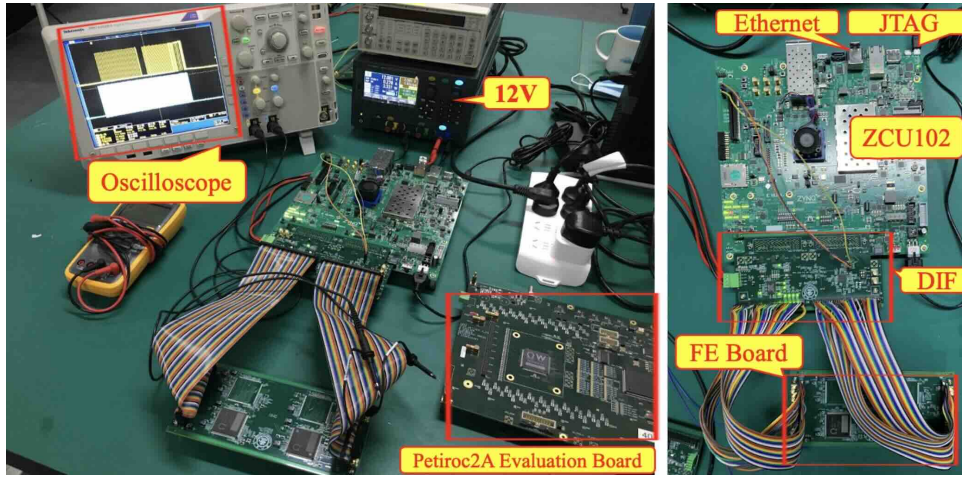
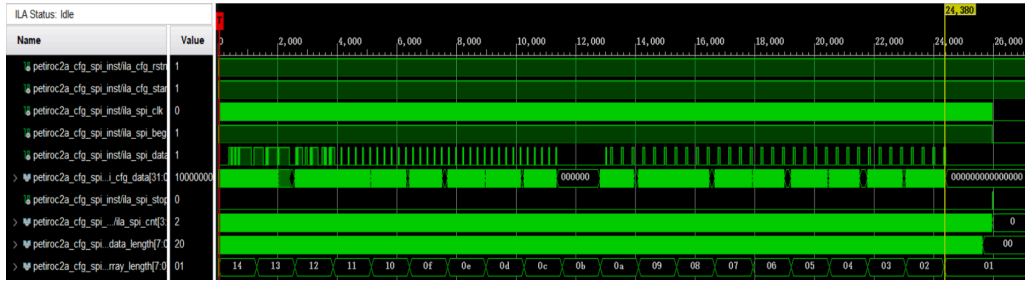


Fig. B.20 Setup for the configuration test of the PETIROC2B. The 648-bit data and clock signals are displayed on the oscilloscope. The test results are compared to those obtained from the PETIROC2A evaluation board.



(a) All Configuration Data for PETIROC2B from ILA.



(a) Part Configuration Data from ILA.

Fig. B.21 Configuration data for PETIROC2B captured by ILA: (a) All 648-bit configuration data, (b) Part 32-bit configuration data and clock signals.

is given by $y = 0.0009x + 1.4697$, while the evaluation board exhibits a similar relationship with $y = 0.0009x + 1.4376$. The near-identical slopes indicate that both systems exhibit the same rate of voltage increase relative to the DAC value. The slight difference in intercept values suggests a minor offset in the baseline voltage, yet the overall linearity is preserved. This confirms that the designed FEB performs reliably and consistently, mirroring the linearity of the evaluation board across the entire range of time threshold settings.

The charge trigger threshold is set by a 10-bit DAC with an output range of 1.01 V to 2.01 V and a resolution of 0.92 mV per unit. Channel-specific masking allows for individual

trigger output control, while trigger polarity can be set for either positive or negative input signals. The outputs are processed through an Open Collector buffer, generating a NOR32 output. These DAC thresholds can be adjusted by setting the slow control parameters in the software. Similarly, for the charge threshold evaluation, a 10-bit DAC was used to verify the linearity between the DAC settings and the output voltage, as depicted in Figure B.22 (b). The FEB produced a linear relationship described by $y = 0.0009x + 1.0173$, closely matching the evaluation board linear fit of $y = 0.0009x + 0.9971$. The identical slopes in both cases indicate that the charge threshold increases uniformly across the DAC range for both systems. The small difference in intercept values reflects a slight variation in baseline voltage, but the overall linearity remains consistent. These results demonstrate that the designed FEB maintains precise and stable charge threshold behavior, equivalent to that of the evaluation board, confirming the reliability of its design.

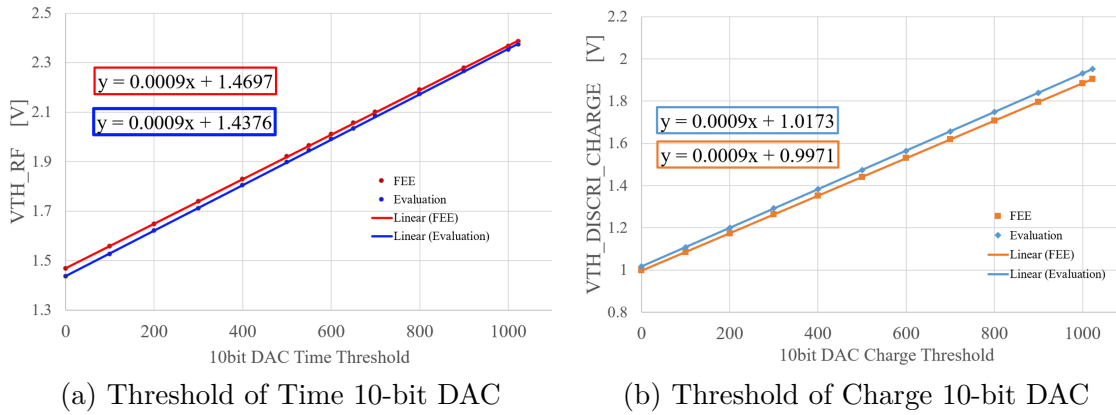


Fig. B.22 Comparison of the linearity for the time (a) and charge (b) 10-bit DAC thresholds. Evaluation denotes the results from the OMEGA board while FEE for the designed FEB. Linear fits are applied to the data points in each evaluation. Good linearity is observed for both charge and time thresholds.

The successful configuration of the FEB is confirmed through the validation of time and charge thresholds. Figure B.23 illustrates the setup for the injection signal test, where the FEB is enclosed by two aluminum panels, acting as a Faraday cage to mitigate noise interference and provide a stable testing environment. Two grounding cables connect the FEB and DIF boards to the FPGA, ensuring effective grounding and maintaining signal integrity. The time performance was measured using a periodic pulse signal with an amplitude of 2V, a frequency of 20 kHz, a leading edge of 62.5 μ s, and a trailing edge of 2 ns, injected into the FEB through SMA connectors. In addition to the data obtained through the software, the data can also be monitored using the ILA, as shown in Figure B.24.

