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Upgrade of the ATLAS tracking detector and measurement of the Higgs boson production cross-section at 13.6 TeV

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In loving memory of my uncle, Dr. Raghunath Nakkalil, whose legacy continues to inspire me every day, and to my mom — Amma, we did it! This one's for you!

Abstract

Title: Upgrade of the ATLAS tracking detector and measurement of the Higgs boson production cross-section at 13.6 TeV

High-energy physics explores the fundamental particles of the universe and their interactions by creating and analyzing collisions at particle accelerators operating at the highest energies. The Large Hadron Collider (LHC), the world's most powerful accelerator, has achieved groundbreaking successes since it began operations. Most notably, during Run 1 (2010-2012) at center-of-mass energies of 7-8 TeV, the ATLAS and CMS collaborations discovered the Higgs boson in 2012, confirming the last missing piece of the Standard Model. This discovery opened new avenues for studying this fundamental particle. In Run 2 (2015-2018), the LHC increased its collision energy to 13 TeV, enabling precise measurements of the Higgs boson's properties, including its mass, and decay into fermions such as bottom quarks and tau leptons. Run 2 also provided insights into rare processes, such as the production of final states containing multiple top quarks and precise measurements of the top quark and W boson masses. Run 3 (2022-present) features even higher energy (13.6 TeV) and increased collision rates, aiming to explore rare processes, improve precision measurements, and search for physics beyond the Standard Model. This thesis presents the first measurement of the Higgs boson production cross-section at 13.6 TeV using $\approx 30\text{fb}^{-1}$ of pp collision data collected in 2022 with the ATLAS detector.

The past 16 years have been remarkable for high-energy physics, marked by the successes of LHC experiments in advancing our understanding of fundamental particles. Significant upgrades are planned to enhance and extend the LHC's discovery potential. The High-Luminosity LHC (HL-LHC) upgrade aims to achieve instantaneous luminosities five times greater than the LHC's nominal value, enabling the ATLAS and CMS experiments to collect ten times more data. This increase will allow precision tests of the Higgs boson's properties and improve sensitivity to new physics scenarios, ensuring effective operation of LHC until the 2040s. The current tracking detectors of the ATLAS and CMS experiments will be replaced with more radiation-hard, faster detectors of higher granularity. The inner detector of the ATLAS will be upgraded to an all-silicon tracker (ITk) featuring a new strip detector and pixel detector.

The focus of this thesis is on the upgrade activities of the ATLAS tracking detectors, particularly addressing radiation damage challenges, a critical concern for the HL-LHC upgrade. Radiation damage affects the performance of silicon tracking detectors, with signal reduction being the most critical issue. Generating simulated data that accurately reflects performance evolution as luminosity and fluence accumulate is crucial. The ATLAS collaboration has developed algorithms to correct simulated Monte Carlo (MC) events for radiation damage effects, achieving impressive agreement between collision data and simulated events in Run 3.

In preparation for the HL-LHC, a faster ATLAS MC production algorithm is imperative due to escalating collision rates, events, tracks, and particle hit rates, imposing stringent constraints on computing resources. This thesis presents a novel lightweight algorithm based on Look-Up Tables to model radiation damage effects. This algorithm has been studied for ITk planar pixel sensors and has the potential for extension to strip and 3D pixel sensors. Additionally, this thesis includes studies on realistically modeling the ITkPix readout chip within the ATLAS software framework, Athena, and pixel quad module development at the Laboratoire de Physique Nucléaire et des Hautes Énergies.

Keywords: ATLAS, HL-LHC, ATLAS inner tracker (ITk), Radiation Damage, ITkPix Readout chip, Higgs boson, $H \rightarrow \gamma\gamma$ fiducial cross-section, LHC Run 3 data

Résumé

Titre: Amélioration du détecteur de traces (ITk) pour la phase haute luminosité d'ATLAS et mesure de la section efficace de production du boson de Higgs at 13.6 TeV

La physique des hautes énergies explore les particules fondamentales de l'Univers et leurs interactions en produisant et analysant des collisions dans des accélérateurs de particules fonctionnant aux énergies les plus élevées. Le Grand Collisionneur de Hadrons (LHC), situé au CERN près de Genève en Suisse, représente l'accélérateur de particules le plus puissant au monde. Depuis le début de ses opérations, le LHC a connu des succès révolutionnaires. Notamment, lors de la Run 1 (2010-2012) à des énergies de centre de masse de 7-8 TeV, les collaborations ATLAS et CMS ont découvert le boson de Higgs en 2012, confirmant le dernier élément manquant du Modèle Standard de la physique des particules. Cette découverte a ouvert de nouvelles perspectives pour l'étude de cette particule fondamentale, qui joue un rôle crucial dans notre compréhension de la nature de la matière et des forces fondamentales. Lors de la Run 2 (2015-2018), le LHC a augmenté son énergie de collision à 13 TeV, permettant des mesures précises des propriétés du boson de Higgs, y compris sa masse et sa désintégration en fermions tels que les quarks bottom et les leptons tau. Cette phase a également fourni des informations sur des processus rares, comme la production de états finaux avec multiples quarks top, ainsi que des mesures précises de la masse du quark top et du boson W. Actuellement, le Run 3 (2022-présent) du LHC opère à une énergie encore plus élevée de 13.6 TeV, avec des taux de collisions accrus. Cette phase vise à explorer des processus rares, à améliorer les mesures de précision et à rechercher des phénomènes au-delà du Modèle Standard de la physique des particules. Cette thèse présente la première mesure de la section efficace de production du boson de Higgs à 13.6 TeV en utilisant $\approx 30\text{fb}^{-1}$ de données de collision pp collectées en 2022 avec le détecteur ATLAS.

Les 16 dernières années ont été remarquables pour la physique des hautes énergies, marquées par les succès des expériences du LHC dans l'avancement de notre compréhension des particules fondamentales. Ces succès ont motivé des mises à niveau significatives pour le LHC afin d'améliorer et d'étendre son potentiel de découverte. L'une des avancées majeures prévues est la mise à niveau vers le Grand Collisionneur de Hadrons à Haute Luminosité (HL-LHC), visant à atteindre des luminosités instantanée cinq fois supérieures à celles du LHC actuel. Cette amélioration permettra aux expériences ATLAS et CMS de collecter dix fois plus de données, essentielles pour des tests de précision encore plus poussés du boson de Higgs et pour accroître la sensibilité à de nouvelles physique au-delà du Modèle Standard, assurant ainsi un fonctionnement efficace du LHC jusqu'aux années 2040. Dans le cadre de ces mises à niveau, les détecteurs de traces d'ATLAS et de CMS seront remplacés par de nouvelles technologies plus avancées, capables de résister à des environnements plus irradiés et d'offrir une meilleure résolution spatiale. Par exemple, le trajectographe d'ATLAS sera remplacé par un nouveau détecteur en silicium - le Inner Tracker (ITk) - comprenant un nouveau détecteur à bandes et un détecteur pixel. Cela permettra non seulement de maintenir, mais aussi d'améliorer les performances de détection nécessaires pour les expériences au HL-LHC.

Le principal objectif de cette thèse est de contribuer aux activités de mise à niveau du trajectographe d'ATLAS, en se concentrant particulièrement sur les défis posés par les dommages de rayonnements. Les détecteurs en silicium utilisés dans les trajectoires sont sensibles aux dommages causés par les hadrons énergétiques, ce qui entraîne une réduction du signal détecté et une dégradation des performances au fil du temps. La génération de données simulées joue un rôle crucial dans la compréhension et la correction de ces effets de dommages. La collaboration ATLAS a développé des algorithmes pour ajuster les événements Monte-Carlo (MC) afin de reproduire fidèlement les conditions expérimentales réelles, ce qui est essentiel pour interpréter correctement

les données de collision.

En prévision du HL-LHC, il est impératif de développer des algorithmes MC plus rapides pour ATLAS, afin de pouvoir simuler et analyser un volume accru d'événements de collision. Cette thèse présente un nouvel algorithme rapide basé sur des tables de consultation pour modéliser les effets des dommages de rayonnements dans les détecteurs pixel planaires ITk. Cet algorithme offre non seulement des gains significatifs en termes de temps de calcul, mais il a également le potentiel d'être étendu à d'autres types de détecteurs, tels que les capteurs à bandes et les pixels 3D. De plus, cette thèse inclut des études détaillées sur la modélisation du comportement des puces de lecture ITkPix dans le cadre du logiciel d'analyse ATLAS, ainsi que le développement de modules pixel quad au Laboratoire de Physique Nucléaire et des Hautes Énergies.

Mots clefs: ATLAS, HL-LHC, détecteur ITk, dommages de rayonnements, Puce de lecture ITkPix, boson de Higgs, section efficace fiduciale de $H \rightarrow \gamma\gamma$, Données du Run 3

Résumé étendu

La physique des hautes énergies (HEP) représente l'intersection entre la rigueur scientifique et une curiosité profonde, où la quête de compréhension des composantes fondamentales de l'univers stimule à la fois l'innovation et la découverte. Ce domaine explore les plus petits constituants de la matière et les forces fondamentales qui régissent leurs interactions, en utilisant des accélérateurs de particules avancés pour recréer des conditions similaires à celles de l'univers primitif. Au cœur de cette démarche se trouve le Modèle Standard (SM) de la physique des particules, un cadre théorique qui classe toutes les particules élémentaires connues et leurs interactions. Il fournit une description complète des forces fondamentales, à l'exception de la gravité, et a été crucial pour orienter la recherche expérimentale.

S'appuyant sur cette base théorique, le Grand Collisionneur de Hadrons (LHC) du CERN est à l'avant-garde de la recherche expérimentale en physique des hautes énergies. En tant que l'accélérateur de particules le plus puissant au monde, le LHC a joué un rôle central dans la confirmation des aspects clés du Modèle Standard, y compris la découverte marquante du boson de Higgs en 2012. L'expérience ATLAS (A Toroidal LHC ApparatuS), l'une des principales expériences du LHC, a été essentielle dans l'étude du boson de Higgs et l'exploration de nouvelles frontières en physique des particules.

En perspective de 2029, le LHC entrera dans sa phase de Haute Luminosité (HL-LHC), une transition qui promet à la fois des avancées significatives et des défis complexes. La mise à niveau du HL-LHC vise à augmenter la luminosité intégrée d'un facteur 10 par rapport à la valeur de conception initiale du LHC, permettant d'accumuler jusqu'à 3000 fb^{-1} de données d'ici la fin de sa durée de vie opérationnelle. Cette amélioration permettra d'améliorer considérablement la précision des mesures pour les processus rares et d'apporter des perspectives plus approfondies en physique fondamentale. Cependant, l'augmentation de la luminosité entraînera également une hausse des niveaux de radiation, posant des défis substantiels en termes de dommages causés aux composants des détecteurs et à l'électronique. Les détecteurs à pixels en silicium, au centre à la fois des mises à niveau actuelles et prévues du détecteur ATLAS, seront exposés à des niveaux de radiation élevés tout au long de leur durée de vie opérationnelle. Avant le HL-LHC, les couches les plus internes de ces détecteurs devaient accumuler une fluence de radiation dépassant $10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$, tandis que la fluence de radiation devrait augmenter d'un ordre de grandeur au HL-LHC, imposant des exigences encore plus grandes sur les mises à niveau du détecteur pour résister à ces niveaux de radiation plus élevés. La simulation des dommages radiatifs est donc cruciale pour faire des prévisions précises sur les performances actuelles et futures du détecteur.

Cette thèse est organisée en plusieurs chapitres qui alternent entre aspects théoriques et expérimentaux, offrant une exploration complète de diverses études avec un accent principal sur les activités de mise à niveau de l'Inner Tracker (ITk) d'ATLAS pour le HL-LHC.

Le Chapitre 1 offre un aperçu concis du Modèle Standard de la physique des particules, du mécanisme de Higgs et de la phénoménologie de Higgs au LHC, établissant les principes fondamentaux qui régissent le comportement des particules élémentaires et leurs interactions.

Le Chapitre 2 propose une vue d'ensemble complète du LHC et du détecteur ATLAS. Il commence par un examen approfondi du LHC, détaillant ses composants clés et ses principes de fonctionnement. Le chapitre se concentre ensuite sur une exploration approfondie du détecteur ATLAS, en mettant l'accent sur sa conception et ses différents sous-systèmes.

Le Chapitre 3 explore la théorie et la technologie des détecteurs à pixels en silicium, qui sont essentiels pour le détecteur ATLAS et centraux pour la recherche en HEP. Le chapitre commence par un examen des interactions entre les particules chargées et la matière, en se concentrant sur les

mécanismes de perte d'énergie. Il se penche ensuite sur les propriétés des détecteurs en silicium, détaillant leur conception et leurs principes de fonctionnement. La discussion progresse vers la formation du signal, en soulignant la dynamique des porteurs de charge et l'influence de l'angle de Lorentz. De plus, le chapitre aborde la théorie de l'électronique frontale et des systèmes de lecture, qui sont essentiels pour mesurer la perte d'énergie des particules traversant le détecteur en silicium. Enfin, il traite des défis posés par les dommages radiatifs, y compris les mécanismes de dégradation des capteurs et leur impact sur les performances du détecteur.

Le Chapitre 4 présente la mesure de la section efficace inclusive fiducielle de $H \rightarrow \gamma\gamma$ à l'aide des données du début du Run 3 collectées par le détecteur ATLAS en 2022, détaillant les méthodologies employées et les résultats obtenus. Le chapitre commence par une introduction qui décrit la motivation et la stratégie derrière la mesure. Il poursuit par une discussion sur les échantillons de données et de simulation utilisés, y compris la simulation du signal de Higgs, du fond et du bruit de fond. Les sections centrales du chapitre se concentrent sur la mesure de $H \rightarrow \gamma\gamma$, en abordant les processus de reconstruction et de sélection des événements, la modélisation du signal et du fond, et la méthodologie d'ajustement. Mes contributions à ce projet incluent la modélisation du signal (Section 4.3.2.1) et l'étude des incertitudes systématiques associées à la modélisation du signal $m_{\gamma\gamma}$ (Section 4.3.3.1). La section des résultats comprend une analyse complète et la présentation des sections efficaces mesurées. Notamment, le chapitre propose également une discussion sur les résultats combinés des mesures de section efficace avec le canal $H \rightarrow ZZ^* \rightarrow 4\ell$. Le chapitre se termine par une perspective sur les futures orientations de la recherche. D'autres détails et mes contributions supplémentaires, y compris des vérifications croisées sur les différences NNLOPS vs. MINLO, les facteurs de correction inclusifs et les facteurs d'acceptation, sont détaillés dans l'Annexe A.

Le Chapitre 5 se concentre sur le HL-LHC et les mises à niveau du détecteur ATLAS, avec un accent particulier sur l'Inner Tracker. Le chapitre commence par une vue d'ensemble du projet HL-LHC, détaillant ses objectifs et son potentiel physique attendu. Ensuite, le chapitre discute de la mise à niveau de la Phase II d'ATLAS, en mettant en avant les avancées dans plusieurs composants : l'Inner Tracker, le Calorimètre, le Spectromètre à Muons, les systèmes de déclenchement et d'acquisition de données, ainsi que l'introduction du Détecteur de Synchronisation à Haute Granularité (HGTD). La dernière partie du chapitre fournit une description détaillée de l'Inner Tracker d'ATLAS. Elle couvre la disposition de l'ITk, les performances de suivi attendues, y compris les efficacités et la résolution des paramètres de suivi, et des détails sur le détecteur à pixels de l'ITk. Cela inclut un examen des technologies des capteurs à pixels utilisés, des puces de lecture, des modules de pixels et des structures de support mécaniques. Le chapitre couvre également les activités de développement de modules menées au Laboratoire de Physique Nucléaire et de Hautes Énergies (LPNHE), en se concentrant sur la préproduction des modules quad pour le HL-LHC, à laquelle j'ai contribué.

Le Chapitre 6 se penche sur la numérisation des pixels au sein de l'Inner Tracker d'ATLAS, en se concentrant sur deux principaux domaines : la Section 6.1 examine la mise en œuvre de la numérisation pour les modules à pixels de l'ITk dans le cadre du logiciel Athena, tandis que la Section 6.2 aborde la modélisation des effets des dommages radiatifs dans les événements de Monte Carlo pour le HL-LHC. Dans la Section 6.1, après avoir fourni un aperçu du processus de numérisation et une brève introduction au cadre logiciel Athena, la Section 6.1.4 détaille la mise en œuvre de la correction du time-walk la Section 6.1.4 détaille la mise en œuvre de la correction du time-walk. La Section 6.1.5 présente ensuite une discussion approfondie sur la conversion charge en Time-over-Threshold (ToT), en se concentrant sur les méthodes utilisant une seule table de correspondance (LUT) ou plusieurs LUTs. De plus, le chapitre aborde l'impact des dommages radiatifs sur les détecteurs en silicium, en présentant le développement d'un nouveau numériseur des dommages radiatifs utilisant des LUTs, spécifiquement pour le HL-LHC, avec un accent sur les capteurs de pixels planaires dans la Section 6.2.2. La discussion comprend la méthodologie,

l'intégration avec Allpix-Squared, les entrées de simulation, la génération de LUTs, et la validation à travers des tests de fermeture.

Le chapitre de Synthèse et Perspectives propose une vue d'ensemble concise des divers projets discutés dans cette thèse et offre des perspectives sur les futurs développements dans le domaine.

Mesure de la section efficace fiducielle de $H \rightarrow \gamma\gamma$ dans les collisions pp à $\sqrt{s} = 13.6$ TeV

La première partie de cette thèse présente la première mesure des sections efficaces du boson de Higgs à une énergie dans le centre de masse de 13.6 TeV via le canal de désintégration en deux photons, en utilisant environ $\approx 30\text{fb}^{-1}$ de données de collisions pp collectées par l'expérience ATLAS au LHC lors de la première année (2022) du Run 3 (voir Chapitre 4).

Le Run 3 du LHC est actuellement en cours avec des performances de la machine stables, et selon le dernier calendrier, il devrait se poursuivre jusqu'en novembre 2026. À la suite de cette période, le troisième long arrêt (LS3) commencera, au cours duquel le détecteur ATLAS subira une mise à niveau complète en préparation pour l'ère du HL-LHC. La période de prise de données de 2024 s'est avérée être la plus réussie à ce jour, surpassant à la fois la luminosité délivrée par le LHC et la luminosité intégrée enregistrée par le détecteur ATLAS par rapport aux luminosités du Run 2. Les mesures de sections efficaces dans le canal $H \rightarrow \gamma\gamma$ et la mesure combinée avec le canal $H \rightarrow ZZ^* \rightarrow 4\ell$, utilisant les premières données de collisions pp du Run 3, de 31.4fb^{-1} et 29.0fb^{-1} respectivement, enregistrées par le détecteur ATLAS en 2022, permettent d'évaluer les performances du détecteur ATLAS dans les nouvelles conditions d'acquisition de données du Run 3 du LHC et facilitent l'étude de la physique du boson de Higgs à l'énergie sans précédent de 13.6 TeV.

La section efficace est mesurée de manière inclusive à travers différents modes de production et est obtenue par un ajustement analytique du spectre de masse invariante di-photon reconstruit. Pour minimiser la dépendance au modèle, la mesure est limitée à un espace de phase cinématique des produits de désintégration du boson de Higgs défini au niveau particulaire, correspondant étroitement aux critères de sélection utilisés au niveau de la reconstruction, et est corrigée pour les effets du détecteur. Les mesures sont ainsi effectuées dans une région fiducielle définie par l'acceptance du détecteur $|\eta| < 2.37$, excluant la plage $1.37 < |\eta| < 1.52$. Les photons sélectionnés doivent également répondre à des critères d'identification et d'isolation et doivent avoir un moment transverse supérieur à 35% et 25% de la masse invariante di-photon. La section efficace fiducielle inclusive mesurée, multipliée par le rapport de branchement, est $\sigma_{\text{fid},\gamma\gamma} = 76_{-13}^{+14}$ fb, ce qui est compatible avec la prédiction du Modèle Standard de 67.5 ± 3.4 fb. En supposant l'acceptance du Modèle Standard et la fraction de branchement di-photon, la mesure fiducielle est extrapolée à l'espace de phase complet, aboutissant à une section efficace totale de $\sigma(pp \rightarrow H) = 67_{-12}^{+13}$ pb à 13.6 TeV. De plus, en combinant cela avec les mesures du canal $H \rightarrow ZZ^* \rightarrow 4\ell$, on obtient une section efficace totale de $\sigma(pp \rightarrow H) = 58.2 \pm 8.7$ pb, comparée à la prédiction du Modèle Standard de 59.9 ± 2.6 pb.

Mise à niveau du détecteur de trajectographie ATLAS pour le HL-LHC

L'objectif central de cette thèse, décrit dans la deuxième partie de cette dissertation, porte sur trois études liées aux activités de mise à niveau de l'Inner Tracker d'ATLAS pour l'ère de la haute luminosité du LHC. La première étude détaille ma tâche de qualification ATLAS (voir Section 6.1), axée sur la mise en œuvre du module de digitalisation pour le détecteur à pixels ITk dans le cadre du logiciel Athena. La digitalisation du détecteur à pixels ITk dans Athena est initialement basée sur la puce de lecture FEI4, actuellement utilisée dans la couche IBL du détecteur interne d'ATLAS. Pour le HL-LHC, le plan est de passer à une puce de lecture de type RD53 (ITkPix), optimisée pour fonctionner dans l'environnement à haute radiation attendu au HL-LHC.

Cette tâche de qualification aborde deux aspects centraux de la digitalisation des pixels ITk. La Section 6.1.4 détaille la mise en œuvre de la correction du "time-walk", une caractéristique clé de la puce de lecture de type RD53. La Section 6.1.5 se concentre sur la modélisation réaliste de la réponse charge-Temps sur Seuil (ToT) de la puce de lecture dans Athena en utilisant des tables de correspondance (LUTs). Des données préliminaires de la puce de lecture ITkPix V1.0, fournies par des collaborateurs d'ATLAS de l'Université de l'Oregon et du Lawrence Berkeley National Laboratory, sont utilisées pour évaluer la faisabilité d'une approche multi-LUT pour une modélisation précise charge-ToT de la puce de lecture.

Le ITkPix FE est une nouvelle puce de lecture conçue pour le détecteur à pixels ITk, sans connaissance communautaire préalable de son comportement. Comparée à ses prédécesseurs, comme les FEI3 et FEI4, cette puce présente une résolution ToT plus faible et une plus grande dispersion du ToT. La Section 6.1.5.4 décrit les défis actuels, les obstacles potentiels et les solutions proposées pour la mise en œuvre d'une calibration de charge réaliste en utilisant une approche multi-LUT dans Athena. Une modélisation précise de cette puce dans Athena nécessite une compréhension approfondie de son fonctionnement. Des études en cours sur les performances de trajectographie visent à finaliser un modèle de calibration de charge efficace basé sur ces nouvelles connaissances.

La deuxième étude examine davantage les aspects de la mise à niveau de l'Inner Tracker d'ATLAS, en se concentrant sur la modélisation des effets des dommages causés par les radiations (voir Section 6.2). Les dommages causés par les radiations ont un impact significatif sur les performances des détecteurs de trajectographie en silicium dans les expériences du LHC comme ATLAS et CMS, la réduction du signal étant une conséquence critique. Bien que l'ajustement de la tension de polarisation des capteurs et des seuils de détection puisse aider à atténuer ces effets, il est essentiel de générer des données simulées qui reflètent avec précision les changements de performances à mesure que la luminosité et le flux de radiations s'accumulent. La collaboration ATLAS a développé et mis en œuvre des algorithmes pour corriger les événements MC simulés pour les effets des dommages causés par les radiations dans les Run 2 et 3, atteignant une concordance impressionnante avec les données de collision, dans une marge de 1% lors du Run 3 (voir Section 6.2.1). Malgré le succès considérable du digitaliseur de dommages radiatifs du Run 3, la préparation pour le HL-LHC nécessite un algorithme de production MC ATLAS plus rapide. Cela est crucial en raison des taux croissants de collisions, d'événements, de trajectoires et d'impacts de particules, qui imposent des contraintes strictes sur les ressources informatiques disponibles. L'objectif du digitaliseur de dommages radiatifs est d'estimer quels pixels enregistreront un signal des charges déposées et l'ampleur de ce signal. Pour atteindre cet objectif lors de la collecte des données ATLAS pendant le HL-LHC, une nouvelle stratégie basée sur des LUTs générées avec Allpix-Squared est proposée et détaillée dans la Section 6.2.2. Initialement, les événements MC ATLAS seront simulés en utilisant un capteur de pixels idéal, non endommagé, avec des effets de dommages radiatifs incorporés ultérieurement par des corrections basées sur les LUTs. Des tests de fermeture réalisés sur divers intervalles de pseudorapidité et de moment transverse montrent que les événements simulés avec le nouvel algorithme sont en accord avec les événements entièrement simulés à quelques pourcents près. Dans un avenir proche, des données provenant de modules à pixels ITk équipés de la nouvelle puce de lecture seront disponibles, permettant une comparaison entre les simulations basées sur les LUTs et les résultats des tests sur faisceau.

Enfin, la troisième contribution aux activités de mise à niveau ITk décrites dans cette thèse concerne l'assemblage de modules quadruples au Laboratoire de Physique Nucléaire et de Hautes Énergies (LPNHE) à Paris. La Section 5.4.4.1 donne un aperçu des étapes impliquées dans le processus d'assemblage des modules quadruples pour le détecteur à pixels ITk. Ce travail a été entrepris dans le cadre du processus de qualification du site pour la production de modules quadruples ITk.

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Introduction

"Somewhere, something incredible is waiting to be known."

— Carl Sagan

High-energy physics (HEP) represents the intersection of scientific rigor and profound curiosity, where the pursuit of understanding the universe's fundamental components drives both innovation and discovery. This field delves into the smallest building blocks of matter and the fundamental forces that govern their interactions, utilizing advanced particle accelerators to recreate conditions similar to those of the early universe. Central to this endeavor is the Standard Model (SM) of particle physics, a theoretical framework that classifies all known elementary particles and their interactions. It provides a comprehensive description of the fundamental forces—except gravity—and has been crucial in guiding experimental research.

Building upon this theoretical foundation, the Large Hadron Collider (LHC) at CERN stands at the forefront of experimental high-energy physics research. As the world's most powerful particle accelerator, the LHC has played a pivotal role in confirming key aspects of the Standard Model, including the landmark discovery of the Higgs boson in 2012. The ATLAS (A Toroidal LHC ApparatuS) experiment, one of the major experiments at the LHC, has been instrumental in studying the Higgs boson and exploring new frontiers in particle physics.

Looking ahead to 2029, the LHC will enter its High-Luminosity phase (HL-LHC), a transition that promises both significant advancements and complex challenges. The HL-LHC upgrade aims to increase the integrated luminosity by a factor of 10 beyond the LHC's original design value, enabling the accumulation of up to 3000 fb^{-1} of data by the end of its operational life. This enhancement will dramatically improve the precision of measurements for rare processes and provide deeper insights into fundamental physics. However, the increased luminosity will also lead to increased radiation levels, posing substantial challenges in terms of radiation damage to detector components and electronics. Silicon pixel detectors, central to both the current and planned upgrades of the ATLAS detector, will face substantial radiation exposure over their operational lifetime. Prior to the HL-LHC, the innermost layers of these detectors are expected to accumulate a radiation fluence exceeding $10^{15} n_{\text{eq}}/\text{cm}^2$ while the radiation fluence is projected to increase by an order of magnitude at HL-LHC, imposing even greater demands on the detector upgrades to withstand these higher levels of radiation over their lifespan. Simulating radiation damage is thus crucial in order to make accurate predictions for current and future detector performance of the detector.

This thesis is organized into several chapters that alternate between theoretical and experimental aspects, offering a comprehensive exploration of various studies with a primary focus on the ATLAS Inner Tracker (ITk) upgrade activities for the HL-LHC.

Chapter 1 offers a concise overview of the Standard Model of particle physics, the Higgs mechanism, and Higgs phenomenology at the LHC, establishing the foundational principles that govern the behavior of elementary particles and their interactions.

Chapter 2 provides a comprehensive overview of the LHC and the ATLAS detector. It begins with an in-depth examination of the LHC, detailing its key components and operational principles. The chapter then shifts to a thorough exploration of the ATLAS detector, focusing on its design and various subsystems.

Chapter 3 explores the theory and technology of silicon tracking detectors, which are integral to the ATLAS detector and central to HEP research. The chapter starts with an examination of

the interactions between charged particles and matter, focusing on energy loss mechanisms. It then delves into the properties of silicon detectors, detailing their design and operational principles. The discussion progresses to signal formation, highlighting charge carrier dynamics and the influence of the Lorentz angle. Additionally, the chapter covers the theory behind front-end electronics and readout systems, which are essential for measuring the energy loss of particles traversing the silicon detector. Finally, it addresses the challenges posed by radiation damage, including the mechanisms of sensor degradation and its impact on detector performance.

Chapter 4 presents the measurement of the $H \rightarrow \gamma\gamma$ inclusive fiducial cross-section using the early Run 3 dataset collected by the ATLAS detector in 2022, detailing the methodologies employed and results achieved. The chapter begins with an introduction that outlines the motivation and strategy behind the measurement. It proceeds with a discussion on the data and simulation samples used, including Higgs boson signal, background, and pileup simulation. The core sections of the chapter focus on the $H \rightarrow \gamma\gamma$ measurement, addressing event reconstruction and selection processes, signal and background modeling, and the fit methodology. My contributions to this project include conducting signal modeling (Section 4.3.2.1) and studying systematic uncertainties associated with the $m_{\gamma\gamma}$ signal modeling (Section 4.3.3.1). The result section includes a comprehensive analysis and presentation of the measured cross-sections. Notably, the chapter also features a discussion of the combined results of cross-section measurements with the $H \rightarrow ZZ^* \rightarrow 4\ell$ channel. The chapter concludes with an outlook on future research directions. Further details and my additional contributions, including supplementary cross-checks on NNLOPS vs. MINLO differences, inclusive correction factors, and acceptance factors, are outlined in the Appendix A. Additionally, I was responsible for producing the uxAODs for signal, background, and data samples used in this analysis; however, this aspect is not discussed within the thesis.

Chapter 5 focuses on the HL-LHC and the upgrades to the ATLAS detector, with a particular emphasis on the Inner Tracker. The chapter starts with an overview of the HL-LHC project, detailing its objectives and anticipated physics potential. Following this, the chapter discusses the ATLAS Phase II upgrade, highlighting advancements across several components: the Inner Tracker, Calorimeter, Muon Spectrometer, Trigger and Data Acquisition systems, and the introduction of the High Granularity Timing Detector (HGTD). The latter part of the chapter provides a detailed description of the ATLAS Inner Tracker. It covers the ITk layout, expected tracking performance, including efficiencies and track parameter resolution, and details on the ITk Pixel Detector. This includes a look at pixel sensor technologies used, readout chips, pixel modules, and the mechanical support structures. The chapter also covers the module development activities carried out at the Laboratoire de Physique Nucléaire et de Hautes Énergies (LPNHE), focusing on the quad module preproduction for the HL-LHC, to which contributions were made.

Chapter 6 delves into pixel digitization within the ATLAS Inner Tracker, focusing on two main areas: Section 6.1 examines the implementation of digitization for the ITk pixel modules within the Athena software framework, while Section 6.2 addresses the modeling of radiation damage effects in Monte Carlo events for the HL-LHC. In Section 6.1, after providing an overview of the digitization process and a brief introduction to the Athena software framework, Section 6.1.4 details the implementation of time-walk correction. Section 6.1.5 then presents a thorough discussion of realistic charge-to-Time-over-Threshold (ToT) conversion, with a focus on single-Look-Up Table (LUT) and multi-LUT methods. Additionally, the chapter addresses the impact of radiation damage on silicon detectors, presenting the development of a new radiation damage digitizer using LUTs specifically for the HL-LHC, with an emphasis on planar pixel sensors in Section 6.2.2. The discussion includes the methodology, integration with Allpix-Squared, simulation inputs, LUT generation, and validation through closure tests.

The Summary and Outlook chapter offers a concise overview of the various projects discussed in this thesis and provides insights into future prospects in the field.

Particle Physics at Hadron Colliders

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This chapter presents the essential theoretical framework for particle physics at hadron colliders. The Standard Model of Particle Physics (SM) provides the current best understanding of the fundamental particles of the universe. In Section 1.1, an overview of the Standard Model's structure is presented, with further elaboration on the formalism predicting the Higgs boson provided in Section 1.2. Section 1.3 discusses the phenomenology associated with Higgs boson measurements at the LHC. Lastly, Section 1.4 details the methodologies used to develop theoretical predictions for collider experiments.

1.1 The Standard Model of Particle Physics

The Standard Model (SM) is a landmark achievement in particle physics, offering a comprehensive description of fundamental particles and their interactions. Developed primarily in the second half of the 20th century, it has demonstrated an unparalleled ability to predict experimental measurements with remarkable precision.

The fundamental particles experimentally observed from the SM are shown in Figure 1.1. The SM classifies fundamental particles into fermions and bosons based on their intrinsic angular momentum (i.e., spin). Particles with half-integer spin adhere to Fermi-Dirac statistics and are referred to as fermions, while those with integer spin conform to Bose-Einstein statistics and are termed bosons. Fermions exist in three generations. The first-generation particles constitute all stable matter, while the second and third-generations can be considered heavier versions of the first-generation fermions. The second and third-generation charged fermions are unstable and eventually decay into their first-generation counterparts. Fermions with color charge are called quarks. Up-type quarks possess an electric charge of $+\frac{2}{3}|e|$ and are available in three flavors: up (u), charm (c), and top (t). Conversely, down-type quarks have a charge of $-\frac{1}{3}|e|$ and come in three flavors: down (d), strange (s), and bottom (b). Leptons are fermions without color charge and can have an electric charge of $\pm|e|$ or no electric charge. The charged leptons include the electron (e), muon (μ), and tau-lepton (τ). Each charged lepton has a neutral counterpart, known as a neutrino, denoted as ν_e , ν_μ , and ν_τ .

Fundamental particles interact through four fundamental forces: the strong, electromagnetic, weak, and gravitational forces. Gravity is excluded from the SM formalism due to its negligible effects on fundamental particles and the lack of a quantum theory of gravity that can be unified with the quantum field theory governing the other three forces mediated by spin-1 particles, known as gauge bosons. The electromagnetic force is mediated by the photon (γ), a massless particle with

no charge that interacts exclusively with particles possessing electric charge. The strong force is mediated by gluons (g), which are massless particles carrying color charge [1], and they interact with particles possessing color charge. Lastly, the weak force is mediated by the massive charged $W^\pm$ bosons and the neutral Z boson [2]. The final component of the SM is the Higgs boson (H) - the Nobel Prize-winning discovery in 2012 [3, 4] - a spin-0 massive boson that arises from the Higgs field, which imparts mass to particles in the Standard Model.

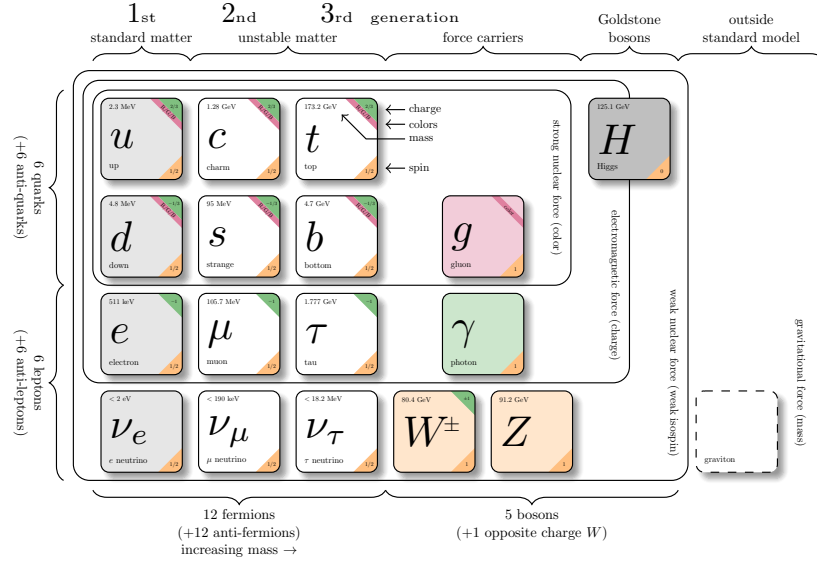


Figure 1.1: The Standard Model of Particle Physics. Figure taken from [5].

The Standard Model is a quantum field theory (QFT) that describes particles as perturbations in quantum fields, which adhere to specific field equations. The theory is built upon the Lagrangian formalism and is an extension of Quantum Electrodynamics (QED). The Lagrangian density, which describes the dynamics of a field $\psi(x)$, is given by:

$$\mathcal{L} = \mathcal{L}(\psi(x), \partial_\mu \psi(x)) \quad (1.1.1)$$

Global and local symmetries play a crucial role in this formalism. A global symmetry implies that the Lagrangian density remains invariant under a transformation that is constant across all space-time points. The invariance of the Lagrangian under these transformations leads to conserved quantities via Noether's theorem. In contrast, a local symmetry allows the transformation to vary as a function of space-time. To maintain invariance under local transformations, gauge fields are introduced, leading to gauge theories such as electromagnetism, represented by QED, discussed further below.

The formulation of the SM begins by considering the dynamics of free fermions, which are governed by the Dirac equation [6] of quantum mechanics, given by:

$$(i\gamma^\mu \partial_\mu - m)\psi(x) = 0 \quad (1.1.2)$$

Here, $\psi(x)$ represents a Dirac spinor field—a multi-component field representing fermions. γ^μ denotes a set of matrices known as gamma matrices that satisfy Clifford Algebra [7]. The partial derivative ∂_μ indicates differentiation with respect to the spacetime coordinates x^μ , and m represents the fermion's mass. The four components of the Dirac spinor can be understood as representing particle and antiparticle states, each with two possible spin states: spin-up and spin-down. Consequently, the Dirac equation yields four solutions, with two corresponding to negative

energies. These negative energy solutions are interpreted as antiparticles. The Dirac equation corresponds to a Lagrangian density, given by :

$$\mathcal{L}_{\text{Dirac}} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi \quad (1.1.3)$$

Here, $\bar{\psi}$ is the Dirac adjoint spinor, defined as $\bar{\psi} = \psi^\dagger \gamma^0$, where $\psi^\dagger$ is the Hermitian conjugate of the Dirac spinor ψ . The Lagrangian is required to be invariant under a U(1) local transformation, a condition also known as gauge invariance. This transformation can be expressed as:

$$\psi \rightarrow \psi' = e^{iq\alpha(x)}\psi, \quad (1.1.4)$$

where, $e^{iq\alpha(x)}$ represents a complex, space-time dependent phase. To maintain the gauge invariance of the Lagrangian, the partial derivative ∂_μ can be substituted with the covariant derivative D_μ :

$$\partial_\mu \rightarrow D_\mu = \partial_\mu + iqA_\mu \quad (1.1.5)$$

Here A_μ is a vector field, which transforms under U(1) as :

$$A_\mu \rightarrow A'_\mu = A_\mu - \partial_\mu \alpha \quad (1.1.6)$$

The vector field A_μ can be interpreted as the gauge field for the electromagnetic interaction, representing the massless photon, with an interaction strength denoted by q . Typically, the invariance of a Lagrangian under a gauge transformation leads to the introduction of spin-1 particles (gauge bosons) in the theory. These gauge bosons act as mediators of specific interactions. In this formalism, mass terms of the form $m^2 A_\mu A^\mu$ are not gauge invariant, necessitating that the mediators be massless. Given the above requirements of gauge invariance under U(1) transformations, the QED Lagrangian can be expressed as:

$$\begin{aligned} \mathcal{L}_{\text{QED}} &= \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi + q\bar{\psi}\gamma^\mu A_\mu\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \\ &= \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} \end{aligned} \quad (1.1.7)$$

Here, $F_{\mu\nu}$ is the electromagnetic field tensor, $\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$ is the kinetic term of the gauge field, and $q\bar{\psi}\gamma^\mu A_\mu\psi$ term describes the interaction between the fermion and the gauge boson.