The preliminary results from the signal injection test are presented in Figure B.25 and Figure B.26. The Gray-encoded data is first decoded to binary format and then converted into decimal format, which is subsequently used to calculate the absolute time using Equation B.1. As discussed in previous Section B.3.1, the data fields, consisting of 10 bits for fine time and charge, 9 bits for coarse time, and 1 bit for the hit signal, are depicted in the figures. Various time thresholds and attenuators were utilized during these preliminary tests. In Figure B.25, a 2V

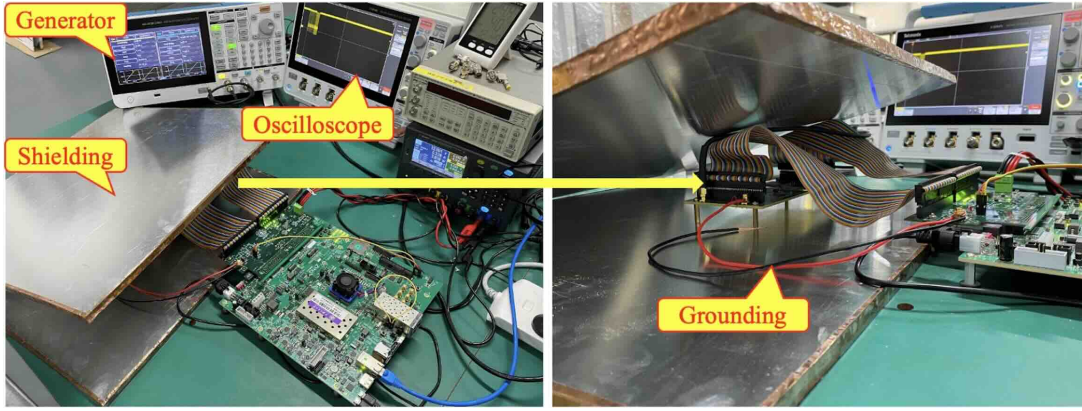


Fig. B.23 Setup for the injection signal test of the whole system including the shielding and the grounding.

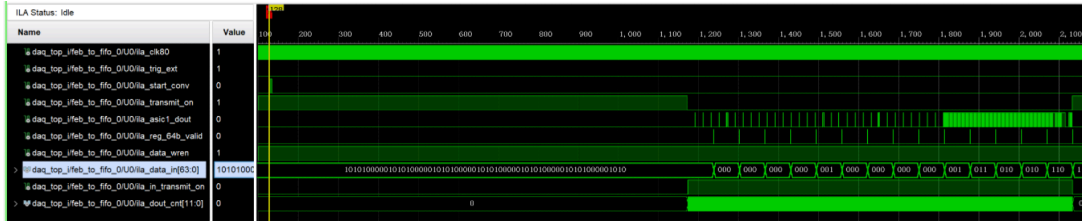


Fig. B.24 Output data directly captured by ILA from "Dout" pin of PETIROC2B.

amplitude signal with a 40 dB attenuator was injected into channel 0 of ASIC 1 at $\text{DAC}_{10\text{-bit}} = 500$ and 600, while $\text{DAC}_{6\text{-bit}} = 32$ was applied uniformly across all 32 channels. At a time threshold of 500, the hit information indicates that all channels register hits simultaneously, despite the signal being injected only into channel 0. When the time threshold is raised to 600, all channels except channel 4 register hits. This behavior suggests the presence of crosstalk between the channels of PETIROC2B.

To further investigate the crosstalk, the time threshold was increased to its maximum values of $\text{DAC}_{10\text{-bit}} = 1023$ and $\text{DAC}_{6\text{-bit}} = 63$, corresponding to $V_{\text{th}} = 2.373$ V. The mask function was applied to certain channels to isolate and analyze the crosstalk. The results of the decoded output data, obtained from the software, are displayed in Figure B.26. Even at the highest thresholds with a small amplitude signal, crosstalk remained in the last few channels, as shown in Figure B.26 (a). Channels 24-28 and 30 were masked to further assess crosstalk, as shown in Figure B.26 (b). Despite masking, crosstalk persisted in channel 29, indicating that the interference originated from channel 0 of PETIROC2B within the FEB design.

B.6 Advanced Version of the System

To deal with the crosstalk from the FEB V1, the FEB V2 was designed through integrating the FEB and DIF boards into one single board. The stackup layer and the real pictures of FEB V2 was shown in Figure B.27. The components contain two PETIROC2B ASICs, Si5345, LTM4644, DC Power, two FMCs and SMA Connectors.

Fine time	Coarse time	Hit	Charge	Counter
0	0	0	0	0
1	1	1	1	1
2	2	2	2	2
3	3	3	3	3
4	4	4	4	4
5	5	5	5	5
6	6	6	6	6
7	7	7	7	7
8	8	8	8	8
9	9	9	9	9
10	10	10	10	10
11	11	11	11	11
12	12	12	12	12
13	13	13	13	13
14	14	14	14	14
15	15	15	15	15
16	16	16	16	16
17	17	17	17	17
18	18	18	18	18
19	19	19	19	19
20	20	20	20	20
21	21	21	21	21
22	22	22	22	22
23	23	23	23	23
24	24	24	24	24
25	25	25	25	25
26	26	26	26	26
27	27	27	27	27
28	28	28	28	28
29	29	29	29	29
30	30	30	30	30
31	31	31	31	31
32	32	32	32	32
33	33	33	33	33
34	34	34	34	34
35	35	35	35	35
36	36	36	36	36
37	37	37	37	37
38	38	38	38	38
39	39	39	39	39
40	40	40	40	40
41	41	41	41	41
42	42	42	42	42
43	43	43	43	43
44	44	44	44	44
45	45	45	45	45
46	46	46	46	46
47	47	47	47	47
48	48	48	48	48
49	49	49	49	49
50	50	50	50	50
51	51	51	51	51
52	52	52	52	52
53	53	53	53	53
54	54	54	54	54
55	55	55	55	55
56	56	56	56	56
57	57	57	57	57
58	58	58	58	58
59	59	59	59	59
60	60	60	60	60
61	61	61	61	61
62	62	62	62	62
63	63	63	63	63

(a) Decoded data: Fine time, Charge, Coarse time, Hit at V_{time} , threshold = 1.921 V

Fine time	Coarse time	Hit	Charge	Counter
0	0	0	0	0
1	1	1	1	1
2	2	2	2	2
3	3	3	3	3
4	4	4	4	4
5	5	5	5	5
6	6	6	6	6
7	7	7	7	7
8	8	8	8	8
9	9	9	9	9
10	10	10	10	10
11	11	11	11	11
12	12	12	12	12
13	13	13	13	13
14	14	14	14	14
15	15	15	15	15
16	16	16	16	16
17	17	17	17	17
18	18	18	18	18
19	19	19	19	19
20	20	20	20	20
21	21	21	21	21
22	22	22	22	22
23	23	23	23	23
24	24	24	24	24
25	25	25	25	25
26	26	26	26	26
27	27	27	27	27
28	28	28	28	28
29	29	29	29	29
30	30	30	30	30
31	31	31	31	31
32	32	32	32	32
33	33	33	33	33
34	34	34	34	34
35	35	35	35	35
36	36	36	36	36
37	37	37	37	37
38	38	38	38	38
39	39	39	39	39
40	40	40	40	40
41	41	41	41	41
42	42	42	42	42
43	43	43	43	43
44	44	44	44	44
45	45	45	45	45
46	46	46	46	46
47	47	47	47	47
48	48	48	48	48
49	49	49	49	49
50	50	50	50	50
51	51	51	51	51
52	52	52	52	52
53	53	53	53	53
54	54	54	54	54
55	55	55	55	55
56	56	56	56	56
57	57	57	57	57
58	58	58	58	58
59	59	59	59	59
60	60	60	60	60
61	61	61	61	61
62	62	62	62	62
63	63	63	63	63

(b) Decoded data: Fine time, Charge, Coarse time, Hit at V_{time} , threshold = 2.011 V**Fig. B.25**

Decoded output data from PETIROC2B obtained by the software, with only channel 0 injected with a 2V amplitude signal. The data includes fine time (10-bit), coarse time (9-bit), hit (1-bit), and charge (10-bit) data in red box. (a) and (b) display the results from different time thresholds 500 with $V_{\text{th}} = 1.921$ V and 600 with $V_{\text{th}} = 2.011$ V respectively. Crosstalk exists between the channels, as only channel 0 registers hits.