The mechanism described above can be extended to other symmetry groups, including non-Abelian groups where the generators do not commute. An example of a non-Abelian group is SU(3), which underlies Quantum Chromodynamics (QCD) and describes the strong interaction. In QCD, the conserved quantum number is the color charge. Within the Standard Model, only quarks possess color charge, which can be red, blue, or green. The QCD Lagrangian is given by:

$$\mathcal{L}_{\text{QCD}} = \sum_q \sum_a \bar{\psi}_q^a (i\gamma^\mu D_\mu^{ab} - m_q \delta^{ab}) \psi_q^b - \frac{1}{4} \sum_a G_{\mu\nu}^a G_a^{\mu\nu}, \quad (1.1.8)$$

Here, q corresponds to the sum over the quarks and a represents the summation over the three colors of the quarks in the SU(3) color space. Similar to QED, a covariant derivative can be defined to ensure invariance under SU(3) transformations:

$$D_\mu^{ab} = \delta^{ab} \partial_\mu - ig_s (T^c)^{ab} A_\mu^c \quad (1.1.9)$$

Here, δ^{ab} represents the Kronecker delta, ensuring correct color index structure. g_s is the coupling constant of the strong interaction, which determines the interaction strength between quarks and gluons. This coupling constant is related to the dimensionless strong coupling parameter α_s as $\alpha_s = \frac{g_s^2}{4\pi}$. T^c represents the generators of the SU(3) color group, typically represented by the Gell-Mann matrices, $\lambda^c/2$, where c runs from 1 to 8, representing the eight different gluon color states and A_μ^c represents the gluon field. From these fields, the strong interaction tensor can be defined as:

$$G_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g_s f^{abc} A_\mu^b A_\nu^c \quad (1.1.10)$$

Here, f^{abc} are the structure constants of the SU(3) color group, indicating the strength of the interaction between different color charges. The term $g_s f^{abc} A_\mu^b A_\nu^c$ represents the interaction term, depicting the self-interaction of gluons due to the non-Abelian nature of the SU(3) gauge group in QCD, thereby resulting in a phenomenon referred to as color confinement [8–10]. Quarks and gluons cannot exist in isolation but are instead confined within color-neutral bound states, such as mesons (quark-antiquark pairs) or baryons (three-quark combinations). This confinement phenomenon arises from the increasing strength of the strong force with distance, prohibiting the observation of free quarks and gluons. Consequently, the observable particles in nature, excluding leptons, are bound states known as hadrons, produced through a process called hadronization (see Section 1.4) in high-energy collisions. Furthermore, in QCD calculations, the coupling strength α_s strongly depends on the energy at which it is measured. α_s is large at low energies (below 1 GeV) or large distances, and it becomes weaker at higher energies or, equivalently, shorter distances. This behaviour is referred to as asymptotic freedom. At energies above 100 GeV, α_s becomes sufficiently small to permit perturbative calculations in deriving QCD predictions. These higher-order correction terms, such as quark self-energy corrections via loop Feynman diagrams, can introduce infinities into the calculations. These divergences that arise in loop diagrams of perturbative calculations at very high energies are referred to as ultraviolet divergences, as they correspond to the high-energy (short-wavelength) end of the spectrum. These divergences are handled through the process of renormalization, which involves regularizing the theory and redefining parameters to absorb the infinities. The corrections depend on arbitrary scale parameters, known as the renormalisation scale μ_R and the factorisation scale μ_F [11, 12]. μ_R represents the energy scale at which the parameters of the theory are defined and influences the running of coupling constants (i.e., the dependence of the coupling constant on μ_R), while μ_F is introduced to distinguish between long-distance (non-perturbative) effects and short-distance (perturbative) effects in processes involving hadrons.

The second non-Abelian symmetry group relevant to the Standard Model is $SU(2) \times U(1)$, which unifies the electromagnetic and weak forces within the SM. A local SU(2) transformation is defined as:

$$\psi \rightarrow \psi' = e^{ig\alpha^a(x)\frac{\sigma^a}{2}} \psi, \quad (1.1.11)$$

Here, σ^a represents the Pauli matrices, which serve as the generators of the $SU(2)$ group. Similar to the previous discussions on QED and QCD, a covariant derivative can be defined to ensure gauge invariance:

$$D_\mu = \partial_\mu + ig\frac{\sigma^a}{2}W_\mu^a \quad (1.1.12)$$

W_μ^a represents the gauge field associated with the SU(2) group, where a is the group index ranging from 1 to 3 and g is the gauge coupling constant, determining the strength of the interaction between the gauge bosons and the matter fields.

In the SM, the weak interaction is described by the $SU(2)_L$ gauge group. The subscript L indicates that the charged-current interaction involving the $W^\pm$ bosons couples exclusively to left-handed (LH) particle states and right-handed (RH) antiparticle states. This left-handed coupling is a fundamental characteristic of the weak interaction. The fermionic fields can be split into their left- and right-handed components using the projection operators P_L and P_R as follows:

$$\psi = P_L\psi + P_R\psi = \frac{1 - \gamma^5}{2}\psi + \frac{1 + \gamma^5}{2}\psi = \psi_L + \psi_R \quad (1.1.13)$$

In the SM, the left-handed fermions are organized into doublets under $SU(2)_L$, whereas the right-handed fermions are singlets, as given by:

$$\begin{aligned} \text{Leptons: } \mathcal{L}_L &= \begin{pmatrix} \nu_L \\ e_L \end{pmatrix} & e_R \\ \text{Quarks: } \mathcal{Q}_L &= \begin{pmatrix} u_L \\ d_L \end{pmatrix} & u_R, d_R \end{aligned} \quad (1.1.14)$$

Here, $\mathcal{L}_L$ and $\mathcal{Q}_L$ are $SU(2)_L$ doublets while e_R , u_R and d_R are singlets. The SM of particle physics, as originally formulated, does not include right-handed neutrinos and treats neutrinos as massless particles, only incorporating left-handed neutrinos and right-handed antineutrinos. However, experimental observations such as neutrino oscillations [13], which imply that neutrinos have mass, suggest the need for extensions to the SM. These extensions often introduce right-handed neutrinos through mechanisms like the seesaw mechanism [14] or as Dirac neutrinos [15] to account for the observed neutrino masses and mixing.

In the SM, the weak interaction is characterized by weak isospin charges, where LH particles possess a weak isospin I_W of $\frac{1}{2}$ with the third component I_W^3 being $\pm\frac{1}{2}$, while RH particles have a weak isospin I_W and I_W^3 of 0. Thus, the W_μ^a gauge bosons exclusively couple to LH particles. The charged-current interactions involving the $W^\pm$ bosons are linear combinations of the $SU(2)_L$ gauge fields. The physical $W^\pm$ bosons are related to the gauge fields W_μ^1 and W_μ^2 by:

$$W_\mu^\pm = \frac{1}{\sqrt{2}} (W_\mu^1 \mp iW_\mu^2) \quad (1.1.15)$$

While it has been experimentally observed that the W boson only interacts with left-handed particles, the Z boson has been observed to interact with both left- and right-handed particles. As a result, an additional symmetry group $U(1)_Y$ is introduced to account for this observation within the SM framework. This is known as the weak hypercharge symmetry group, and it introduces an additional gauge field B_μ , with the coupling g' - representing the strength of the coupling between particles with weak hypercharge and the $U(1)_Y$ gauge boson. The weak hypercharge (Y), the generator of the $U(1)_Y$ group, represents a combination of electric charge and weak isospin, and is defined as:

$$Y = 2(Q - I_W^3) \quad (1.1.16)$$

Here Q denotes the electromagnetic charge. The covariant derivative for the $SU(2) \times U(1)$ group is given by:

$$D_\mu = \partial_\mu + ig\frac{\sigma_a}{2}W_\mu^a + ig'\frac{Y}{2}B_\mu \quad (1.1.17)$$

The Glashow-Salam-Weinberg (GSW) model [16–18] is based on the gauge symmetry group $SU(2) \times U(1)$. The GSW model begins with two gauge fields: B_μ from $U(1)_Y$, which couples to weak hypercharge interactions, and W_μ^3 from $SU(2)_L$, which couples to weak isospin interactions. The weak mixing angle θ_W is a fundamental parameter of the GSW model that determines the strength of the mixing between the B_μ and W_μ^3 gauge fields. The physical electromagnetic photon (A_μ) and the Z boson (Z_μ) result from a linear combination of the B_μ and W_μ^3 fields, given by:

$$\begin{pmatrix} A_\mu \\ Z_\mu \end{pmatrix} = \begin{pmatrix} \cos \theta_W & \sin \theta_W \\ -\sin \theta_W & \cos \theta_W \end{pmatrix} \begin{pmatrix} B_\mu \\ W_\mu^3 \end{pmatrix} \quad (1.1.18)$$

In the GSW model, the coupling strengths of the weak interaction (g_W and g_Z) and the electromagnetic interaction (e) are related to each other through θ_W , given by:

$$e = g_W \sin \theta_w = g_Z \sin \theta_W \cos \theta_W \quad (1.1.19)$$

In the SM, the unification of electroweak and QCD theories is achieved under the gauge group $SU(3)_C \times SU(2)_L \times U(1)_Y$. However, in gauge theory, local gauge invariance requires that all gauge bosons must be massless, ensuring that the gauge symmetry is preserved at all energy scales. Additionally, the fermionic fields are split into left-handed and right-handed components, which breaks the gauge invariance of the simple mass term in the electroweak Lagrangian. Experimentally, it is observed that fermions and W and Z bosons have non-zero masses. This contradicts the initial prediction of massless gauge bosons and massless fermions in a gauge-invariant theory. Therefore, an additional mechanism needs to be incorporated into the electroweak sector of the SM, which spontaneously breaks the symmetry and gives rise to particle masses: the Brout-Englert-Higgs mechanism [19–22].

1.2 The Higgs Mechanism

The Higgs mechanism is a process by which gauge bosons acquire mass through spontaneous symmetry breaking. This mechanism is a fundamental part of the SM, providing a way to explain the masses of the W and Z bosons while keeping the photon massless. Spontaneous symmetry breaking occurs when the ground state (vacuum) of a system does not share the symmetry of the underlying theory, and in the SM, this is achieved by the Higgs field acquiring a non-zero vacuum expectation value (VEV). The Higgs field ϕ , represented as a complex doublet under $SU(2)_L$ with one neutral field ϕ^0 and one charged field ϕ^+ , can be expressed in terms of complex scalar fields with four degrees of freedom as :

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix} \quad (1.2.1)$$

The corresponding Lagrangian is given by :

$$\mathcal{L}_{\text{Higgs}} = (D_\mu \phi)^\dagger (D^\mu \phi) - V(\phi), \quad (1.2.2)$$

where $(D_\mu \phi)^\dagger (D^\mu \phi)$ denotes the kinetic term of the Lagrangian, with D_μ being the covariant derivative defined in Equation 1.1.17, and $V(\phi)$ represents the Higgs potential, given by:

$$V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2, \quad (1.2.3)$$

Here, μ and λ are scalar constants. The quadratic term in the Higgs potential, $\mu^2 \phi^\dagger \phi$, denotes the mass term, while the quartic term $\lambda (\phi^\dagger \phi)^2$ describes the self-interaction among the scalar fields. The minimum of the potential corresponds to the vacuum state.

The sign of μ^2 determines the nature of the symmetry breaking. If $\mu^2 > 0$, the potential has a single minimum at $\phi = 0$ as illustrated in Figure 1.2a, and the symmetry is unbroken. If $\mu^2 < 0$, the potential takes on a "Mexican hat" shape as depicted in Figure 1.2b, leading to spontaneous symmetry breaking. Thus, a set of degenerate minima can be found at a circumference of:

$$(\phi^\dagger \phi) = \frac{1}{2}(\phi_1^2 + \phi_2^2 + \phi_3^2 + \phi_4^2) = \frac{v^2}{2} = \frac{|\mu|^2}{2\lambda} \quad (1.2.4)$$

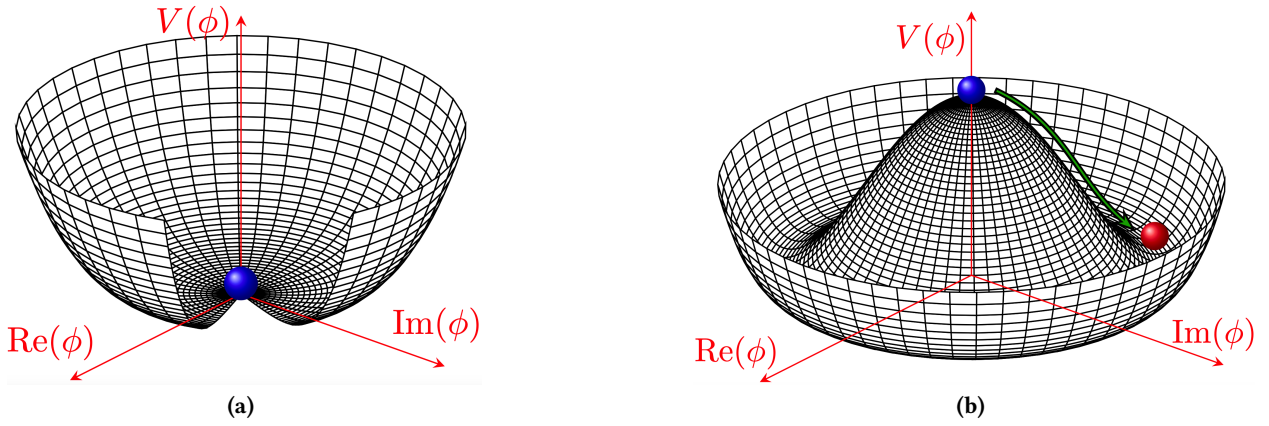


Figure 1.2: Visualization of Higgs potential with (a) $\mu \geq 0$ and (b) $\mu < 0$. Adapted from [23, 24].

The magnitude of the Higgs field ϕ at each minimum is given by the term $v = \sqrt{\frac{|\mu|^2}{\lambda}}$, which represents the VEV of the field ϕ . All the available minima are equivalent and connected by an $SU(2)_L$ transformation. The choice of the vacuum state breaks the symmetry of the Lagrangian. The following choice of vacuum state, with $\phi_1 = \phi_2 = \phi_4 = 0$ and $\phi_3 = v$, leads to a VEV of:

$$\langle 0|\phi|0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix} \quad (1.2.5)$$

After spontaneous symmetry breaking, the Higgs field $\phi(x)$ can be expanded around the VEV and can be expressed as:

$$\phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi_1(x) + i\phi_2(x) \\ v + \eta(x) + i\phi_4(x) \end{pmatrix} \quad (1.2.6)$$

In this parametrization, the Higgs field is described by one real physical field, $\eta(x)$, which represents the physical Higgs boson, and three unphysical fields, $\phi_1(x)$, $\phi_2(x)$, and $\phi_4(x)$, corresponding to the Goldstone bosons. The term $v + \eta(x)$ represents the field's fluctuation around its vacuum expectation value (VEV), leading to mass generation for the gauge bosons through the Higgs mechanism. The Goldstone bosons are "eaten" by the W and Z bosons, giving them mass, while the physical Higgs boson $\eta(x)$ remains an observable scalar particle. Mathematically, this is achieved

by selecting a specific gauge, called the unitary gauge, where the vector fields absorb the Goldstone fields. In this case, the expansion of the Higgs field around the vacuum simplifies to :

$$\phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + h(x) \end{pmatrix} \quad (1.2.7)$$

Using Equation 1.2.7, the Lagrangian in Equation 1.2.2 can be expressed as :

$$\begin{aligned} \mathcal{L}_{\text{Higgs}} = & \frac{1}{2}(\partial_\mu h)(\partial^\mu h) \\ & + \frac{1}{4}g_W^2(W_\mu^+ W^{\mu-})(v + h)^2 \\ & + \frac{g_W^2 + g'^2}{8}(Z_\mu Z^\mu)(v + h)^2 \\ & - \frac{\mu^2}{2}(v + h)^2 - \frac{\lambda}{4}(v + h)^4 \end{aligned} \quad (1.2.8)$$

The term $\frac{1}{2}(\partial_\mu h)(\partial^\mu h)$ describes the kinetic energy of the physical Higgs boson, h , which represents fluctuations around the VEV. The second term, $\frac{1}{4}g_W^2(W_\mu^+ W^{\mu-})(v + h)^2$, represents the interaction between the Higgs field and the charged $W^\pm$ bosons, while the third term, $\frac{g_W^2 + g'^2}{8}(Z_\mu Z^\mu)(v + h)^2$, describes the interaction with the neutral Z boson. In both cases, the boson masses arise from the Higgs field's VEV, along with additional interaction terms involving the Higgs boson h . The physical field for the massive neutral Z boson can be identified as a linear combination of the fields W_μ^3 and B_μ , defined in Equation 1.1.18, as:

$$Z_\mu = \frac{g_W W_\mu^3 - g' B_\mu}{\sqrt{g_W^2 + g'^2}} \quad (1.2.9)$$

Similarly, the physical field of the photon, with no associated mass term, can be expressed as:

$$A_\mu = \frac{g' W_\mu^3 + g_W B_\mu}{\sqrt{g_W^2 + g'^2}} \quad (1.2.10)$$

When $h = 0$, the masses of the heavy bosons arising from the Higgs mechanism can be written as:

$$m_W = \frac{g_W v}{2}, m_Z = \frac{v}{2} \sqrt{g_W^2 + g'^2} = \frac{m_W}{\cos \theta} \quad (1.2.11)$$

The Higgs boson mass, as well as the trilinear and quartic couplings, are derived by expanding the remaining terms in the potential part of the Lagrangian in Equation 1.2.8. This is given by:

$$\begin{aligned} \frac{\mu^2}{2}(v + h)^2 + \frac{\lambda}{4}(v + h)^4 = & \frac{\mu^2}{2}(v^2 + 2vh + h^2) \\ & + \frac{\lambda}{4}(v^4 + 4v^3h + 6v^2h^2 + 4vh^3 + h^4) \end{aligned} \quad (1.2.12)$$

Here, the term $\frac{\mu^2}{2}v^2 + \frac{\lambda}{4}v^4$ is a constant and does not influence the dynamics of the field. The linear term in h , given by $(\mu^2 v + \lambda v^3)h$, shifts the minimum of the Higgs potential. Consequently, the potential has a minimum at $h = 0$ if and only if :

$$(\mu^2 v + \lambda v^3) = 0 \implies \mu^2 = -\lambda v^2 \quad (1.2.13)$$

The quadratic term in h , $\frac{1}{2}(\mu^2 + 3\lambda v^2)h^2$, represents the Higgs boson mass term. Inserting Equation 1.2.13 results in $-\mu^2 h$. Therefore, the excitation of the Higgs field h can lead to the production of an additional massive boson, the Higgs boson, with a mass given by:

$$m_H = \sqrt{2|\mu|^2} \quad (1.2.14)$$

The Higgs trilinear and quartic coupling terms involve interactions among three and four Higgs fields, respectively, and arise from the expansion of the potential term $\frac{\lambda}{4}(v+h)^4$ in the Lagrangian, as shown in Equation 1.2.8. The trilinear coupling term is $\lambda v h^3$ with a coupling constant of λv , while the quartic coupling term is $\frac{\lambda}{4}h^4$, with a coupling constant of λ .