The signal used for testing the timing performance of the system is a periodic pulse wave with a frequency of 20 kHz, generated by a function generator with a negative peak-to-peak amplitude of 30.0 mV. The pulse features a leading edge with a rise time of 1.000 μs and a very sharp trailing edge of 2.00 ns, indicating quick transitions between its high and low states. With a duty cycle of 95%, the pulse remains high for the majority of the time, allowing precise and consistent testing conditions when injected into the ASICs. This configuration ensures that the system response to fast, high-frequency pulses can be thoroughly evaluated under controlled conditions. The time performance was evaluated by analyzing the time differences from neighboring and coincident hits, specifically between channel 0 in one ASIC and channel 0 between two ASICs. The results, presented in Figure B.28, demonstrate that the system achieved a time resolution of 50 ps RMS for the neighboring hits, which is less than 100 ps RMS from the simulation in Figure B.3. The observed resolution is composed of the intrinsic time resolution and the jitter resolution of other sources ($\sigma_{\text{observe}}^2 = \sigma_{\text{intrinsic}}^2 + \sigma_{\text{jitter}}^2$). In general, we could assume that the intrinsic and jitter show the similar time resolution, and the intrinsic time resolution can be expressed as $\sigma_{\text{intrinsic}} = \sigma_{\text{observe}}/\sqrt{2}$. The observe value denotes the RMS value from the distribution of the time differences. Therefore, the intrinsic time resolution of the readout system is about 36 ps

0	LineInfo	11111111	Decade	0000000110	TAC	681	ChargeInfo	0000001010	Decade	0000001100	ADC	12	61	CoarseTime	110010001	Decade	0000000000	Counter	368	HLT
1	LineInfo	0000000110	Decade	0000000110	TAC	682	ChargeInfo	0000001010	Decade	0000001100	ADC	12	62	CoarseTime	101010001	Decade	0000000000	Counter	369	HLT
2	LineInfo	0000000110	Decade	0000000110	TAC	683	ChargeInfo	0000001010	Decade	0000001100	ADC	12	63	CoarseTime	101010001	Decade	0000000000	Counter	370	HLT
3	LineInfo	0000000110	Decade	0000000110	TAC	684	ChargeInfo	0000001010	Decade	0000001100	ADC	12	64	CoarseTime	101010001	Decade	0000000000	Counter	371	HLT
4	LineInfo	0000000110	Decade	0000000110	TAC	685	ChargeInfo	0000001010	Decade	0000001100	ADC	12	65	CoarseTime	101010001	Decade	0000000000	Counter	372	HLT
5	LineInfo	0000000110	Decade	0000000110	TAC	686	ChargeInfo	0000001010	Decade	0000001100	ADC	12	66	CoarseTime	101010001	Decade	0000000000	Counter	373	HLT
6	LineInfo	0000000110	Decade	0000000110	TAC	687	ChargeInfo	0000001010	Decade	0000001100	ADC	12	67	CoarseTime	101010001	Decade	0000000000	Counter	374	HLT
7	LineInfo	0000000110	Decade	0000000110	TAC	688	ChargeInfo	0000001010	Decade	0000001100	ADC	12	68	CoarseTime	101010001	Decade	0000000000	Counter	375	HLT
8	LineInfo	0000000110	Decade	0000000110	TAC	689	ChargeInfo	0000001010	Decade	0000001100	ADC	12	69	CoarseTime	101010001	Decade	0000000000	Counter	376	HLT
9	LineInfo	0000000110	Decade	0000000110	TAC	690	ChargeInfo	0000001010	Decade	0000001100	ADC	12	70	CoarseTime	101010001	Decade	0000000000	Counter	377	HLT
10	LineInfo	0000000110	Decade	0000000110	TAC	691	ChargeInfo	0000001010	Decade	0000001100	ADC	12	71	CoarseTime	101010001	Decade	0000000000	Counter	378	HLT
11	LineInfo	0000000110	Decade	0000000110	TAC	692	ChargeInfo	0000001010	Decade	0000001100	ADC	12	72	CoarseTime	101010001	Decade	0000000000	Counter	379	HLT
12	LineInfo	0000000110	Decade	0000000110	TAC	693	ChargeInfo	0000001010	Decade	0000001100	ADC	12	73	CoarseTime	111110110	Decade	0000000000	Counter	380	HLT
13	LineInfo	0000000110	Decade	0000000110	TAC	694	ChargeInfo	0000001010	Decade	0000001100	ADC	12	74	CoarseTime	111110110	Decade	0000000000	Counter	381	HLT
14	LineInfo	0000000110	Decade	0000000110	TAC	695	ChargeInfo	0000001010	Decade	0000001100	ADC	12	75	CoarseTime	111110110	Decade	0000000000	Counter	382	HLT
15	LineInfo	0000000110	Decade	0000000110	TAC	696	ChargeInfo	0000001010	Decade	0000001100	ADC	12	76	CoarseTime	111110110	Decade	0000000000	Counter	383	HLT
16	LineInfo	0000000110	Decade	0000000110	TAC	697	ChargeInfo	0000001010	Decade	0000001100	ADC	12	77	CoarseTime	111110110	Decade	0000000000	Counter	384	HLT
17	LineInfo	0000000110	Decade	0000000110	TAC	698	ChargeInfo	0000001010	Decade	0000001100	ADC	12	78	CoarseTime	111110110	Decade	0000000000	Counter	385	HLT
18	LineInfo	0000000110	Decade	0000000110	TAC	699	ChargeInfo	0000001010	Decade	0000001100	ADC	12	79	CoarseTime	111110110	Decade	0000000000	Counter	386	HLT
19	LineInfo	0000000110	Decade	0000000110	TAC	700	ChargeInfo	0000001010	Decade	0000001100	ADC	12	80	CoarseTime	111110110	Decade	0000000000	Counter	387	HLT
20	LineInfo	0000000110	Decade	0000000110	TAC	701	ChargeInfo	0000001010	Decade	000										

(a) No Mask at Max $V_{\text{time, th}} = 2.373$ V

1	2.FineLine	0000000110	Decode	0000000110	ADC	1	ChargeInfo	0000000110	Decode	0000000110	ADC	44	CoarseTime	1000000110	Decode	1010100001	Counter	506	HLT	6
2	2.FineLine	0000000110	Decode	0000000110	ADC	2	3.ChargeInfo	0000000111	Decode	0000000111	ADC	45	45.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
3	2.FineLine	0000000110	Decode	0000000110	ADC	3	5.ChargeInfo	0000001000	Decode	0000001000	ADC	46	46.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
4	2.FineLine	0000000110	Decode	0000000110	ADC	4	7.ChargeInfo	0000001001	Decode	0000001001	ADC	47	47.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
5	2.FineLine	0000000110	Decode	0000000110	ADC	5	9.ChargeInfo	0000001010	Decode	0000001010	ADC	48	48.CoarseTime	0011001101	Decode	1000101101	Counter	93	HLT	6
6	2.FineLine	0000000110	Decode	0000000110	ADC	6	11.ChargeInfo	0000001011	Decode	0000001011	ADC	49	49.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
7	2.FineLine	0000000110	Decode	0000000110	ADC	7	13.ChargeInfo	0000001011	Decode	0000001011	ADC	50	50.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
8	2.FineLine	0000000110	Decode	0000000110	ADC	8	15.ChargeInfo	0000001011	Decode	0000001011	ADC	51	51.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
9	2.FineLine	0000000110	Decode	0000000110	ADC	9	17.ChargeInfo	0000001011	Decode	0000001011	ADC	52	52.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
10	2.FineLine	0000000110	Decode	0000000110	ADC	10	19.ChargeInfo	0000001001	Decode	0000001001	ADC	53	53.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
11	2.FineLine	0000000110	Decode	0000000110	ADC	11	21.ChargeInfo	0000001011	Decode	0000001011	ADC	54	54.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
12	2.FineLine	0000000110	Decode	0000000110	ADC	12	23.ChargeInfo	0000001011	Decode	0000001011	ADC	55	55.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
13	2.FineLine	0000000110	Decode	0000000110	ADC	13	25.ChargeInfo	0000001011	Decode	0000001011	ADC	56	56.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
14	2.FineLine	0000000110	Decode	0000000110	ADC	14	27.ChargeInfo	0000001011	Decode	0000001011	ADC	57	57.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
15	2.FineLine	0000000110	Decode	0000000110	ADC	15	29.ChargeInfo	0000001011	Decode	0000001011	ADC	58	58.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
16	2.FineLine	0000000110	Decode	0000000110	ADC	16	31.ChargeInfo	0000001011	Decode	0000001011	ADC	59	59.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
17	2.FineLine	0000000110	Decode	0000000110	ADC	17	33.ChargeInfo	0000001011	Decode	0000001011	ADC	60	60.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
18	2.FineLine	0000000110	Decode	0000000110	ADC	18	35.ChargeInfo	0000001011	Decode	0000001011	ADC	61	61.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
19	2.FineLine	0000000110	Decode	0000000110	ADC	19	37.ChargeInfo	0000001011	Decode	0000001011	ADC	62	62.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
20	2.FineLine	0000000110	Decode	0000000110	ADC	20	39.ChargeInfo	0000001011	Decode	0000001011	ADC	63	63.CoarseTime	1111100001	Decode	1010100001	Counter	336	HLT	6
21	2.FineLine	0000000110	Decode	0000000110	ADC															