In the SM, the Higgs mechanism not only provides masses to the gauge bosons but also generates fermion masses through Yukawa interactions. These interactions are specified in the Lagrangian and remain invariant under transformations in the $SU(2)_L \times U(1)_Y$ gauge group, represented as:

$$\mathcal{L}_{\text{Yukawa}} = -y_f \bar{\psi}_L \Phi \psi_R - y_f \bar{\psi}_R \Phi^\dagger \psi_L \quad (1.2.15)$$

Here, y_f is the Yukawa coupling constant for the fermion f , while ψ_L and ψ_R are the left-handed and right-handed components of the fermion field f , respectively. Φ is the Higgs doublet field, as given by Equation 1.2.7. Substituting this parametrization of the Higgs doublet into the Yukawa Lagrangian in Equation 1.2.15 yields:

$$\mathcal{L}_{\text{Yukawa}} = -y_f \left(\frac{v+h}{\sqrt{2}} \right) (\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L) \quad (1.2.16)$$

The mass term for the fermion f arises from the VEV of the Higgs field and is expressed as :

$$\mathcal{L}_{\text{Yukawa, mass}} = -y_f \frac{v}{\sqrt{2}} (\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L) \quad (1.2.17)$$

The mass of the fermion f is then given by:

$$m_f = y_f \frac{v}{\sqrt{2}} \quad (1.2.18)$$

The interaction term involving the Higgs boson h is:

$$\mathcal{L}_{\text{Yukawa, int}} = -y_f \frac{h}{\sqrt{2}} (\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L) \quad (1.2.19)$$

Combining the mass and interaction terms, the Yukawa interaction Lagrangian for all fermions can be generalized as:

$$\mathcal{L}_{\text{Yukawa}} = - \sum_f m_f (\bar{f}_L f_R + \bar{f}_R f_L) - \sum_f \frac{m_f}{v} h (\bar{f}_L f_R + \bar{f}_R f_L) \quad (1.2.20)$$

In the quark sector of the SM, the transition between the weak interaction eigenstates and the mass eigenstates is described by the Cabibbo-Kobayashi-Maskawa (CKM) matrix [25]. This complex unitary matrix accounts for the mixing of quark flavors in weak interactions and is given by:

$$V_{\text{CKM}} = \begin{pmatrix} V_{ud} & V_{cd} & V_{td} \\ V_{us} & V_{cs} & V_{ts} \\ V_{ub} & V_{cb} & V_{tb} \end{pmatrix} \quad (1.2.21)$$

The elements of the CKM matrix describe the probability amplitudes for the transition of one type of quark to another type during weak interactions. The matrix elements are measured experimentally, revealing an almost diagonal structure with small off-diagonal entries. This indicates that transitions between quarks of the same generation are preferred in charged-current interactions (e.g., $c \rightarrow s$), while transitions between different generations (e.g., $c \rightarrow d$) occur at a lower rate. The CKM matrix also contains a complex phase that introduces CP violation [26] in weak interactions, creating an asymmetry between the behavior of particles and antiparticles under the combined transformations of charge conjugation (C) and parity (P). CP violation is observed in specific particle decays, such as those of neutral kaons and B mesons.

The SM, complemented by the Higgs mechanism, stands as the most successful theory to date in describing the fundamental particles and their interactions. This formalism explains the strong and electroweak interactions through particle properties such as color charge, electric charge, isospin, and hypercharge. Additionally, the SM provides a mechanism by which massive bosons and fermions acquire mass. Despite its success, the SM contains several parameters not predicted by theory. These parameters must be determined experimentally. Precise measurement of these parameters is a primary objective of modern particle physics. These measurements refine the understanding of fundamental interactions and test the predictions of the SM. The free parameters of the theory are:

- The mass of the Higgs boson (m_H).
- The 3 gauge couplings: g_s for the strong interaction, g_W and g' for the electroweak interaction.
- The Yukawa couplings for the fermions, which determine the masses and mixing angles of the quarks and leptons. These include 9 parameters for the charged fermion masses (3 charged leptons, 6 quarks) and 4 parameters for the CKM matrix (3 mixing angles and 1 CP-violating phase).

1.3 Higgs Phenomenology at the LHC

The LHC has played a crucial role in observing and studying the Higgs boson, a fundamental part of the SM of particle physics. At a pp collider, the Higgs boson can be created in different ways and measured through various decay channels, which are discussed in the following section. The Higgs boson's coupling to other particles increases with their mass, resulting in stronger coupling with more massive particles, a key to studying both its production and decay modes.

The hard scattering interactions at pp collider occur between the partons (quarks or gluons) within the proton. Therefore, due to the nature of the proton as a composite particle consisting of quarks and gluons bound by the strong force, the longitudinal momentum of the colliding partons is not precisely known. The uncertainty in the longitudinal momentum of the colliding partons leads to uncertainty in the kinematics of the hard scattering process. Specifically, the precise values of the parton momenta along the beam axis (p_z) are unknown before the collision, thereby complicating the precise prediction of final-state observables. The partonic cross-section $\hat{\sigma}_{ab \rightarrow X}$ for two partons a and b , which carry fractions x_1 and x_2 of the proton momentum, respectively, describes the probability of their transition from the initial state to a final state X and can be computed from the interaction Lagrangian. The inclusive cross-section for the specific process $pp \rightarrow X$ can be

defined according to the factorization theorem [12], that allows the cross-section to be written as a convolution of the parton distribution functions and the partonic cross-section. Mathematically, this is given by:

$$\sigma_{pp \rightarrow X} = \sum_{a,b} \int_0^1 dx_1 \int_0^1 dx_2 f_a(x_1, \mu_F) f_b(x_2, \mu_F) \int d\sigma_{ab \rightarrow X}(x_1 P_1, x_2 P_2, \mu_R, \mu_F) \quad (1.3.1)$$

$\sum_{a,b}$ denotes the sum over all possible parton types a and b (quarks, antiquarks, and gluons) within the protons. The parton distribution functions (PDFs), $f_i(x_i, \mu_F)$, describe the probability of a parton i participating in a hard scattering interaction with a momentum $p_i = x_i P_i$, where P_i is the proton momentum. The PDFs depend on the energy scale at which the collisions occur but are independent of the specific outcomes of the interactions. The energy scale is parametrized in terms of the factorization scale μ_F , which represents the scale that separates long-distance (non-perturbative) and short-distance (perturbative) physics. μ_F can be interpreted as the maximum value of transverse momentum where partons are still considered as part of the proton. For transverse momenta greater than μ_F , the partons are treated as free particles participating in the hard scattering process. An example of the process $ab \rightarrow X$ can be a specific production mode of the Higgs boson, which contributes to the inclusive cross-section $pp \rightarrow H$.

There are four main Higgs production modes relevant in proton-proton collisions at the LHC: gluon-gluon fusion (ggF), vector boson fusion (VBF), associated production with a vector boson (VH or Higgsstrahlung), and associated production with top quarks ($t\bar{t}H$), as depicted in Figure 1.3. The production cross-sections depend on the center-of-mass energy as shown in Figure 1.4a, with higher energies generally leading to increased production rates. While the aforementioned four production modes are dominant at the LHC, other production modes exist with lower cross-sections, such as the associated production of the Higgs boson with a pair of bottom quarks ($b\bar{b}H$) and the production of the Higgs boson in association with a single top quark (tH).

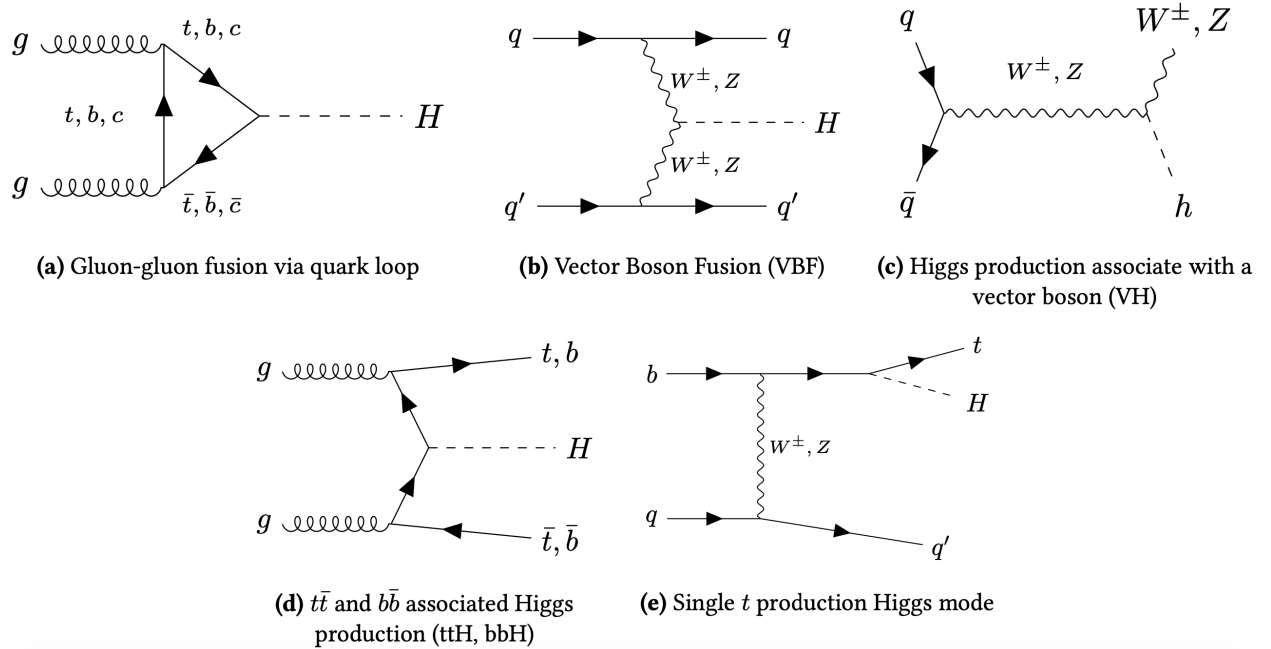


Figure 1.3: Leading order (LO) Feynman diagrams for the main Higgs boson production modes at the LHC for a Higgs mass of 125 GeV: (a) gluon fusion (ggF), (b) Vector Boson Fusion (VBF), (c) Higgs production associated with a vector boson (VH), (d) Higgs production associated with $t\bar{t}$ ($t\bar{t}H$), (e) Higgs production associated with single t

ggF is the most predominant Higgs production mode at the LHC, with the largest production cross-section of $\sigma_{ggF} = 52.7 \pm 2.6 \text{ pb}$ [27] at $\sqrt{s} = 13.6 \text{ TeV}$. The abundance of gluons in the protons amplifies the likelihood of gluon-gluon interactions, thereby increasing the ggF cross-section. Since gluons are massless particles, Higgs bosons are produced via a top quark loop in the ggF production mode, as depicted in Figure 1.3. Other kinds of loops involving lighter fermions are theoretically possible in the ggF production mode, but their contributions are much smaller compared to the top quark loop due to the significantly lower masses of these other fermions, which results in weaker coupling to the Higgs boson.

The second most common Higgs production mode at LHC is the vector boson fusion (VBF), with a cross-section of $4.075^{+0.088}_{-0.089} \text{ pb}$ at $\sqrt{s} = 13.6 \text{ TeV}$ [27]. In this process, two quarks scatter in an interaction mediated by two off-shell vector bosons (W or Z), which subsequently produce a Higgs boson. Experimentally, this production mode is easier to identify as it is characterized by the presence of two forward jets in the event, in addition to the decay products of the Higgs boson [28].

In the VH production mode, the Higgs boson is produced in association with a W or Z boson. This process has a relatively small cross-section, with $\sigma_{WH} = 1.453^{+0.029}_{-0.028} \text{ pb}$, $\sigma_{q\bar{q} \rightarrow ZH} = 0.806^{+0.033}_{-0.029} \text{ pb}$, and $\sigma_{gg \rightarrow ZH} = 0.136^{+0.034}_{-0.026} \text{ pb}$ [27]. Furthermore, the VH production mode can provide a very clean signature in the detector when selecting events with a leptonic decay of the vector boson, significantly reducing the QCD background. Consequently, it is the most sensitive for searching for Higgs decays into quarks and is commonly used in the searches for Higgs decays into b - and c -quarks.

The fourth main production mode is the associated production of Higgs bosons with top quark pairs ($t\bar{t}H$). This mode has a very small cross-section of $\sigma_{t\bar{t}H} = 0.569^{+0.040}_{-0.057} \text{ pb}$ [27], making it very rare. However, it offers a unique opportunity to probe the Higgs coupling to top quarks directly.

The Higgs boson has an extremely short lifetime, predicted to have a total width of around 4.07 MeV in the SM [27], translating to a lifetime on the order of 10^{-22} seconds. As a result, the Higgs boson can only be detected through its decay products. The relative decay rates of particles are described by a branching ratio (BR), which represents the probability that a parent particle P decays into a specific final state X_i . Mathematically, the branching ratio is calculated as the ratio of the decay rate for the specific final state X_i ($\Gamma(P \rightarrow X_i)$) to the total decay rate of the parent particle P (Γ_P) and, is given by:

$$BR(P \rightarrow X_i) = \frac{\Gamma(P \rightarrow X_i)}{\Gamma_P} = \frac{\Gamma(P \rightarrow X_i)}{\sum_j \Gamma(P \rightarrow X_j)} \quad (1.3.2)$$

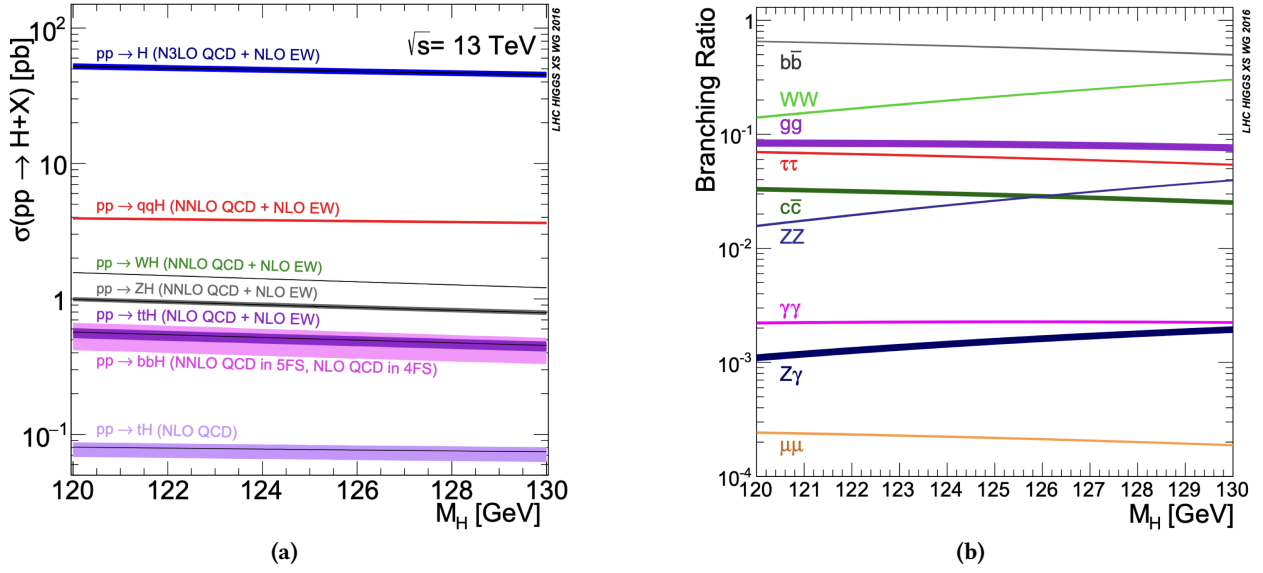


Figure 1.4: (a) Predicted SM Higgs boson production cross-sections at $\sqrt{s} = 13$ TeV and (b) SM Higgs boson decay branching ratios as functions of the Higgs boson mass. From [29].

Figure 1.4b depicts the expected BRs of the Higgs boson as a function of Higgs boson mass. The BR for the decay into a pair of bottom quarks ($H \rightarrow b\bar{b}$) constitutes 58% of the Higgs decays, while the decay into a pair of photons ($H \rightarrow \gamma\gamma$) accounts for only 0.23% for a Higgs mass of 125 GeV. The other dominant decay modes of the Higgs boson include decays into a pair of W or Z bosons, which subsequently decay into leptons or quarks.

A particle with properties consistent with the SM Higgs boson was discovered in 2012 by the ATLAS and CMS collaborations, using the $H \rightarrow \gamma\gamma$, $H \rightarrow ZZ \rightarrow 4l$, and $H \rightarrow WW^* \rightarrow 2l2\nu$ channels [3, 4]. These channels have excellent sensitivity and provide clean signatures to identify the Higgs boson candidate. Chapter 4 presents the measurement of the inclusive fiducial cross-section of the Higgs boson in the di-photon decay channel at a center-of-mass energy of 13.6 TeV. Since the discovery, many more Higgs boson production and decay modes have been measured, with summaries of the results shown in Figures 1.5 and 1.6 at center of mass energy of 13 TeV. The Higgs boson production cross-sections and the measured couplings to different particles show good agreement with the SM expectations.

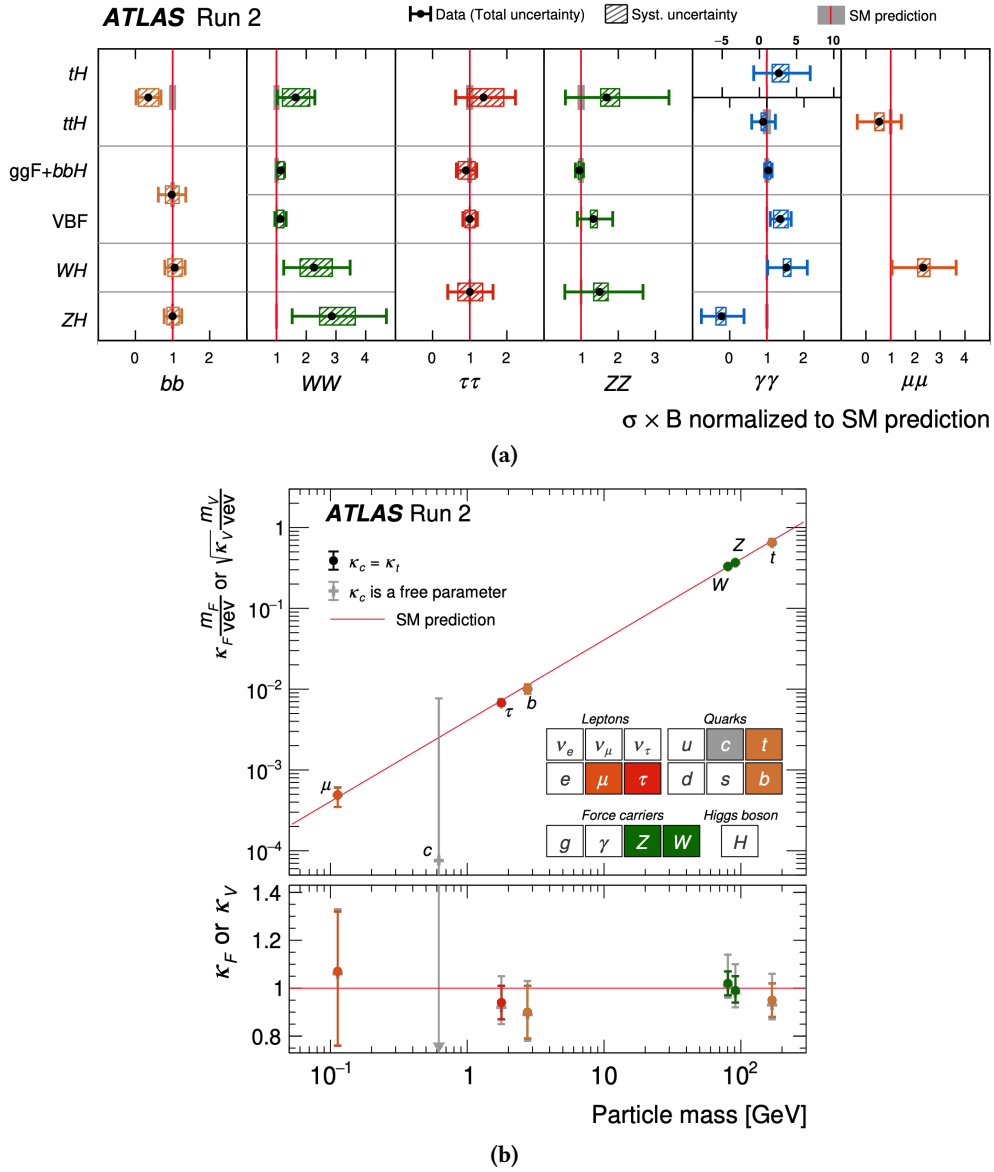


Figure 1.5: (a) Ratio of observed rate to predicted SM event rate for different combinations of Higgs boson production and decay processes. The horizontal bar on each point denotes the 68% confidence interval. The narrow grey bands indicate the theory uncertainties in the SM cross-section times the branching fraction predictions. The p -value for compatibility of the measurement and the SM prediction is 72%. (b) Reduced Higgs boson coupling strength modifiers and their uncertainties are defined as $\kappa_F \frac{m_F}{\text{vev}}$ for fermions ($F = t, b, \tau, \mu$) and $\sqrt{\kappa_V} \frac{m_V}{\text{vev}}$ for vector bosons as a function of their masses m_F and m_V . Two fit scenarios are shown: $\kappa_c = \kappa_t$ (colored circle markers), or κ_c left free-floating in the fit (grey cross markers). Loop-induced processes are assumed to have the Standard Model (SM) structure, and Higgs boson decays to non-SM particles are not allowed. The vertical bar on each point denotes the 68% confidence interval. The p -values for compatibility of the combined measurement and the SM prediction are 56% and 65% for the respective scenarios. The lower panel shows the values of the coupling strength modifiers. The grey arrow points in the direction of the best-fit value and the corresponding grey uncertainty bar extends beyond the lower panel range. Figures taken from [30]

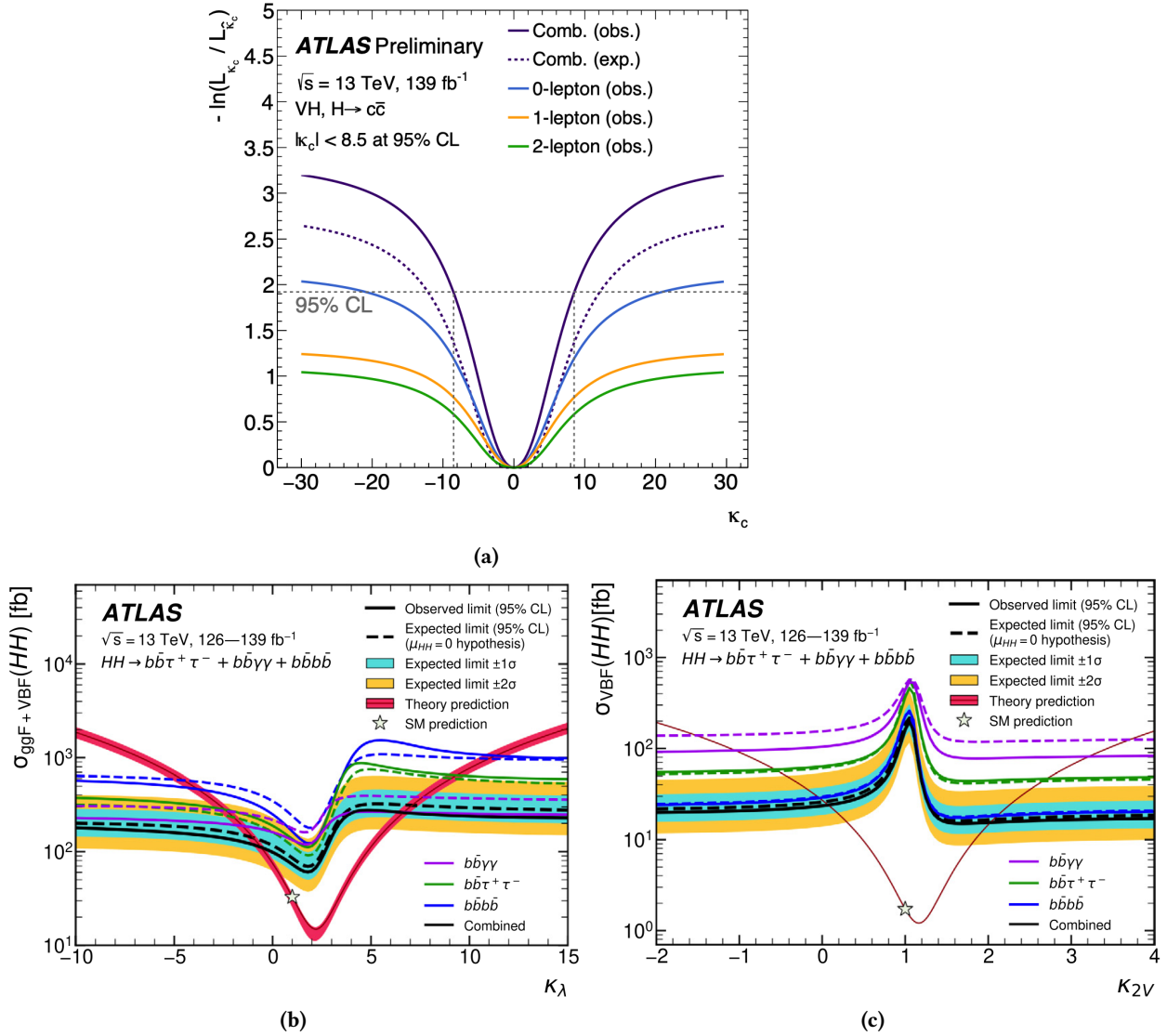


Figure 1.6: (a) Expected and observed profile likelihood scans for Higgs-charm coupling modifier, k_c . The per-channel likelihoods are obtained using a five-POI fit, in which each channel has a separate $VH(\rightarrow c\bar{c})$ parameter of interest. The combination allows an observed (expected) constraint to be set of $|k_c| < 8.5(12.4)$ at the 95% confidence level (CL). Further details on the analysis are available in [31]. (b) Observed and expected 95% CL exclusion limits on the production cross-sections of the combined ggF HH and VBF HH processes as a function of the coupling modifier k_λ . The parameter k_λ is defined as the ratio of the Higgs boson self-coupling to its SM value [32]. (c) Observed and expected 95% CL exclusion limits on the production cross-sections of the VBF HH process as a function of the coupling modifier, k_{2V} , for the three double-Higgs search channels ($b\bar{b}b\bar{b}$, $b\bar{b}\tau^+\tau^-$, and $b\bar{b}\gamma\gamma$) and their combination. The expected limits assume no HH production or no VBF HH production respectively. The red line in Figure 1.6b illustrates the theoretical prediction for the combined ggF HH and VBF HH cross-section as a function of k_λ , with all parameters and couplings set to their SM values except for k_λ . In Figure 1.6c, the red line represents the predicted VBF HH cross-section as a function of k_{2V} . The bands surrounding the red cross-section lines indicate the theoretical uncertainty on the predicted cross-section. The uncertainty band in Figure 1.6c is smaller than the width of the plotted line. The combination of the double-Higgs analyses sets an upper limit of $\mu_{HH} < 2.4$ at 95% CL on the double-Higgs production cross-section normalized to its SM prediction. Combining the single-Higgs and double-Higgs analyses, with the assumption that new physics affects only the Higgs boson self-coupling, values outside the interval $-0.4 < k_\lambda < 6.3$ are excluded at 95% CL. For further details of this analysis, please refer to [32].

1.4 Theoretical Predictions for Hadron Colliders

In HEP measurements, the collected collision data is compared to theoretical predictions. Computing theoretical predictions for pp collisions is a highly complex task involving solving multi-dimensional integrals such as Equation 1.3.1 and the calculation of QCD interactions in the hard scattering process. An illustration of a pp collision is depicted in Figure 1.7. Given the complexity of these computations, numerical methods known as Monte Carlo (MC) techniques [33] are employed, which rely on generating random numbers to sample different possible outcomes of a process and provide an estimate of the desired quantity by averaging over many such samples. The simulation of pp collision events is done in several steps.

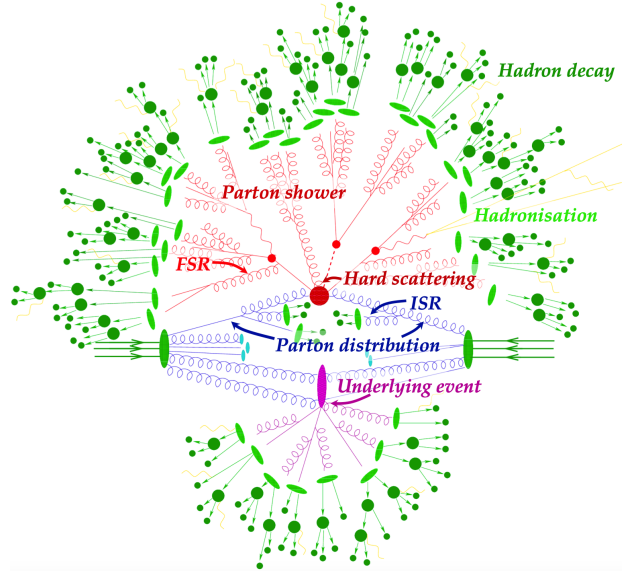


Figure 1.7: Visualization of a proton-proton collision as simulated in a Monte Carlo event generator. Figure taken from [34].

The hard scattering interaction in pp collisions is computed first through the calculation of the hadronic cross-section, $\sigma_{pp \rightarrow X}$, as shown in Equation 1.3.1. This includes the calculation of the matrix element, $\sigma_{ab \rightarrow X}$, based on the interaction Lagrangian using PDFs. Additionally, it takes into account hadronisation—the energy scale at which quarks and gluons transition into hadrons such as protons and pions—and factorisation scales (μ_F , see Section 1.3). The high-energy particles produced in the hard scatter, such as gluons and quarks, are initially too energetic to form bound states. They produce additional quarks and gluons through radiation or gluon splitting, a process simulated separately using perturbative QCD known as parton shower generation. Once the energy of the emitted gluons and quarks is reduced to around $\mathcal{O}(1\text{GeV})$, the partons begin to form bound states through the hadronization process. At these lower energy scales, perturbative QCD is no longer applicable. Instead, phenomenological QCD models convert parton showers into outgoing hadrons. The initial state radiation (ISR) and final state radiation (FSR) involve the emission of gluons (or, less frequently, photons) from the incoming and outgoing partons before and after the hard scatter occurs, respectively. These emissions are considered in the simulation to accurately account for the energy and momentum distributions of the partons involved. In addition to the hard scattering, the remaining partons within the protons can also interact. These interactions constitute the underlying event, which includes all the activity in the collision not associated with the primary hard scatter. At the LHC, multiple protons collide simultaneously in each bunch crossing. As a result, several interactions can happen at the same time, leading to pile-up [35]. Pile-up adds additional complexity to the analysis and is accounted for by adding soft QCD events (interactions involving low-momentum transfer) to the simulated event before further processing.

Several MC generators are available for this chain of computations. These generators can either

simulate all the steps described above or be interfaced with one another to simulate the various stages. Further details on the MC generators used in this thesis are provided in Section 4.2.

Once the events are generated, a detailed simulation of the ATLAS detector is performed to ensure that the simulated data can be accurately compared to real collision data. The ATLAS simulation chain, implemented within the ATHENA [36, 37] software framework, consists of four steps. First, events are generated using MC generators, where the matrix element for the hard scatter process is calculated along with the parton shower and hadronization processes. The truth information for each stable particle is recorded at this stage. Next, the detector simulation, the most computationally intensive step, is performed using GEANT4 [38], which accurately models the full geometry and material composition of the ATLAS detector. Particles are propagated through the detector, and their interactions with the sensitive detector material are recorded as *hits*, with the energy deposit, position, and timing information stored for each interaction. These hits are then transformed into digital signals in the digitization step, simulating the electronic readout of the detector, and stored as Raw Data Objects (RDOs). Further details regarding ITk pixel digitization can be found in Section 6.1. Finally, the reconstruction step employs specific algorithms [39] to convert the digital signals into identified particles, reconstructing their trajectories and properties. This reconstructed data is stored in the Analysis Object Data (AOD) format, facilitating detailed physics analyses and enabling precise comparisons with experimental measurements.

The LHC and the ATLAS detector

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Particle colliders have played a crucial role in the pursuit of discovering the particles predicted by the Standard Model of particle physics over the past decades. A prominent example of these ambitious endeavors is the Large Hadron Collider (LHC) [40, 41], located at the European Organization for Nuclear Research (CERN¹) on the border between Switzerland and France. With a circumference of 26.7 km, the LHC stands out as the world’s largest particle accelerator, housing four main experiments — A Large Ion Collider Experiment (ALICE) [42], A Toroidal LHC Apparatus (ATLAS) [43], the Compact Muon Solenoid (CMS) [44], and the Large Hadron Collider beauty (LHCb)[45]. This section serves as an introductory overview of the LHC and the ATLAS detector, emphasizing their pivotal roles in advancing our comprehension of the fundamental constituents of the universe.

¹<https://home.cern>

2.1 The Large Hadron Collider

The LHC, designed to accelerate and collide protons or heavy ions, features two counter-circulating particle beams situated in a tunnel 100 meters underground, which formerly housed the LEP collider [46]. The protons used in the LHC are sourced from a hydrogen gas bottle and then pre-accelerated by a series of accelerators, as illustrated in Figure 2.1 and detailed in Section 2.1.2.

Upon entering the LHC, the protons in adjacent, oppositely moving beams are individually accelerated to a maximum energy, currently set at 6.8 TeV since 2022. The acceleration process involves the use of resonant frequency cavities to propel the two hadron beams to extremely high energies and superconducting magnets to guide the beams along separate circular paths. The parallel beams converge at four crossing points along the LHC, where ATLAS, CMS, ALICE and LHCb detectors are positioned as depicted in fig. 2.1.

At these interaction points, protons collide, generating a center-of-mass energy that has evolved over different runs, starting at 7 TeV (2010-2011) and 8 TeV (2012) during Run-1, increasing to 13 TeV in Run-2 and reaching 13.6 TeV in Run-3, which commenced on July 5th, 2022.

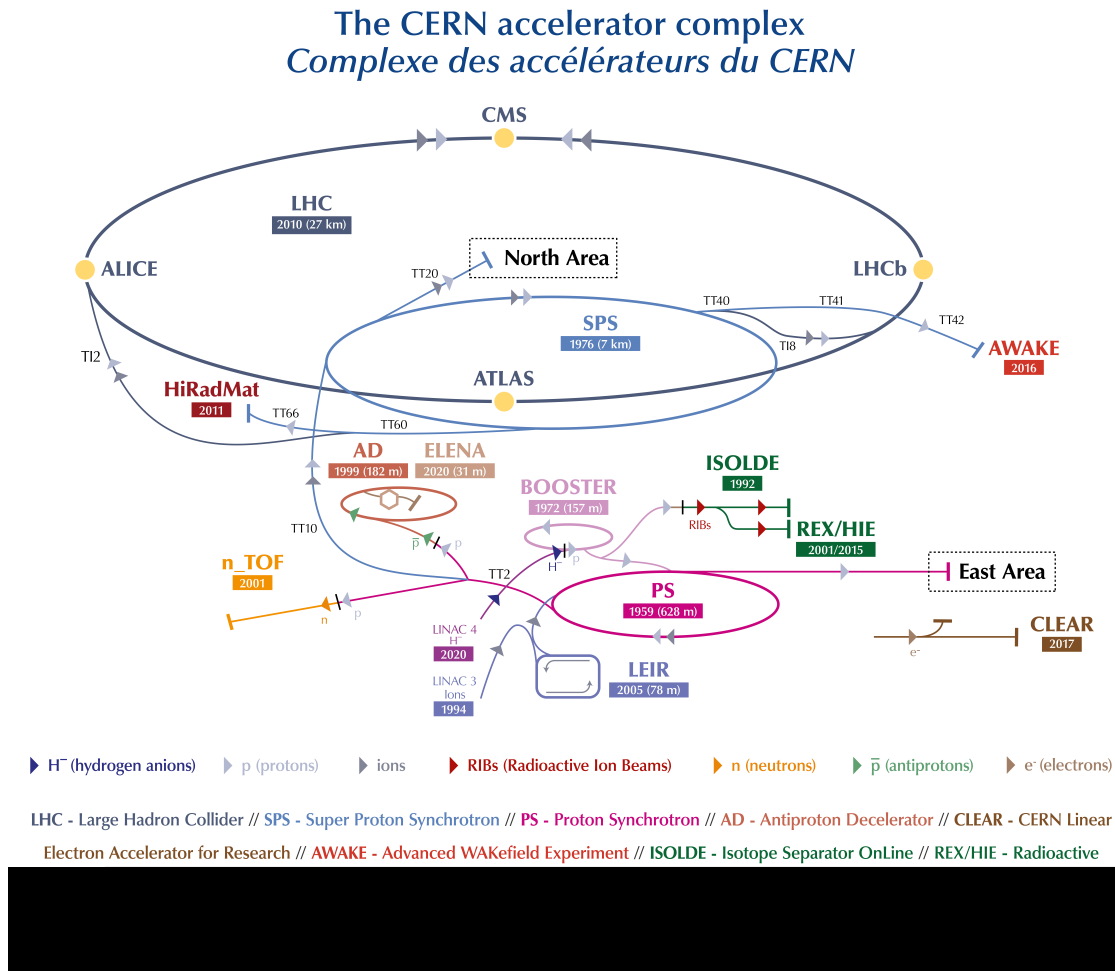


Figure 2.1: Sketch of the CERN accelerator complex and pre-accelerator stages of the LHC. Proton-proton collisions commence in LINAC4 and progress through the Booster, Proton Synchrotron (PS), and Super Proton Synchrotron (SPS). Protons are injected into the LHC from two directions and converge at four designated intersection points for collisions [47].

2.1.1 LHC Magnets

Within the Large Hadron Collider (LHC), two primary types of superconducting magnets play crucial roles: dipoles, responsible for bending particle beams, and quadrupoles, dedicated to focusing the beams. The LHC ring houses a total of 1,232 dipole magnets, each extending 15 m, and 392 quadrupole magnets, each 3 m long, to facilitate the precise bending and focusing of particle beams within the collider. To ensure the stability of proton beams along their circular trajectory, an additional 6000 correcting magnets are employed. Operating on copper-stabilized NbTi Rutherford cables or single strands, these superconducting magnets function within a superfluid helium environment maintained at 1.9 K. The dipole magnets are designed for a nominal operation current of about 11 600 A for a central field of 8.3 T, with possibility to reach 9 T (ultimate field) and the corresponding field gradient of the main focusing quadrupole magnets is 220 T m^{-1} [48].