(b) Masked Channels 24-28 and 30 at Max $V_{\text{time, th}} = 2.373$ V

Fig. B.26

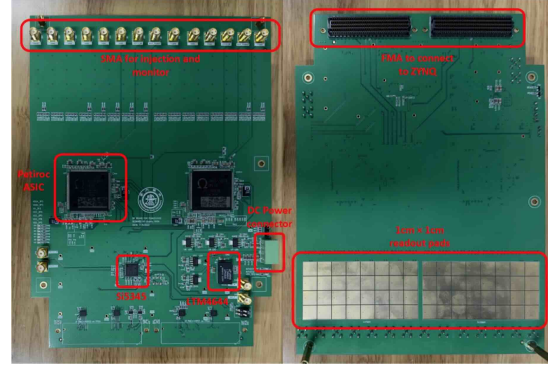
Decoded output data from PETIROC2B obtained by the software, with only channel 0 injected with a 2V amplitude signal. The data includes fine time (10-bit), coarse time (9-bit), hit (1-bit), and charge (10-bit) fields, highlighted in the red box. (a) and (b) depict the results from the maximum time threshold at $V_{th} = 2.373$ V, without and with masking channels 24-28 and 30, respectively. Despite masking certain channels, a few unmasked channels still register hits, indicating the presence of crosstalk.

divided by $\sqrt{2}$ while the resolution from coincidence hits is about 75 ps.

The time resolution of the system using PETIROC2B can be verified very well, which indicates that the system is able to achieve a time resolution better than 100 ps for the intrinsic time resolution. The next plan is to design the large size of the FEB for the MGRPCs and develop the data acquisition system for the Time-SDHCAL.

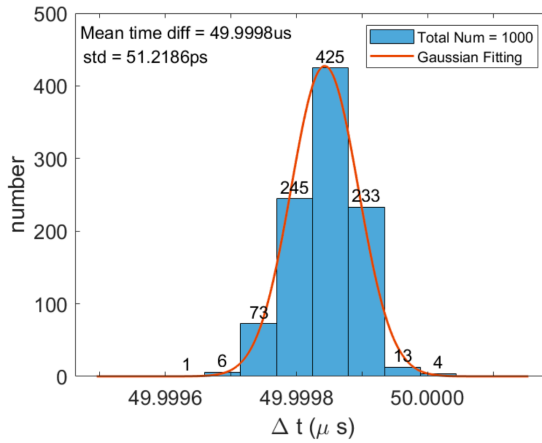


(a) Stackup of FEB V2

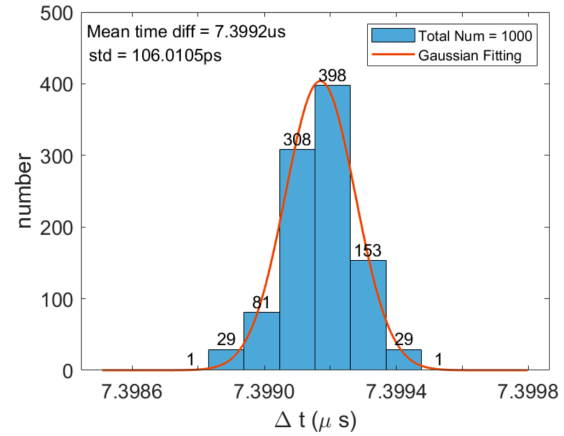


(b) Pictures of FEB V2

Fig. B.27 Upgraded version of FEB: (a) Stackup for the FEB V2, (b) Real pictures of FEB V2 integrating the FEB and DIF boards.



(a) Hits from Neighbor Channel



(b) Hits from Coincidence Channel

Fig. B.28 Results from injection tests: (a) Time difference from the neighbor hits of channel 0, (b) Time difference from the coincidence hits between two PETIROC2B ASICs.



Search for the rare Higgs boson decays to $Z\gamma$

The latest result of the $H \rightarrow Z\gamma$ analysis, combining ATLAS and CMS data from the full LHC Run-2, provides evidence at a significance level of 3.4 standard deviations for this rare Higgs boson decay [21]. While this result focuses solely on the leptonic decay channel of the Z boson, exploring hadronic and invisible decays (i.e. to neutrinos) of the Z boson could further enhance the sensitivity of the measurement. As Run-3 progresses, with a targeted luminosity of more than 200 fb^{-1} during full Run-3 period, the search for $H \rightarrow Z\gamma$ decays remains an intriguing area of study, in particular given that the measured signal yield, 2.2 ± 0.7 times the standard model prediction, is larger than (though compatible with) the expectation. The detailed status of Run-3 data-taking has been presented in Section 2.3.2. To broaden the scope of the $H \rightarrow Z\gamma$ analysis, a trigger for the invisible decay channel has been developed for the first time in ATLAS. However, this effort poses significant challenges due to the reliance on soft missing transverse energy ($E_{\text{T}}^{\text{miss}}$) and photon transverse momentum (p_{T}) and the small branching ratio of the decay channel. As discussed in Section 2.2.6, the ATLAS trigger system operates as a two-level architecture, consisting of Level-1 and the HLT. The investigations for the invisible decay channel focus on the HLT and certain Level-1 seeds, aiming to optimize data collection for Run-3 and potentially for the HL-LHC. This chapter will present preliminary results related to this development.

C.1 Efficiency of Run-3 Triggers for $H \rightarrow Z(\nu\nu)\gamma$ Events

First of all, the efficiencies of the triggers already existing in the current Run-3 trigger menu were computed. The main input quantities exploited by a trigger for $H \rightarrow Z(\nu\nu)\gamma$ events are those related to the kinematics of the photon and of the reconstructed missing transverse momentum vector. For processes like VBFH and WH , ZH with hadronic W or Z boson decays there are additional jets in the event that could be further leveraged upon at trigger level. The

criteria for such triggers were investigated first by studying the expected trigger efficiency in simulation. Simulated event samples of Higgs bosons decaying to $Z(\nu\nu)\gamma$ were produced for the following production modes: ggFH, VBFH, WmH, WpH, qqZH, and ggZH. For each production mode, 1400 events were simulated, with detector conditions corresponding to the Run-3 data taking.