Figure 2.2a displays a sequence of LHC magnets, offering a perspective one might observe while exploring the tunnel housing the accelerator at CERN, with different colors indicating the various types of magnets. The distinctive blue hue is predominantly a result of unwritten guidelines, emphasizing the selection of vibrant colors for optimal visibility in the dimly lit surroundings within the LHC tunnels. The familiar blue tone alternates with a radiant white shade employed for the vacuum vessels containing the LHC's quadrupole magnets and the rich, deep red associated with the triplet quadrupole magnets, which further focus the beam around the collision points. In the upcoming years, these colors will be complemented by dark blue, representing the future High-Luminosity LHC's (see Section 5.1) 11.4 T magnets, which are currently in the testing phase. The deeper hue is intended to signify these magnets' stronger magnetic field strength compared to the regular LHC dipoles, which are characterized by a lighter blue color [49].

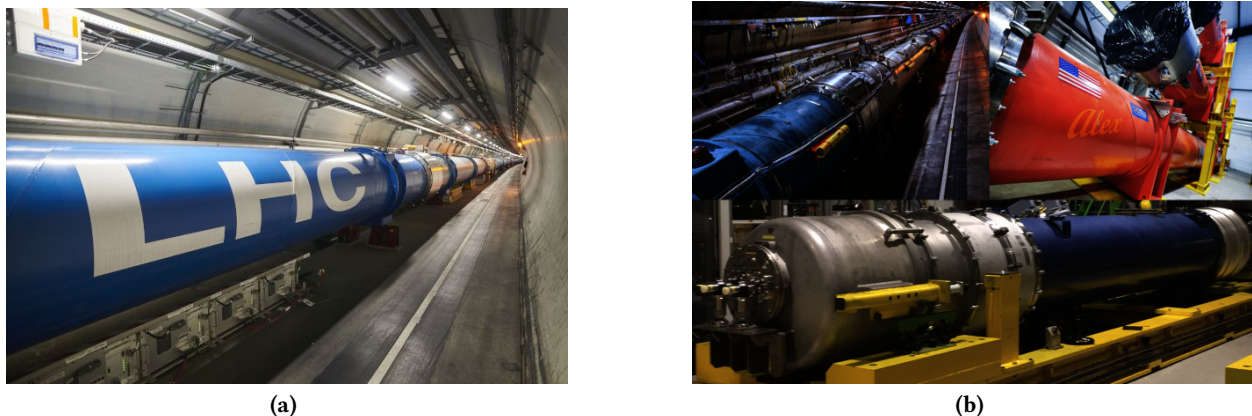


Figure 2.2: (a) A chain of LHC dipole magnets inside the tunnel at point 1 (ATLAS) [50]. (b) The LHC with its blue dipole magnets and white quadrupole magnets (top left), a red LHC triplet quadrupole magnet before installation (top right) and a prototype of the dark blue 11.4 T HL-LHC dipole magnet (bottom) [51].

2.1.2 The CERN Accelerator Complex

The performance of the LHC and its successor, the HL-LHC, relies on the injector chain (see Figure 2.1), the four accelerators that pre-accelerate the beams before injecting them into the 26.7-kilometre ring. The injector chain starts with a linear accelerator (LINAC4), designed to boost negative hydrogen ions to high energies, and has been the source of proton beams for the LHC since 2020 (replacing LINAC2 [52]). LINAC4, comprising a H^- ions source and a series of conducting cylindrical accelerating structures operate by accelerating hydrogen anions to 160 MeV, preparing them for entry into the Proton Synchrotron Booster (PSB) using radiofrequency cavities to charge the cylindrical conductors. The ions pass through the conductors, alternately charged positively or negatively. The conductors behind them push particles, and the conductors ahead of them pull,

causing the particles to accelerate. Small quadrupole magnets ensure the hydrogen ions remain in a tight beam. After leaving LINAC4, the hydrogen anions are stripped of their two electrons, and the bare protons are injected into the PSB for acceleration in the rest of the chain [53].

The Proton Synchrotron Booster (PSB) [54], a synchrotron, is the first and smallest circular proton accelerator in the accelerator chain at the CERN injection complex, delivering beams to the LHC. Comprising of four superimposed synchrotron rings with accelerated and eventually recombined after extraction to 2 GeV before injecting into the Proton Synchrotron (PS). The PSB does not only act as a proton injector for the PS but also provides protons at an energy of 1.4 GeV to its sole direct user, the Isotope mass Separator On-Line facility (ISOLDE), a facility dedicated to the production of a large variety of radioactive ion beams for many different experiments in the fields of nuclear and atomic physics, solid-state physics, materials science and life sciences [55].

The Proton Synchrotron (PS) [56] stands as a vital cornerstone within CERN's accelerator complex, primarily tasked with accelerating protons delivered by the PSB or heavy ions from the Low Energy Ion Ring (LEIR). Spanning a circumference of 628 m, the PS boasts 277 conventional (room-temperature) electromagnets, including 100 dipoles to guide beams around its circular track. Operating at energies reaching up to 26 GeV, the accelerator has facilitated the acceleration of a diverse array of particles, including alpha particles, oxygen, Sulphur, Argon, Xenon, and Lead nuclei, as well as electrons, positrons, and antiprotons.

As the second-largest machine within CERN's accelerator complex, the Super Proton Synchrotron (SPS) [57] boasts a circumference of nearly 7 km with the primary function of receiving particles from the PS and subsequently accelerating them to produce beams for the LHC, NA61/SHINE [58], NA62 [59], COMPASS [60], and the AWAKE [61] experiment. Since its inauguration in 1976, the SPS has emerged as a cornerstone in CERN's particle physics program, with the most significant milestone being the Nobel-prize-winning discovery of W and Z particles, with the SPS running as a proton-antiproton collider. Operating at energies up to 450 GeV, the SPS is equipped with 1317 conventional electromagnets, including 744 dipoles to bend beams around the ring. The accelerator has accommodated a diverse range of particles, including Sulphur and Oxygen nuclei, electrons, positrons, as well as protons and antiprotons.

Finally, the beams are injected into the LHC, where the protons circulate in two separate vacuum chambers in opposite directions within a single beam pipe. The proton beams are organized into regularly spaced bunches containing approximately 10^{11} protons. The structure of these beams depends on the capabilities of the injectors, as detailed in Section 2.1.3. A standard LHC fill takes about 30 minutes per ring from the SPS and waits up to 15 minutes on the LHC 450 GeV injection plateau before the 28 minutes ramp to energy of 6.5 TeV and ≈ 5 minutes for the beam squeeze. High energy beams circulate within the LHC for 10 – 20 hours, colliding at a rate of 40 MHz until the number of proton bunches runs out. Then, the beams are dumped, the magnets are ramped down, and the entire system goes through ≈ 30 minutes of rest, and a new cycle begins [62].

2.1.3 LHC Filling Scheme

The filling scheme of an accelerator ring is dictated by the capabilities of its RF system and the injector chain (see Section 2.1.2). The LHC's RF operates at ≈ 400 MHz, establishing the smallest particle-containing interval at 2.5 ns or roughly 75 cm. Given the extensive length of the LHC ring (27 km), this translates to 35640 possible slots, referred to as buckets. However, owing to injector limitations, the nominal bunch spacing is fixed at 25 ns, permitting the filling of only one out of every ten buckets, which defines a bunch, resulting in 3564 available bunch positions in the ring. The time measurement at the LHC commonly employs a bunch as the basic unit, corresponding to 25 ns. Collisions occur when two bunches cross each other at the four experimental interaction points. The collisions are independent so the particle interactions within one bunch crossing is

called an event and each event is identified by a Bunch Crossing Identifier (BCID) that runs from 0 to 3563. Out of the 3564 possible positions, only 2808 are nominally filled due to dead-times resulting from various systems, as depicted in Figure 2.3. Time must be allocated for the rise time of the kicker magnets — a pulsed dipole magnets with very fast rise and/or fall times typically ranging from 50 ns to 1 μ s — used to inject and extract beams at each stage of the acceleration chain. The rise times are ≈ 225 ns or 9 empty bunches for PS to SPS and ≈ 950 ns or 39 empty bunches for SPS to LHC [63].

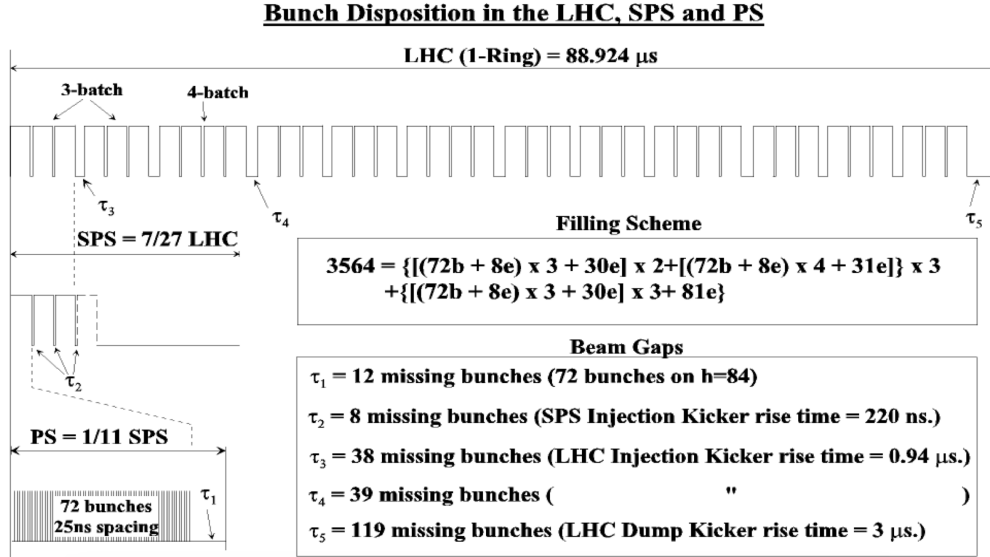


Figure 2.3: Illustration depicting the nominal filling sequence at LHC, showcasing proton bunches in the PS, SPS, and one LHC ring. The RF cavity facilitates 3564 bunch slots of 25 ns; however, not all slots can be filled due to the kicker rise time of the SPS and LHC [63].

2.1.4 Luminosity and Pile-up

In collider physics, the instantaneous luminosity ($\mathcal{L}_{inst}$) is a fundamental metric representing the number of particle collisions occurring per unit area per second at a given interaction point. It directly correlates the occurrence rate of a specific physics process ($\frac{dN}{dt}$) with the process's cross-section (σ) and is given by :

$$\frac{dN}{dt} = \mathcal{L}_{inst} \times \sigma \quad (2.1.1)$$

Increasing the instantaneous luminosity enhances the probability of occurrence for rare events. Consequently, the instantaneous luminosity serves as a measure of a particle accelerator's performance and can be computed from collider parameters as:

$$\mathcal{L}_{inst} = \frac{N_1 N_2 f N_b}{4\pi \sigma_x \sigma_y} \quad (2.1.2)$$

Here, N_1 and N_2 represent the number of protons in each of the two colliding bunches of particles, f is the revolution frequency of the collider, N_b is the number of bunches, and σ_x, σ_y are the widths of the beam density distributions in the x and y direction, respectively. The Run 1 of the LHC achieved a peak instantaneous luminosity of $0.8 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$ [48]. Subsequently, in the second and third runs of the LHC, the luminosity further increased to $2.1 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$ [64, 65].

The integrated luminosity is a key metric to quantify the total data delivered. The expected number of events (N) for a process with a cross section (σ) is determined as:

$$N = \mathcal{L}_{\text{int}} \times \sigma \quad (2.1.3)$$

Here, $\mathcal{L}_{\text{int}}$ represents the integrated luminosity, which is defined as the integral of the instantaneous luminosity $\mathcal{L}_{\text{inst}}$ over the time interval from t_1 to t_2 :

$$\mathcal{L}_{\text{int}} = \int_{t_1}^{t_2} \mathcal{L}_{\text{inst}}(t) dt \quad (2.1.4)$$

Figure 2.4a illustrates the cumulative integrated luminosity versus time delivered by the LHC, recorded by the ATLAS experiment and certified to be good quality data in Run 2 (2015 and 2018). The delivered luminosity accounts for the luminosity delivered from the start of stable beams until the LHC requests ATLAS to put the detector in a safe standby mode to allow a beam dump or beam studies. The recorded luminosity accounts for inefficiencies in the Data Acquisition (DAQ) system (see Section 2.2.7), as well as the inefficiencies associated with the 'warm start' process when the stable beam flag is raised, the tracking detectors ramp up their high voltage, and the pixel system activates its preamplifiers. Good quality data represents the subset of recorded data that has been verified to meet all criteria for high-quality data, making it "good for physics." Delivered luminosity directly correlates with the radiation dose received by silicon detectors, affecting their longevity and performance due to radiation damage (see Section 3.5), while recorded luminosity determines the amount of data available for physics analyses, impacting both the detector's performance and the statistical power of physics searches. The total Run 2 dataset corresponds to an integrated luminosity of $\mathcal{L}_{\text{int}} = 140.1 \pm 1.2 \text{ fb}^{-1}$ [66]. In Figure 2.4b, the integrated luminosity delivered during Run 3 (January'22 - July'23) is depicted and the total dataset corresponds to an integrated luminosity of $\mathcal{L}_{\text{int}} \approx 66 \text{ fb}^{-1}$.

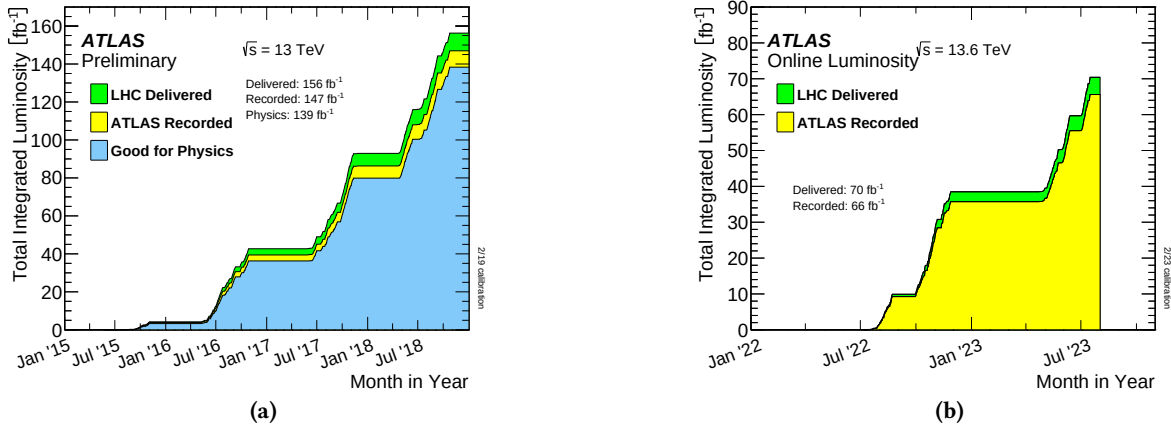


Figure 2.4: (a) Integrated luminosity versus time delivered to ATLAS (green), recorded by ATLAS (yellow), and certified to be good quality data (blue) during stable beams for pp collisions at 13 TeV centre-of-mass energy in LHC Run 2 [64]. (b) Integrated luminosity versus time delivered to (green) and recorded by ATLAS (yellow) during stable beams for p-p collisions at 13.6 TeV centre-of-mass energy in LHC Run 3 (2022-2023) [65].

The head-on collisions between two protons within a bunch-crossing, which produce high-energy (hard) scattering events, are of prime interest in HEP experiments like ATLAS and CMS. However, each hard scatter event is accompanied by additional soft proton-proton interactions known as pile-up. This effect pollutes the final state of the collision and deteriorates the reconstruction performance of the objects in this final state, resulting in increased experimental measurement uncertainties. In-time pile-up are additional soft interactions within the same bunch-crossing, while out-of-time pile-up stems from neighboring bunch crossings. The amount of pile-up events is quantified by the average number of interactions per event, μ , defined as:

$$\mu = \frac{\mathcal{L}_{bunch} \sigma_{inel}}{N_b f} \quad (2.1.5)$$

Here, $\mathcal{L}_{bunch}$ represents the instantaneous luminosity associated with a single bunch crossing and σ_{inel} is the inelastic scattering cross-section for proton-proton collisions (≈ 80 mb at 13 TeV and 13.6 TeV). The average number of interactions per bunch crossing corresponds to the mean of the Poisson distribution representing the number of interactions per crossing, calculated for each bunch. Figure 2.5a and figure 2.5b illustrate this distribution for different data-taking periods in Run 2 and Run 3 of the LHC, respectively. Figure 2.5c depicts the cumulative luminosity delivered to ATLAS for p-p collisions over time. The instantaneous luminosity has increased with each successive run, and the preliminary average pile-up for Run 3 is $\langle \mu \rangle = 42.5$.

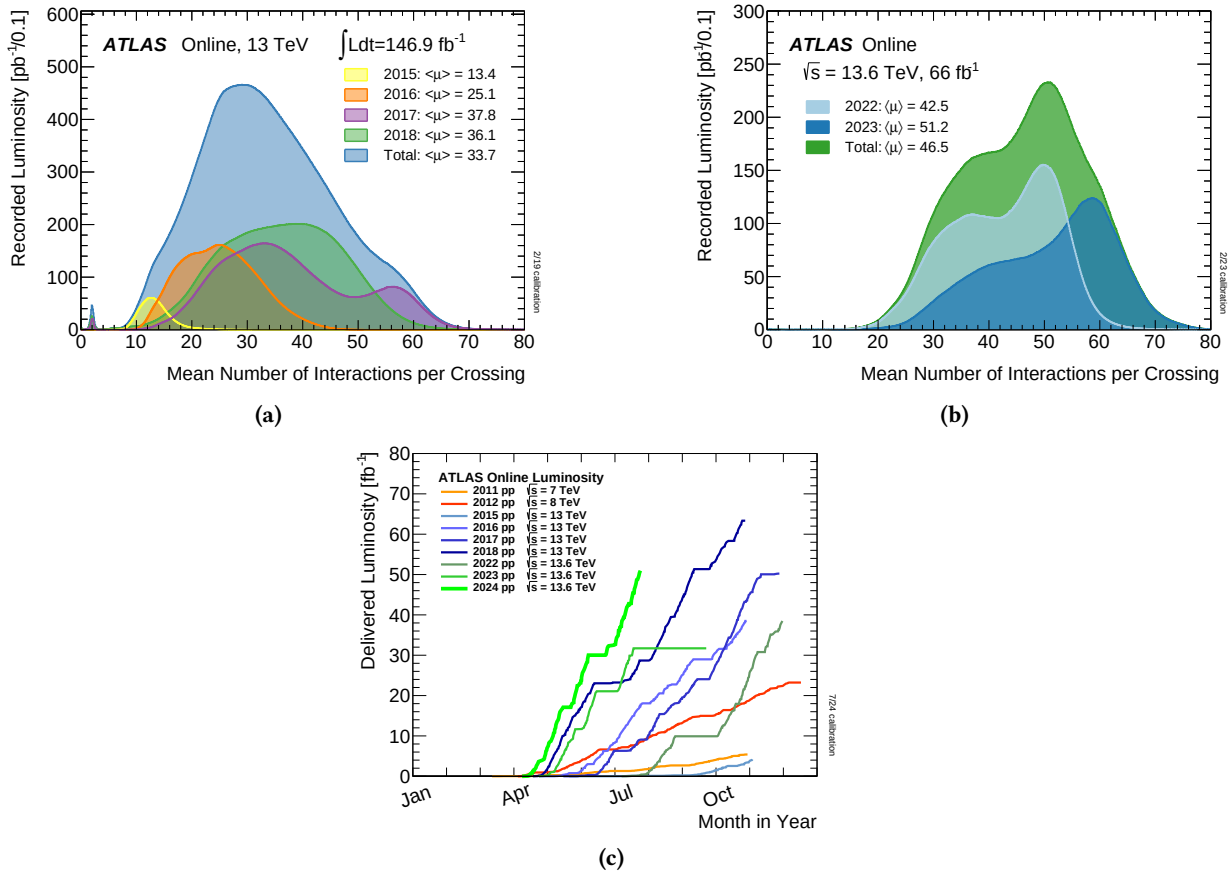


Figure 2.5: (a) Luminosity-weighted distribution of the mean number of interactions per crossing for the 2015-2018 pp collision data at 13 TeV centre-of-mass energy [64]. (b) Luminosity-weighted distribution of the mean number of interactions per crossing for the 2022-2023 pp collision data at 13.6 TeV centre-of-mass energy [65]. (c) Cumulative luminosity versus day delivered to ATLAS during stable beams and for high energy p-p collisions [65].