The trigger efficiency is calculated as the ratio of the number of events passing the trigger selection over the total number of events. All results for the dominant production modes of the Higgs boson are shown in Figure C.1 and Figure C.2. In Figure C.1 (a), the trigger efficiency for ggFH ranges from 1.64% to 2.14% depending on the trigger line, when using triggers that require the presence of tight and isolated photon candidates (with various energy thresholds) combined with missing transverse energy criteria. These results demonstrate that the current trigger configurations are not sufficient for an efficient reconstruction of this production mode. In Figure C.1 (b), the trigger efficiency for VBFH is about 2% efficiency when applying only photon and MET requirements, while the highest performance, approximately 3.8%, is obtained with a trigger requiring the presence of four jets in addition to the photon. However, the overall efficiency remains inadequate for this mode. For vector boson-associated production modes, trigger efficiencies are evaluated based on the decay channels of $W^\pm$ and Z bosons. In Figure C.1 (c), the hadronic WH mode reaches the highest trigger efficiency of approximately 2% using photon and MET requirements, whereas the leptonic WH mode in Figure C.1 (d) achieves efficiencies of around 18% for lepton triggers and 15% for photon and MET selections. Figure C.2 presents the trigger efficiencies for the ZH production mode. The hadronic ZH mode in panel (a) records the highest efficiency of approximately 3.5% when using photon and MET requirements. The leptonic ZH mode in panel (b) achieves an efficiency around 30% for lepton triggers and 20% when using photon and MET requirements. The neutrino ZH mode in panel (c) shows an efficiency of about 15% when using photon and MET requirements.

As a result, the leptonic decay modes of $W^\pm$ and Z bosons demonstrate higher trigger efficiencies compared to their hadronic counterparts. Triggers utilizing lepton final states are notably more efficient, while the hadronic mode is specifically examined within the hadronic channel of $H \rightarrow Z\gamma$. Triggers based on photon and MET selections are primarily used for ggFH and the invisible decays of ZH, while triggers incorporating photon, jet, or MET criteria are applied to VBFH. Consequently, trigger optimizations are focused on the ggFH and VBFH production modes, with additional evaluations for the invisible ZH mode.

C.2 Development of New Dedicated Triggers for $H \rightarrow Z(\nu\nu)\gamma$

New dedicated triggers for $H \rightarrow Z(\nu\nu)\gamma$ with higher efficiency than the existing ones were proposed after studying the kinematic properties of the signal. Both truth-level and reconstruction-level distributions of key variables for each mode are examined. For the ggFH mode, only the photon p_T and E_T^{miss} variables, as shown in Figures C.3, are considered. In contrast, for VBFH, the observables related to photons and jets are presented in Figure C.4, while Figures C.5 and C.6 display the corresponding distributions for WH and ZH modes, respectively.

The development of a new trigger for Run 3 MC samples in the ATLAS experiment is a carefully structured process. According to the kinematics of the final state, the trigger can

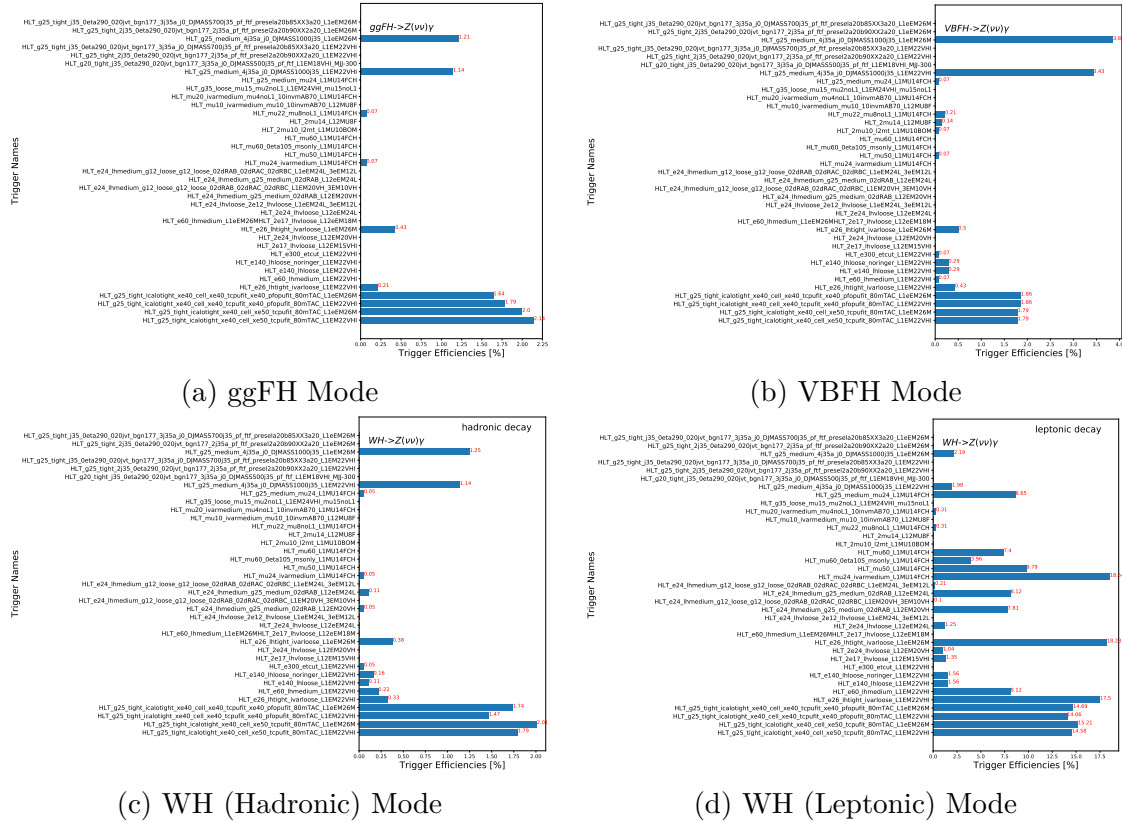


Fig. C.1

Trigger efficiency for each production mode using the current suitable triggers in Run-3 trigger menu. "WH" encompasses both the W^+H and W^-H production modes. Different decay modes of $W^\pm$ are separately evaluated.

be defined following the Run-3 trigger naming convention [188]. Initially, the trigger is introduced into the `MC_pp_run3_v1.py` menu, located within the `TriggerMenuMT` package of the Athena framework. The trigger chain is configured using the `ChainProp` class, which defines essential parameters like kinematic thresholds and Level-1 seeds. Once implemented, the newly added trigger undergoes comprehensive testing through Athena's compilation and trigger validation tools, such as `runTrigART.py`, to verify proper functionality and integration within the existing framework. After passing validation, including assessments of physics efficiency and computational performance, the trigger is added to the development menu for use in Run 3 MC production. Upon further validation and performance monitoring, it may be promoted to the official physics menu.

The evaluation of a new trigger within the ATLAS experiment requires the consideration of several key performance metrics, including the trigger rate, the weighted pre-scale (PS) rate, the unique rate and the trigger efficiency. These metrics are essential for assessing the trigger's efficiency and its overall impact on the system. The trigger rate, defined as the number of events per second that satisfy the trigger criteria, provides a direct measure of how frequently the trigger is activated under experimental conditions. In Run 3, trigger rate estimates are derived from *EnhancedBiasData*, which biases datasets towards events of interest, enabling more efficient