2.1.5 LHC Experiments

The LHC houses four large and five smaller physics experiments situated at various locations along the ring, as shown in figure 2.1. The two largest experiments, ATLAS and CMS, employ general-purpose detectors for exploring a wide range of physics phenomena and cross-confirming new discoveries, while ALICE and LHCb employ specialized detectors focused on specific phenomena. The smallest experiments on the LHC, namely TOTEM [67] and LHCf [68], focus on "forward particles" – protons or heavy ions that skim past each other instead of colliding head-on. TOTEM employs detectors positioned on either side of the CMS interaction point, while LHCf consists of

two detectors situated along the LHC beamline, 140 m on each side of the ATLAS collision point. MoEDAL-MAPP [69] utilizes detectors deployed near LHCb to investigate a hypothetical particle known as the magnetic monopole. FASER [70] and SND@LHC [71], the two most recent LHC experiments, are located near the ATLAS collision point to explore light new particles and study neutrinos.

In the upcoming short overview, focus will be placed on the four main experiments at the LHC — ALICE, ATLAS, CMS, and LHCb — each tailored to investigate specific aspects of particle physics through the use of specialized detectors and methodologies.

ALICE is a dedicated detector at LHC for heavy-ion physics, designed to study the properties of quark-gluon plasma (QGP), pivotal for understanding quantum chromodynamics (QCD) and quark confinement [72–74]. Heavy-ion (Pb-Pb) collisions at LHC generate temperatures hundreds of thousands of times hotter than the center of the sun, recreating post-Big Bang conditions in the laboratory, allowing the study of this primordial state of matter (QGP) before the recombination of quarks and gluons into familiar hadrons like protons and neutrons. The collaboration uses a 10,000-tonne detector measuring approximately 26 m in length, 16 m in height, and 16 m in width to study the QGP as it expands and cools, transitioning into the particles forming our present-day universe. The detector sits in a vast cavern 56 m underground close to the village of St Genis-Pouilly, France.

ATLAS is one of two general-purpose detectors at the LHC that explores a diverse spectrum of physics, ranging from the precise measurement of Higgs boson properties to the search for new physics beyond the Standard Model (BSM), including super-symmetry (SUSY) and searches for dark matter candidates [75–77]. At 46 m long, 25 m high and 25 m wide, the 7000-tonne ATLAS detector is the largest volume particle detector ever constructed and it sits in a cavern 100 m underground near the main CERN site, close to the village of Meyrin in Switzerland. A comprehensive description of the ATLAS detector can be found in Section 2.2.

CMS, the second general-purpose detector at the LHC, shares a closely aligned physics program with the ATLAS experiment, spanning from studying the Standard Model to searching for extra dimensions and dark matter candidates but utilizes distinct technical solutions and a magnet-system design different from that of ATLAS [78–80]. The complete detector is 21 m long, 15 m wide, and 15 m high, with a strong magnetic field of 4 T and is situated in an underground cavern near Cessy, France.

Unlike the other three main detectors at LHC, the LHCb experiment features a unique design with an asymmetric, one-sided forward detector [81–83]. With dimensions measuring 21 m in length, 10 m in height, 13 m in width, and a weight of 5600 tonnes, LHCb focuses on matter anti-matter asymmetry, precise flavor physics measurements, and CP violation studies using bottom (beauty) and charm hadrons decays, primarily produced in forward and backward regions, close to the beam axis. The detector is situated 100 m underground near the town of Ferney-Voltaire, France.

2.2 The ATLAS Detector

The collisions at the LHC produce hundreds to thousands of particles at each bunch crossing. However, only those particles that live long enough to reach the detector can be directly measured. Assuming the particles travel at speeds close to the speed of light and considering the size of the tracker (approximately 1 m), only particles with lifetimes on the order of nanoseconds or longer, such as electrons, protons, neutrons ($\tau \approx 900$ s), muons ($\tau \approx 2.2$ μ s), charged pions ($\tau \approx 25$ ns), and kaons ($\tau \approx 10$ ns to 50 ns), can travel a sufficient distance to be detected directly in the ATLAS detector. In the subsequent discussion, the term "stable particle" encompasses any of these long-lived particles. Neutrinos interact with matter extremely weakly despite being stable, rendering them nearly impossible to detect in ATLAS. Consequently, their presence is inferred in the detector

by observing an imbalance in the energy and momentum of the colliding protons and all detected particles in the transverse plane (perpendicular to the beam) of the ATLAS detector. Particles with short lifetimes, like the Higgs bosons (1.6×10^{-22} s), are indirectly detected through the distinctive signatures left in the detector by their decay products, which often include the aforementioned long-lived particles. Additionally, stable and unstable hadrons produced from the hadronization (see Section 1.4) of quarks and gluons are often not resolved individually and mostly show up as groups of particles called jets.

An effective detector must be able to detect, identify, and distinguish among the diverse particles produced during the collisions at the LHC. The layout of a detector is meticulously designed to accomplish the goals mentioned above and typically involves the following key components:

- **Tracker:** The charged particles are identified, and their momenta are accurately measured by the tracker. To effectively determine the charge and momentum of particles, the tracker needs to be enveloped within a magnetic field and can be enhanced with a specialized particle identification system.
- **Calorimetry System:** After the tracker, a calorimetry system measures the energy of both charged and neutral particles by bringing them to a halt. This system ensures precise energy measurements.
- **Muon Detector:** This detector subsystem serves to identify and measure the properties of muons. Positioned outside the calorimeter, the muon detector is considered crucial, given that muons are minimum ionizing particles (see Section ??) which interacts minimally within the tracker and calorimeter, allowing them to penetrate to the outer layers of the detector.

2.2.1 ATLAS Detector: Design and Requirements

The required performances of the detector are inherently tied to the specific physics objectives it aims to accomplish. Serving as a general-purpose detector, ATLAS has extensive physics goals, encompassing a wide range of objectives, such as:

- W and Z bosons studies, in particular in the leptonic decay channels, requiring a precise measurement of electrons and muons.
- Top quark studies, which relies on the measurements of b-hadrons, requiring a good vertex resolution for an efficient b-jet identification (b-tagging), and the measurement of the associated W bosons decaying to leptons or jets
- Higgs boson studies in various decay modes, such as in a photon pair, requiring a good energy and spatial resolution of photons; four-lepton final states, which provide a clean experimental signature, low background, and precise mass measurement capabilities; τ -lepton pair subsequently decaying in jets or lighter leptons and neutrinos, demanding precise energy measurements of electrons, muons, and jets; and b-quark pair, requiring b-tagging capabilities with good jet energy resolution
- Searches for BSM physics and exotic states, that involve tagging methods that rely on displaced vertices or missing energy in the detector, and a possible high jet multiplicity.

The aforementioned physics goals translate into a set of overarching requirements for the ATLAS detector, that include:

- Large geometrical acceptance
- Enhanced charged particle momentum resolution and improved efficiency in reconstruction.
- Superior electromagnetic (EM) calorimetry for precise electron and photon identification and measurements, complemented by comprehensive full-coverage hadronic calorimetry to ensure

- accurate jet and missing transverse energy measurements.
- Enhanced muon identification with superior momentum resolution across a broad spectrum of momenta, coupled with the capability to unambiguously determine the charge of muons with high transverse momentum, p_T (see Section 2.2.2)
 - Highly efficient triggering on low p_T objects (typically 5 – 10 GeV) coupled with robust background rejection capabilities
 - Fast, radiation-resistant electronics and sensor components, complemented by a high detector granularity aimed at reducing the impact of pile-up events in the LHC radiation environment, characterized by intense radiation from high-energy proton-proton collisions, posing significant challenges for data collection and maintaining detector's performance (see Section 3.5.3).

The schematic of the ATLAS detector, depicted in Figure 2.6, reflects a purposeful alignment with its general-purpose philosophy. This design features barrel detector layers and endcaps, strategically chosen to enable the detection of a diverse array of particles at LHC. In line with the aforementioned physics goals, the ATLAS detector provides full coverage of the entire solid angle, ensuring complete hermeticity. The demand for fast, radiation-resistant sensors, and readout electronics arises from the 25 ns bunch structure of the LHC and the substantial datasets acquired. Additionally, a crucial emphasis on high spatial resolution emerges, facilitating the effective discrimination of multiple simultaneous events. Section 2.2.4, Section 2.2.5, and Section 2.2.6 presents the features and performance of the various ATLAS subdetectors.

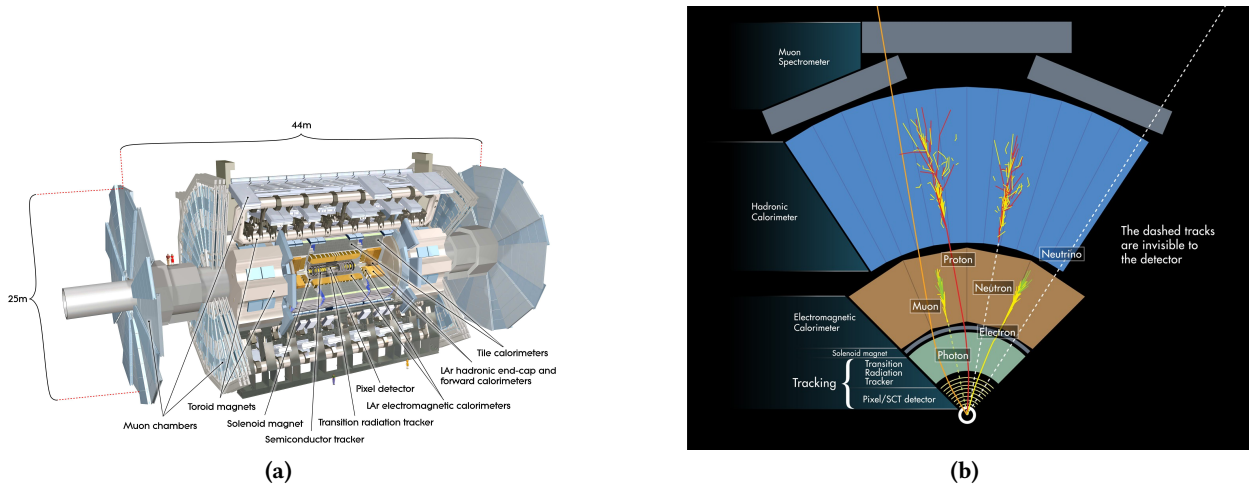


Figure 2.6: (a) Cut-away view of the ATLAS detector. (b) View of the particle paths and experimental signatures in the transverse plane of the ATLAS detector [84, 85].

2.2.2 ATLAS Coordinate System

ATLAS utilizes a right-handed coordinate system, with the origin located at the nominal interaction point (IP) at the center of the detector, as depicted in Figure 2.7. The z -axis is aligned with the beam pipe, the x -axis extends from the IP towards the center of the LHC ring, and the y -axis points upwards from the IP. The transverse plane is conventionally represented as the x - y plane, while any plane containing the z -axis is referred to as the longitudinal plane. In the transverse plane, cylindrical coordinates (r, ϕ) are used, where r is the radial coordinate and $\phi \in [-\pi, \pi]$ is the azimuthal angle around the z -axis. The polar angle, denoted as $\theta \in [0, \pi]$, is the angle relative to the beam axis.

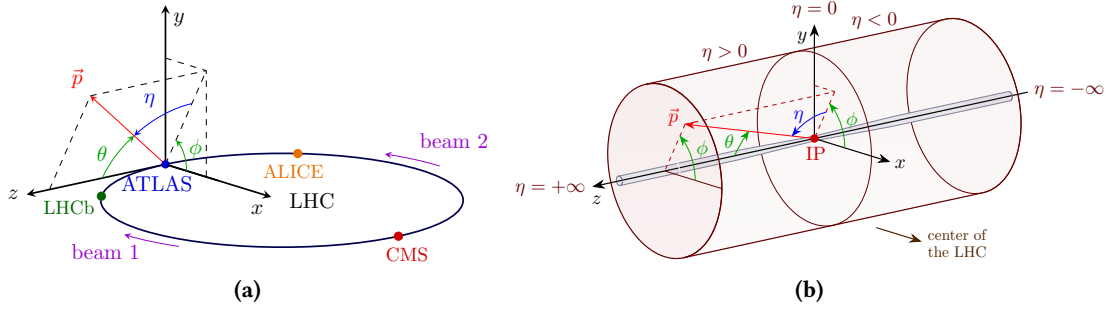


Figure 2.7: A graphical representation depicting the coordinate system of both (left) the LHC and (right) the ATLAS detector [86].

Consider a particle described by the four-momentum $(E, \mathbf{p})$, where E represents the energy, and $\mathbf{p} = (p_x, p_y, p_z)$ denotes the momentum. The components p_x , p_y , and p_z correspond to the momentum projections on the x , y , and z axis, respectively. The particle's transverse momentum, p_T , is derived by projecting the momentum onto the transverse plane, $\mathbf{p}_T = p_x \mathbf{e}_x + p_y \mathbf{e}_y$, where $\mathbf{e}_x$ and $\mathbf{e}_y$ are the unit normal vectors in the direction of the x and y axes, respectively. The relationships between the norm of the transverse momentum, p_T , and the momentum components $\mathbf{p}$ are as follows:

$$p_T = \sqrt{p_x^2 + p_y^2} = |\mathbf{p}| \sin(\theta) \quad (2.2.1)$$

$$p_x = p_T \cos(\phi) = |\mathbf{p}| \sin(\theta) \cos(\phi) \quad (2.2.2)$$

$$p_y = p_T \sin(\phi) = |\mathbf{p}| \sin(\theta) \sin(\phi) \quad (2.2.3)$$

$$p_z = \frac{p_T}{\tan(\theta)} = |\mathbf{p}| \cos(\theta) \quad (2.2.4)$$

In hadron colliders, the longitudinal momentum (p_z) of the partons inside the protons is not directly measurable because only the final state particles are observed, not the detailed internal dynamics of the partons within the protons. Consequently, the precise longitudinal momentum of the partons before and after the collision remains unknown while the vector sum of the transverse momenta of all detected particles should be equal to the total transverse momentum of the initial system, which is zero in symmetric collisions at hadron colliders. Consequently, the transverse momentum is a more useful measure compared to the overall momentum itself. A pivotal quantity is rapidity (y), serving as a measure of a particle's direction, is defined as:

$$y = \frac{1}{2} \ln \left(\frac{E - p_z}{E + p_z} \right) = \tanh^{-1} \left(\frac{p_z}{E} \right), \quad (2.2.5)$$

For ultra-relativistic particles with $p \gg m$, the pseudo-rapidity (η) serves as a suitable approximation of rapidity and depends on the polar angle, θ as:

$$\eta = -\ln \tan(\theta/2) \quad (2.2.6)$$

Furthermore, the intervals of pseudo-rapidity ($\Delta\eta$) remains invariant under Lorentz transformation along the z -axis, rendering it independent of the boost along longitudinal axis. Figure 2.8 illustrates a graphical representation of correlation between pseudorapidity and polar angles. In the transverse plane, η equals to 0, whereas along the beam axis, η tends towards $\pm \infty$.

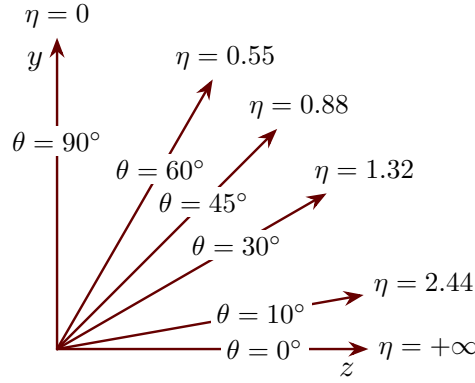


Figure 2.8: The correlation between pseudorapidity η and specific values of the polar angle θ [86].

The angular separation ΔR between two particles can be specified with the differences in azimuthal angles ($\Delta\phi$) and pseudorapidities ($\Delta\eta$), expressed as:

$$\Delta R = \sqrt{(\Delta y)^2 + (\Delta\phi)^2} \underset{\text{massless particle}}{\approx} \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}. \quad (2.2.7)$$

2.2.3 ATLAS Magnet System

One vital element of the ATLAS detector is its magnet system, which plays a crucial role in measuring the momentum of the charged particles as they follow curved trajectories in a magnetic field due to the Lorentz force (see Section 3.3.4). The radius of the particle trajectory R is given by:

$$R = \frac{p \sin \theta}{0.3B} \quad (2.2.8)$$

Here, p represents the particle's momentum in GeV/c, θ is the polar angle, B denotes the magnetic field strength in T, and R represents the radius in m. Thus, high magnetic fields are needed to increase the curvature of high- p_T particles and precisely measure their momentum.

The ATLAS experiment incorporates a sophisticated magnet system featuring four superconducting magnets as illustrated in fig 2.9, shaping the magnetic field within both the inner detector (section 2.2.4) and the muon spectrometer (section 2.2.6). The central solenoid, capable of generating a 2 T magnetic field along the z-axis, effectively deflects particles in the transverse plane while the barrel and endcap toroids integrated into the muon detector, produce a magnetic field between 0.5 to 1 T deflecting muons in longitudinal plane, thereby facilitating precise momentum measurements [43].

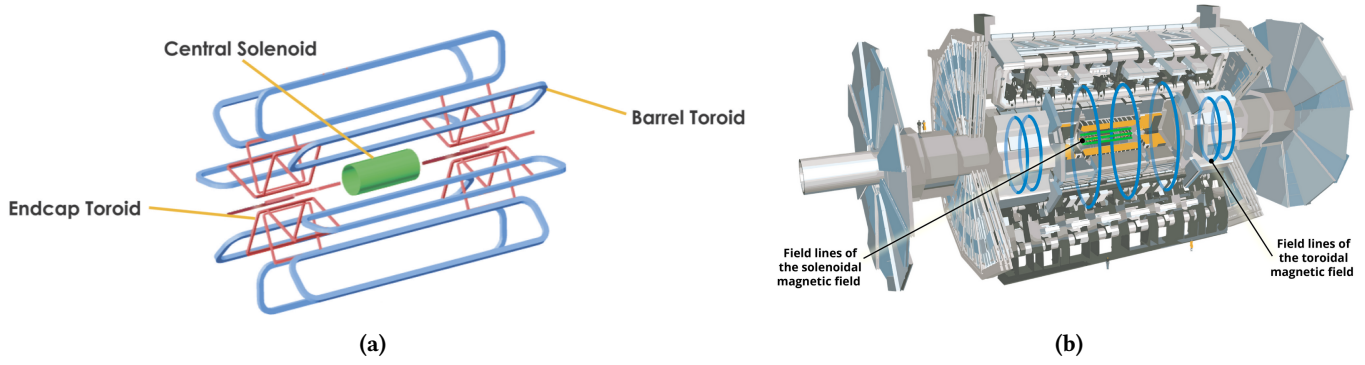


Figure 2.9: (a) Illustration of the central solenoid, barrel toroid, and endcap toroid magnets in the ATLAS detector. (b) Visualization of the generated magnetic field lines: the solenoid produces a parallel field within the tracker (depicted by straight green lines), while the toroidal magnets create a rotating field (illustrated by blue lines). The broader central field lines are from the barrel toroid magnets, and the smaller outer ones result from the combined influence of the endcap magnet field and the barrel toroid [87, 88].