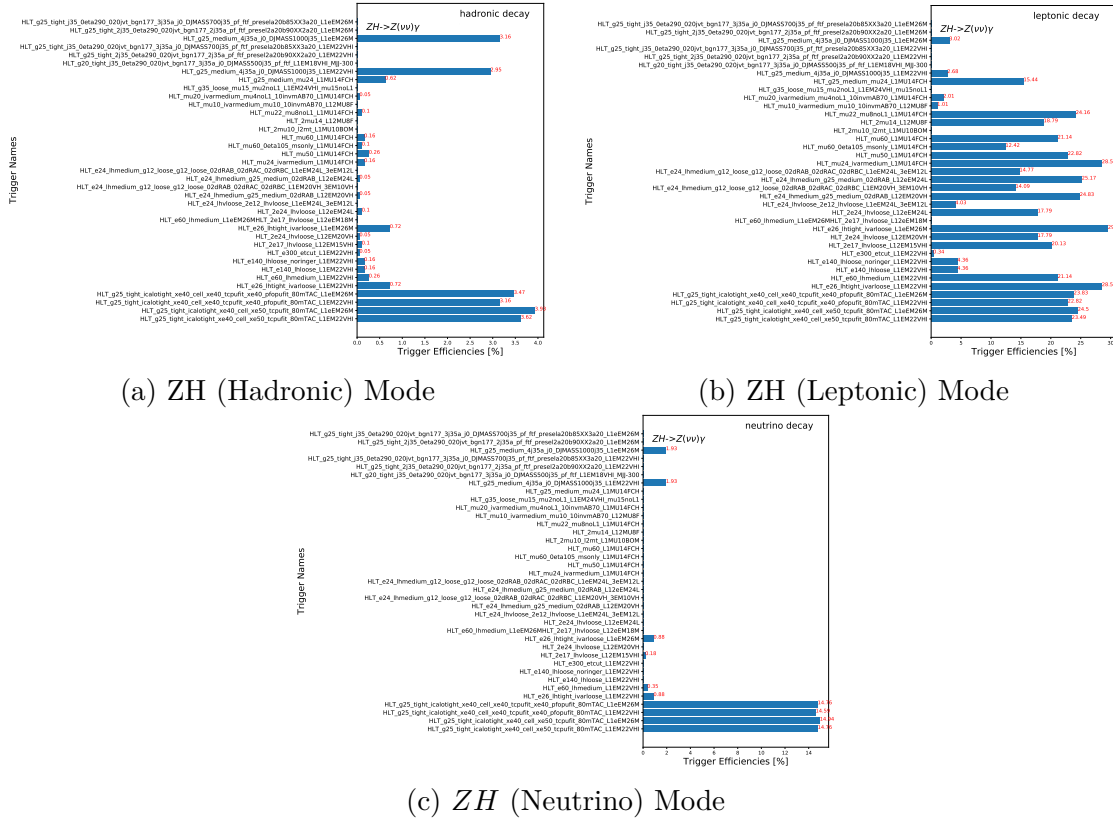


Fig. C.2

Trigger efficiency for each production mode using the current suitable triggers in Run-3 trigger menu. "ZH" refers to both the $ggZH$ and $qqZH$ production modes. Different decay modes of Z bosons are separately evaluated.

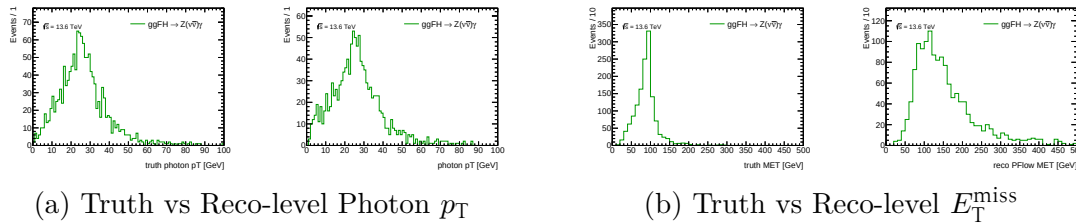


Fig. C.3

Distributions of truth and reconstructed photon p_T and missing transverse energy E_T^{miss} from the full simulation of $ggFH$ decaying to $H \rightarrow Z\gamma$.

rate calculations compared to *ZeroBias* data. These events are accompanied by correction weights to account for the introduced bias. New trigger selections can be tested on reprocessed EnhancedBias AODs. The rate estimation process involves running emulation scripts on these AODs and applying rate corrections to align with online rates. The scaling procedure leverages known trigger rates and luminosity adjustments. Accurate rate predictions depend on proper weighting and the careful selection of events for both the trigger under test and the reference trigger. The weighted pre-scale rate, which incorporates pre-scaling, is calculated by summing the products of event weights associated with the new trigger selection, scaled by the known trigger rate. This result is then normalized by the sum of weights for the known trigger and

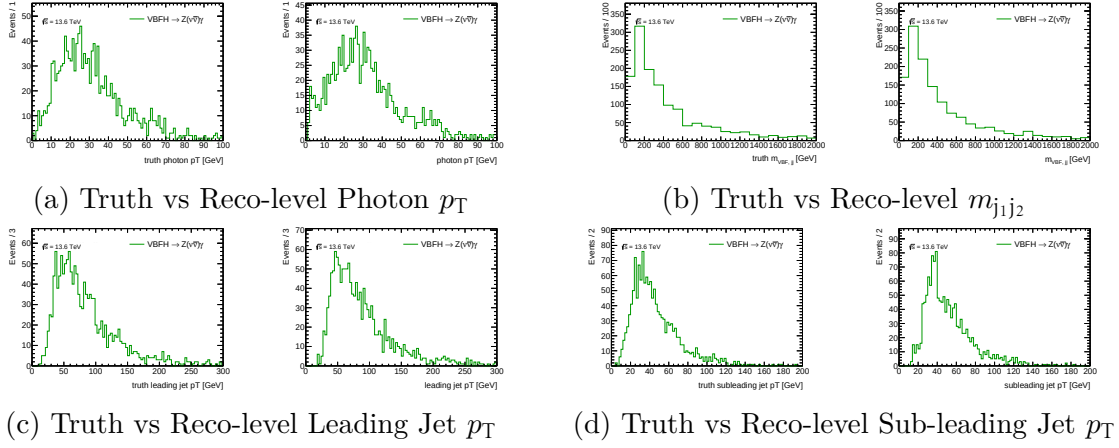


Fig. C.4 Distributions of truth and reconstructed photon p_T (a), invariant mass m_{j1j2} (b), leading and sub-leading jet p_T (c, d) from the full simulation of $VBFH$ decaying to $H \rightarrow Z\gamma$.

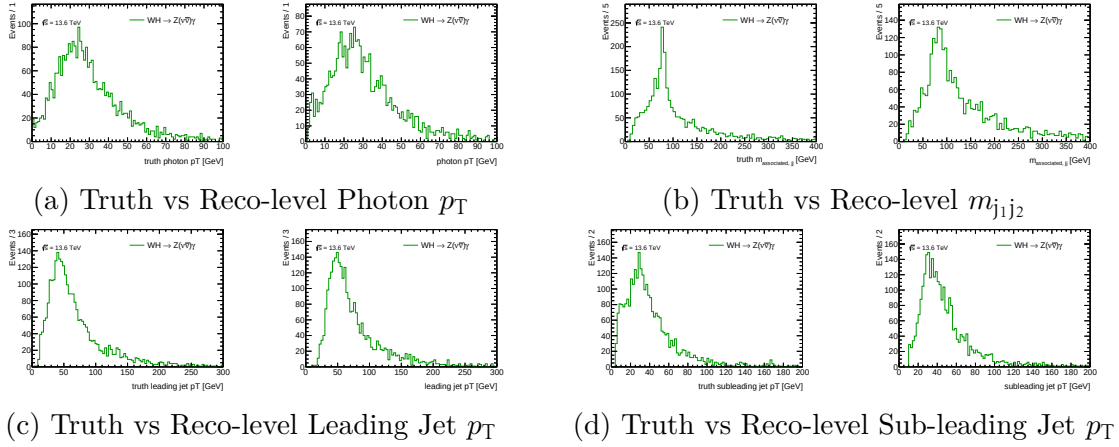


Fig. C.5 Distributions of truth and reconstructed photon p_T (a), invariant mass m_{j1j2} (b), leading and sub-leading jet p_T (c, d) from the full simulation of $W^\pm H$ decaying to $H \rightarrow Z\gamma$.

further adjusted for luminosity scaling, ensuring the rate accurately reflects real-time operating conditions. The unique rate, a critical measure for evaluating a new trigger's contribution, quantifies the additional rate added to the overall trigger menu. Specifically, it measures the rate increase when the new trigger is introduced, compared to the original menu. It is imperative that this unique rate be controlled, typically suppressed to approximately 10 Hz, to preserve system efficiency and prevent oversaturation of the available trigger bandwidth. Collectively, these metrics form a robust framework for the quantitative evaluation of a new trigger, ensuring its performance is optimized within the operational constraints of the ATLAS DAQ system. Trigger efficiency is defined as the ratio of events passing the trigger selection to the total number of events. It is important to note that the trigger selection may differ from the final selection. The efficiency of the new trigger is evaluated using the *TrigDecisionTool*, which is

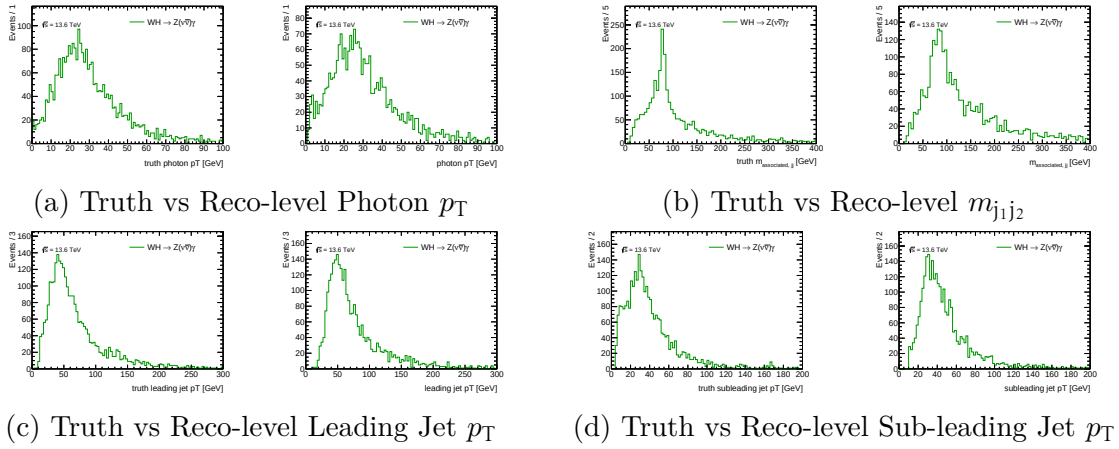


Fig. C.6 Distributions of truth and reconstructed photon p_T (a), invariant mass m_{j1j2} (b), leading and sub-leading jet p_T (c, d) from the full simulation of ZH decaying to $H \rightarrow Z\gamma$.

employed to assess the trigger's performance.

C.3 Performance of the Proposed Triggers

The trigger development primarily targets the dominant Higgs boson production modes, specifically ggFH and VBFH. Trigger efficiencies are detailed in Table C.1, with separate evaluations for each mode. The ggFH mode exhibits relatively low trigger efficiencies, ranging from 2.79% to 5.36%, while VBFH demonstrates significantly higher efficiencies, reaching up to 16%. The photon and MET signals in the invisible decay channel, as depicted in Figure C.3, are significantly softer compared to the Higgs decay to photon and massless dark photon channel [189], posing substantial challenges for trigger development. Additionally, ggFH offers minimal improvement in significance due to the absence of strong signatures in the invisible decay channel. As a result, the ggFH mode will not be further considered in this study. The investigations are focused on the VBFH mode to optimize the trigger rate while keeping the efficiency higher.

In general, higher trigger rates tend to correspond with lower efficiencies, requiring a balance between the two. Based on the kinematic distributions shown in Figure C.4, the Level-1 trigger seed $L1eEM22M_jMJJ-300$ is used, indicating a photon with $p_T > 18$ GeV and a dijet invariant mass (m_{j1j2}) > 300 GeV, to achieve sufficient efficiency. At higher trigger levels, the photon transverse energy is defined as $p_T > 20$ GeV with tight identification and isolation criteria. Additionally, two jets with $p_T > 35$ GeV, or one jet with $p_T > 30$ GeV and another with $p_T > 25$ GeV, are required, along with an invariant mass $m_{j1j2} > 500$ GeV. A trigger utilizing photon, jet, and MET objects is defined and evaluated. The performance results of these triggers for the VBFH mode are summarized in Table C.2. Considering both unique rate and efficiency, the trigger in the second row provides the optimal performance for VBFH, with a unique rate of 24.04 Hz and an efficiency of 15.71%.

Futhermore, the efficiency of the trigger was calculated within the fiducial phase space. The fiducial phase space is defined with the following criteria: photons with transverse momentum

High Level trigger	Weighted PS Rate [Hz] (8k Events)	Efficiency [%]	
		ggFH	VBFH
HLT_g25_medium_xe35_cell_xe40_tcpufit_L1eEM26M	335.9729 ± 100.7682	5.36	15.57
HLT_g25_tight_xe35_cell_xe40_pfopufit_L1XE35	151.8891 ± 67.9269	4.5	13.36
HLT_g25_medium_xe35_cell_xe40_pfopufit_L1XE35	212.6447 ± 80.3721	4.5	14.14
HLT_g25_loose_icaloose_xe35_cell_xe40_pfopufit_L1XE35	212.6447 ± 80.3721	4.86	15.00
HLT_g25_tight_xe30_cell_xe40_pfopufit_L1XE50	60.7556 ± 42.9607	2.79	9.36
HLT_g20_tight_xe30_cell_xe40_pfopufit_L1XE50	60.7556 ± 42.9607	2.79	9.79
HLT_g20_tight_xe35_cell_xe40_pfopufit_L1XE35	151.8891 ± 67.9269	4.57	13.79
HLT_g20_medium_xe35_cell_xe40_pfopufit_L1XE35	212.6447 ± 80.3721	4.57	14.57
HLT_g20_loose_icaloose_xe35_cell_xe40_pfopufit_L1XE35	212.6447 ± 80.3721	5.0	15.57
HLT_g25_medium_2j35a_j0_DJMASS700j35_pf_ftf_L1eEM26M	394.9115 ± 109.5288	3.5	15.07
HLT_g25_loose_icaloose_2j35a_j0_DJMASS700j35_pf_ftf_L1eEM26M	516.4228 ± 125.2509	3.93	16.14
HLT_g25_medium_2j35a_j0_DJMASS1000j35_pf_ftf_L1eEM26M	303.7781 ± 96.0631	2.36	10.86
HLT_g20_medium_2j35a_j0_DJMASS700j35_pf_ftf_L1eEM22M_jMJJ-300	121.5112 ± 60.7556	1.43	13.36
HLT_g20_tight_2j35a_j0_DJMASS700j35_pf_ftf_L1eEM22M_jMJJ-300	91.1334 ± 52.6159	1.43	12.86

Tab. C.1 Weighted PS rate with its uncertainty and efficiency of various photon+MET and photon+jets triggers for ggFH and VBFH production modes. The efficiencies of all triggers for ggFH are quite small (a few percent) while some triggers for VBFH can bring the efficiency up to 16%.

High Level Trigger	Weighted PS Rate [Hz]	Unique Rate [Hz]	Efficiency [%]	VBFH
HLT_g20_tight_2j35a_j0_pf_ftf_L1eEM22M_jMJJ-300	255.9004 ± 55.6882	48.6045 ± 10.5771	21.14	
HLT_g20_tight_2j35a_j0_DJMASS500j35_pf_ftf_L1eEM22M_jMJJ-300	146.5403 ± 42.0990	24.302 ± 6.9817	15.71	
HLT_g20_tight_icaloose_2j35a_j0_DJMASS500j35_pf_ftf_L1eEM22M_jMJJ-300	97.9358 ± 34.3763	<1	15.64	
HLT_g20_tight_j30a_j25a_pf_ftf_xe35_cell_xe40_pfopufit_L1eEM22M_jMJJ-300	36.4534 ± 21.0464	<1	12.36	

Tab. C.2 Weighted PS rate, unique rate, and efficiency of various triggers for the VBFH production mode. Different combinations of photon, jet, and MET objects are employed to assess the rate and trigger efficiency. The trigger in the second row exhibits an optimal balance between unique rate and efficiency. The notation “<1” indicates a unique rate below 1 Hz, either due to limited statistics or overlap with other triggers..

$p_T > 15$ GeV, jets with leading jet $p_T > 30$ GeV, sub-leading jet $p_T > 25$ GeV, and a missing transverse energy $E_T^{\text{miss}} > 40$ GeV. Additionally, the invariant mass of the VBF jets ($m_{j_1 j_2}$) was required to be greater than 300 GeV with the rapidity difference $|\eta| < 4.4$. The trigger efficiency in the fiducial phase space is summarized in Table C.3. To improve this performance, a looser photon isolation condition was introduced by adding *icaloLoose* isolation. This resulted in an improved VBFH trigger efficiency for the last trigger, particularly in the fiducial space, reaching a value of 39.95%. However, due to the complexity of background estimation, accurately assessing the significance of the trigger is challenging. As a result, this trigger will not be considered for data-taking in 2024.

C.4 Outlook

The trigger development for the invisible $H \rightarrow Z(\nu\nu)\gamma$ channel, particularly in the VBF Higgs production mode, faces challenges due to the soft kinematics of the photon, jet, and

High Level Trigger	Weighted PS Rate [Hz]	Estimated Unique Rate [Hz]	VBFH Efficiency [%]	
			Inclusive Space	Fiducial Space
HLT_g20_tight_2j35a_j0_pf_ftf_L1eM22M_jMJJ-300	265.8284 ± 22.3802	98.5373 ± 16.4389	21.14	51.10
HLT_g20_tight_2j35a_j0_DJMASS500j35_pf_ftf_L1eM22M_jMJJ-300	156.0438 ± 21.7854	70.4382 ± 13.0164	15.71	40.12
HLT_g20_tight_icaloose_2j35a_j0_DJMASS500j35_pf_ftf_L1eM22M_jMJJ-300	120.3470 ± 15.7565	59.4865 ± 15.5799	15.64	39.95

Tab. C.3 Trigger evaluation for the VBFH production mode, focusing on the efficiency within the inclusive and fiducial phase space. The last trigger demonstrates improved performance in the fiducial space, with an efficiency of 39.95% and smaller unique rate.

MET signatures. Achieving high efficiency while controlling the unique rate has been difficult. The focus moving forward, especially for Run 3 and the HL-LHC, is on improving both trigger efficiency and rate management. Key optimizations include refining photon identification and MET thresholds, with an emphasis on the fiducial phase space for VBF Higgs events. Future improvements will likely involve implementing photon isolation and adjusting dijet mass cuts, while combining photon and MET triggers is seen as a crucial strategy for increasing sensitivity. The ultimate aim is to enhance signal efficiency without overloading the trigger rate, ensuring the system can handle the higher data volumes expected at increased luminosities.

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Something ends here, Something starts there.

— Qiuping SHEN

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Here, I extend my deepest thanks to all who have helped and supported me along the way. In the future, I will continue to maintain humility and diligence, and repay your trust and care with my actions.

Place: Shanghai, China

Date: November 25, 2024

Signature: **Qiuping SHEN**

LIST OF PERSONAL CONTRIBUTIONS

During Ph.D. I have contributed to the following projects in the ATLAS collaboration:

- Mitigation of the pile-up dependence of the photon identification criteria of the ATLAS experiment for the Run-3 or High-Luminosity LHC data-taking period. For Run-3 and next HL-LHC, the collision will bring much harsher pile-up environment, which may cause the decline of the efficiency of the cut-based photon identification. To mitigate the dependence of pile-up, the selections are optimized using Genetic Algorithm to define a μ -dependent tight menu to be more robust with pile-up. The performances of the menu are evaluated in the $|\eta|$ and p_T as well. The μ -dependent tight menu is also implemented into the ATHENA framework.
- Legacy search for Higgs boson pair production in the $b\bar{b}\gamma\gamma$ final state with the full Run-2 13 TeV pp collision data collected by the ATLAS Experiment. I proposed an innovative method to separate the signals and backgrounds to enhance the signal-to-background ratio and the similar results to the baseline ones are obtained. These results are recorded in the ATLAS internal note. The theoretical and experimental systematic uncertainties are evaluated. The 2D constraint on κ_{2V} and κ_V is derived from the analysis considering the contributions from the Higgs production and decay modes.
- Joint combination analysis for double Higgs boson and single Higgs boson with electroweak next-to-leading order corrections. The combined analysis aims to constraint the Higgs self-coupling κ_λ . I helped to develop the fit tools and study the correlation schemes between those systematic uncertainties as well as contributed to the final fitted results.

Additional contributions to ATLAS Muon Detector and CEPC SDHCAL projects are also listed below:

- ATLAS Muon Phase-II Upgrade Project: The project is based on the ATLAS Muon Phase-I Upgrade Project. Various designs of the resistive plate chamber are simulated with COMSOL for the gas flow and fabricated in the clean rooms. Built all the whole procedure of the fabrication and cosmic-ray test of the resistive plate chamber using glass as substrate and gas as sensitive medium. The detector efficiency for muons in cosmic rays is more than 95%.
- Fast-timing electronics readout design and test applied to MRPC for SDHCAL: The front end board is designed using PETIROC2B ASIC chip and the interface board is developed to connect the FEB and DAQ. The DAQ is implemented using Xilinx FPGA ZCU102 with programmable logic and processing system. The first version is used to test the performance of the board. Some crosstalk from the FEB is found and the second version with two chips is designed and both the power source and clock source are also integrated into one board. The performance is evaluated with the signal from the generator, which can achieve the intrinsic time resolution of 36ps.

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LIST OF PUBLICATIONS**Selected publications from the ATLAS Collaboration and the SDHCAL Collaboration**

- [7]. Qiuping Shen etc, A Prototype of the Timing Electronic System for the CALICE SDHCAL, *IEEE Transactions on Nuclear Science* (2024) 0018-9499
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- [10] *Higgs self-coupling measurement from single Higgs and double Higgs*
Shanghai, China, The 9th China LHC Physics Workshop (CLHCP2023), November 18, 2023
- [9] *Studies of new Higgs boson interactions through non-resonant HH production in the $b\bar{b}\gamma\gamma$ final state in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*
Zhuhai, Guangdong, 14th Workshop of France China Particle Physics Laboratory (FCPPL2023), November 06, 2023
- [8] *Search for Higgs boson pair production in the two bottom quarks plus two photons final state in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector*
Nanjing, Jiangsu, The 8th China LHC Physics Workshop (CLHCP2022), November 25, 2022
- [7] *Search for di-Higgs production with $HH \rightarrow b\bar{b}\gamma\gamma$*
Paris, France, Workshop Physics ATLAS France 2022, September 20, 2022
- [6] *Fast Timing Readout Electronic based on PETIROC ASIC*
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- [4] *Progress of CEPC Semi-Digital HCAL*
Yangzhou, Jiangsu, Joint Workshop of the CEPC Physics, Software and New Detector Concept, April 15, 2021
- [3] *Progress of fast-timing electronics readout design and test for SDHCAL*
Online, CALICE Collaboration Meeting, March 25, 2021
- [2] *Performance Study of SDHCAL Prototype and Future 5D HCAL R&D*
Shanghai, China, 2020 Joint Academic Exchange Conference and Shanghai Symposium on Particle Physics and Nuclear Physics, January 8, 2021
- [1] *Implement timing in a new board to be used for a small SDHCAL prototype*
Online, CALICE Collaboration Meeting, September 29, 2020

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