2.2.4 The Inner Detector

The Inner Detector (ID), positioned closest to the IP, is designed to trace the paths of charged particles from the IP to the calorimeter, determining their momentum by measuring the curvature of their trajectories within the 2 T magnetic field generated by a solenoidal magnet within the pseudorapidity range of $|\eta| < 2.5$. Housed within a cylindrical envelope measuring 7 m in length and a radius of 1.15 m, the ID operates in an environment characterized by a high track density, requiring a detector that is both fast and radiation-tolerant. Additionally, a high granularity is essential for achieving excellent resolution in reconstructing momenta and vertices. Figure 2.10 shows the schematic view of the ID barrel region, highlighting its four distinct subsystems: the Insertable B-Layer (IBL), the Pixel Detector, the Semiconductor Tracker, and the Transition Radiation Tracker.

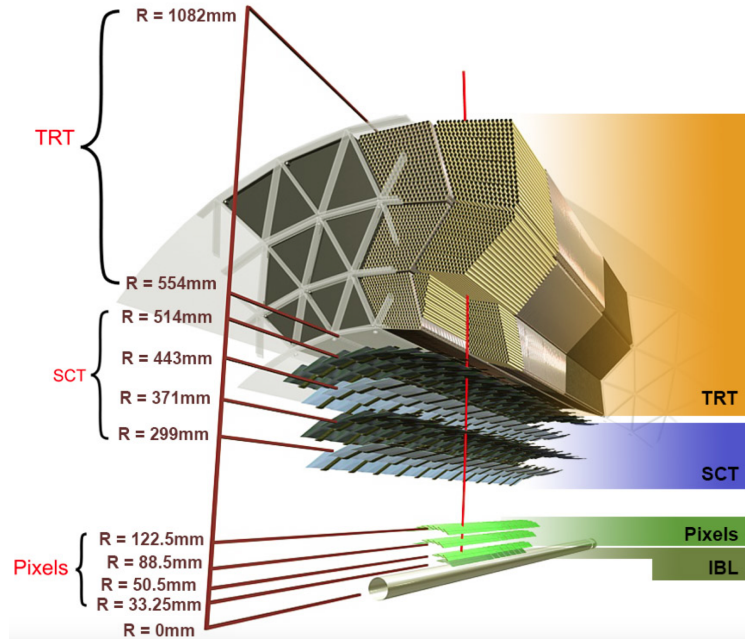


Figure 2.10: 3D representation showcasing the inner detector barrel structure, including the beam pipe, IBL, Pixel layers, four cylindrical layers of the SCT, and three layers of the TRT barrel module. [43].

2.2.4.1 The Insertable B-Layer

The Insertable B-Layer (IBL) [89], innermost part of the ID, was integrated in the first Long Shutdown (LS-1) occurred between Run 1 and Run 2 between the innermost pixel layer (the B-layer at a radius of 50.5 mm) and the beam pipe ($R = 0$ mm) to enhance the tracking performance of the ID in high luminosity scenarios. IBL achieves this by providing an additional hit closer to the primary interaction at a radius of 3.3 cm, with a smaller longitudinal pixel pitch (250 μ m) compared to the Pixel Detector (400 μ m) thereby improving the vertex reconstruction and b-tagging performance of the tracking system. The additional layer of highly segmented pixel sensors in the IBL serves to rectify inefficiencies within the Pixel Detector stemming from irreparable module failures and radiation damage, particularly in the B-Layer, which was originally intended for replacement and effectively mitigates the occurrence of ghost tracks induced by high pile-up backgrounds [90]. Additionally, the closer proximity of the IBL to the beam axis improves the precision of the impact parameter of tracks, thereby enhancing vertex reconstruction and b-tagging performance of the tracking system.

The IBL comprises 14 staves, each accommodating 20 modules arranged longitudinally along the z - or beam-direction, as illustrated in figure 2.11. The staves are tilted by 14° in a classic turbine design to ensure complete azimuthal coverage for high p_T tracks and compensate for the Lorentz angle shift affecting charges drifting in the sensors. Each staff integrates 12 planar sensors in its central region and 8 3D sensors in its forward region (4 on each side), extending the coverage up to $|\eta| = 2.58$.

The IBL utilizes two distinct sensor technologies: an enhanced version of the ATLAS Run 1 n^+ -in-planar pixel sensors with a thickness of 200 μ m, designed to withstand unprecedented operational conditions with reduced inactive edges, and an innovative 3D device design, where n^+ and p^+ electrodes penetrate a 230 μ m thick silicon substrate fully or partially—a pioneering application in high-energy physics. The IBL planar and 3D sensors have been shown to be sufficiently radiation hard up to $5 \times 10^{15} \text{ n}_{\text{eq}} \text{ cm}^{-2}$ [91]. Both sensor implementations share a common footprint for interfacing with the same readout chip, the FEI4, which is produced with CMOS 130 nm technology. This chip is capable of handling very high radiation doses above 250 MRad and coping with the high hit rate encountered in such environments [92]. Two-chip planar sensor tiles match the longitudinal dimension of two single-chip 3D sensors, ensuring a consistent mechanical layout. Both technologies share identical granularity, featuring pixels measuring $250 \mu\text{m} \times 50 \mu\text{m}$, organized in arrays of 80×336 pixels.

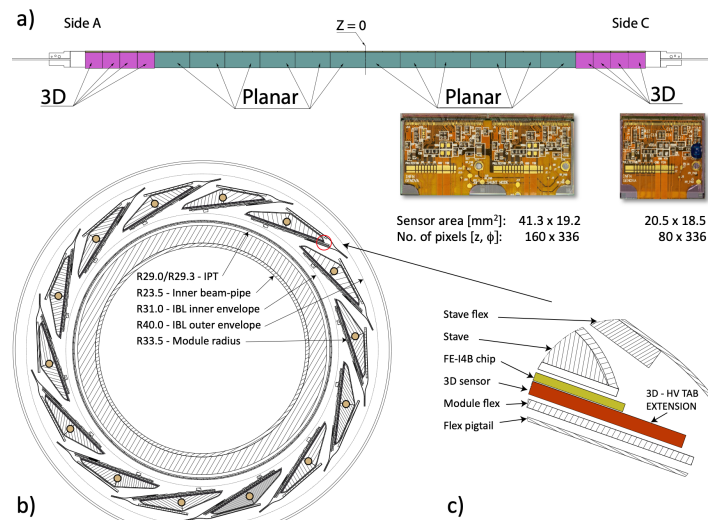


Figure 2.11: (a) Stave layout with the organization of planar and 3D sensor modules. (b) Layout of the IBL detector with the 14 staves around the IBL positioning tube (IPT) and (c) zoom of one stave side where a 3D sensor module is visible [93, 94].

2.2.4.2 The Pixel Detector

The pixel detector [95], positioned around the IP and enveloping the IBL, comprises three barrel layers at average radii of approximately 4 cm, 11 cm, and 14 cm, as well as three end-cap disks with radii ranging from 11 cm to 20 cm. The pixel system provides three or more space points within the complete acceptance of the ID ($|\eta| < 2.5$), enhancing the impact parameter resolution and improving the Inner Detector's ability to identify short-lived particles such as b-quarks and τ -leptons. Figure 2.12 illustrates a schematic of the pixel detector and the barrel cross-sectional view depicting the radial extensions of the pixel detector from the beam line. The three barrel layers consist of 1,456 pixel modules, while the three disks in each end-cap are composed of 288 modules equipped with FE-I3 readout chips, for a total of 80 million readout channels and an active area of 1.7 m^2 . The pixel modules are constructed using $250 \mu\text{m}$ thick n-on-n silicon sensors with 328×144 pixel cells, totaling 47,232 pixels. The standard pixel size is $50 \times 400 \mu\text{m}^2$, except for a subset of long pixels measuring $50 \times 600 \mu\text{m}^2$, which are located in the inter-chip regions. Each module operates at a bias voltage of $150 - 600 \text{ V}$ and is read out using 16 Front-End (FE) chips (FE-I3 ASICs [96]), each with 2,880 readout channels. While the 16 chips read out a total of 46,080 channels, all 47,232 pixels are read out by ganging the pixels in the inter-chip regions together [97].

The FE-I3 chip allows for pulse height measurements using the Time-over-Threshold (ToT) method (see Section 6.1.1), with on-chip zero suppression to streamline data processing by ignoring noise signals and reducing data volume. An event-building chip, the Module Controller Chip (MCC) [98], aggregates data from the 16 readout chips. This data is then converted into optical signals and transmitted via optical fibers to the off-detector electronics at a transfer speed adjustable between 40 and 160 MHz, depending on the expected occupancy. Additionally, the MCC provides clock and control signals to the individual front-end chips.

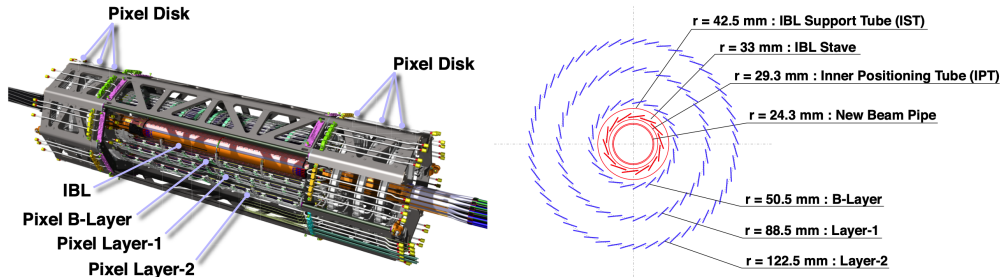


Figure 2.12: Schematic view of the pixel detector and cross-section view [99].

2.2.4.3 The Semi Conductor Tracker (SCT)

The Semiconductor Tracker (SCT) [100] is a precise silicon microstrip detector that extends the tracking volume to radial distances of $299 < r < 560 \text{ mm}$. The SCT consists of 4088 modules of silicon strips arranged in four concentric barrels and two end-caps of nine disks each, for a total surface of 63 m^2 . Each SCT module comprises two (or four) single-sided $285 \mu\text{m}$ thick p-in-n sensors. Two sensors on each side of the modules are wire bonded together, resulting in 768 strips of $\approx 12 \text{ cm}$ in length. A second pair of identical sensors is glued back-to-back with the first pair at a stereo angle of 40 mrad to provide hit reconstruction in two dimensions. Each module also has two arrays of six ABCD chips [101], where each chip is wire-bonded to 128 strips, in order to amplify, shape and discriminate pulses from the charges collected on the strips. A binary threshold of around 1 fC in the detected charge is used to define a 'hit' in the SCT. The SCT is designed to deliver a minimum of four 3D position measurements per track ensuring a precise measurements of track momenta, vertex position, and impact parameter with an accuracy of $17 \mu\text{m}$ in $R - \phi$ and

580 μm in z . Figure 2.13a illustrates the layout of the ATLAS detector, highlighting the SCT barrel and end-caps, and Figure 2.13b depicts a schematic view of one quadrant of the SCT.

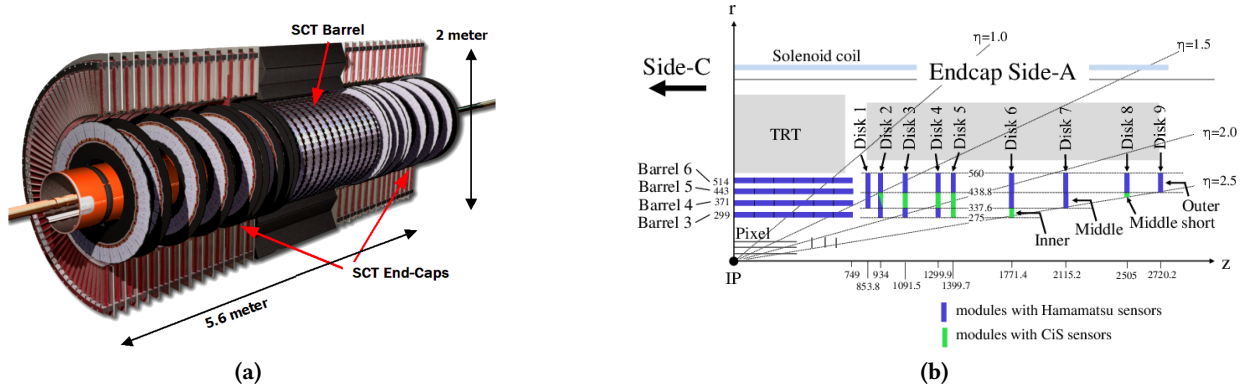


Figure 2.13: (a) Layout of the ATLAS Inner Detector with indications to the SCT barrel and end-caps. Figure sourced from [102]. (b) Schematic view of one quadrant of the SCT. The numbering schemes for the barrel layers and endcap disks are shown, along with the radial and longitudinal coordinates. The disks consist of up to three rings of modules, referred to as inner, middle, and outer, positioned at increasing radii from the beam pipe. The detector is symmetric between Side-A (positive z) and Side-C (negative z). Figure taken from [103].

2.2.4.4 The Transition Radiation Tracker (TRT)

The Transition Radiation Tracker (TRT) [104], the outermost of the three tracking subsystems of the ID, is a straw-tube tracker consisting of 300000 cylindrical drift tubes (straws) with a diameter of 4mm. In the barrel the straws are placed parallel to the beam-line and cover from 560 to 1080mm in radius and $|z| < 720\text{mm}$. The two endcaps where straws are arranged perpendicular to the beam-line cover $827 < |z| < 2774\text{mm}$ and $617 < r < 1106\text{mm}$. The TRT system provides $3 \approx 0$ space points with ≈ 130 micron resolution for charged tracks with $|\eta| < 2$ and $p_T > 0.5 \text{ GeV}/c$ [105].

Each straw in the TRT is equipped with a gold-plated anode wire and was originally filled with a gas mixture of Xe (70%), CO_2 (27%), and O_2 (3%) at the start of LHC and ATLAS operations. However, due to significant, irreparable gas leaks that developed in the gas system, the TRT detector is now flushed with a gas mixture primarily composed of Argon. When a charged particle passes through the tube, it ionizes the gas, causing the resulting electrons to drift towards the anode wire and cascade in the electric field, generating a detectable signal, which can be compared against two adjustable thresholds.

The TRT serves a dual purpose by contributing to the momentum measurement of charged particles and particle identification. The space between the straws is filled with polyethylene and a relativistic particle traversing the boundary between the two materials emits radiation (transition radiation), which depends on the Lorentz boost ($\gamma = E/mc^2$). This enables the determination of the particle mass for particles with the same momentum. The drift tubes measure the transition radiation photons by detecting the photoelectrons they generate, which are identified as characteristic large energy deposits. In the ATLAS detector, the TRT helps in distinguishing between electrons and pions with momenta ranging from 1 to 100 GeV. The TRT on average provide 30 two-dimensional space points with a resolution of 130 μm for charged particle tracks with $|\eta| < 2$ and $p_T > 0.5 \text{ GeV}$ thereby significantly enhancing the p_T resolution of the combined tracking system.

2.2.4.5 Tracking Resolution

Integrating all three components of the ID enables the reconstruction of a charged particle's track within the detector. The trajectory of a particle moving in a uniform magnetic field B can be described using five helix parameters $P = (d_0, z_0, \phi_0, \theta, q/p_T)$ [106] as depicted in Figure 2.14. Here, d_0 represents the transverse impact parameter, which is the closest approach of the particle's trajectory to the origin in the plane perpendicular to the magnetic field (typically the x - y plane), and it provides information about the particle's origin, useful in the identification of primary and secondary vertices. The parameter z_0 denotes the z -coordinate at this point of closest approach, indicating the height along the z -axis where the trajectory is nearest to the beam line, thus helping to understand the vertical displacement from the interaction point. The azimuthal angle ϕ_0 is the angle between the x -axis and the particle's trajectory in the transverse plane at the closest approach. The polar angle θ is the angle between the particle's momentum vector and the z -axis. Finally, q/p_T describes the curvature of the particle's path due to the magnetic field.

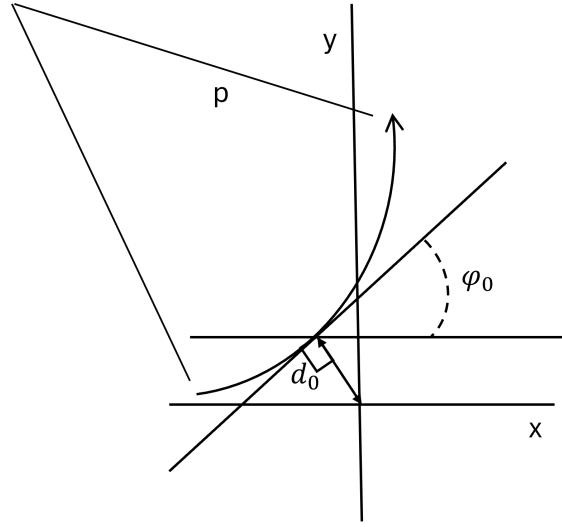


Figure 2.14: The helix parameters of a track moving through the bending plane of a uniform magnetic field. Adapted from [106].

The ID is designed to achieve a transverse impact parameter resolution given by [106] :

$$\sigma_{d_0} = \frac{140 \mu\text{m}}{p_T [\text{GeV}]} \oplus 10 \mu\text{m}$$

and a longitudinal impact parameter resolution of

$$\sigma_{z_0 \cdot \sin \theta} = \frac{209 \mu\text{m}}{p_T [\text{GeV}]} \oplus 91 \mu\text{m}$$

for the reconstructed tracks [106]. The particle's momentum is derived from the track's curvature, and the momentum resolution achieved by the ATLAS ID is approximately

$$\sigma \left(\frac{1}{p_T} \right) = A \oplus \frac{B}{p_T \sqrt{\sin \theta}} = \left(0.00036 \oplus \frac{0.0013}{p_T [\text{GeV}] \sqrt{\sin \theta}} \right) \text{GeV}^{-1},$$

where A represents the intrinsic error in the track parameters, B denotes the error due to multiple scattering, and $\oplus$ denotes addition in quadrature [106].

2.2.5 The Calorimeter

The calorimeter system, enveloping the ID and the 2T solenoid, covers the pseudorapidity range $|\eta| < 4.9$, is used to measure the energy of neutral and charged particles, missing transverse momentum for high- p_T particles that have close to straight trajectories in the ID. ATLAS employs sampling calorimeters, featuring multiple layers of both active and passive materials. The passive component typically consists of a dense material with a high atomic number, inducing cascades of particles known as showers while the active layers are responsible for measuring the energy deposited by these showers, using methods such as ionization or detection of scintillation light. Liquid Argon (LAr) serves as the primary active material in the ATLAS calorimeter [107]. When a particle crosses the LAr, an output signal proportional to its energy is created by the drift of ionization electrons under high voltage. Figure 2.15 illustrates the layout of the ATLAS calorimeter system.

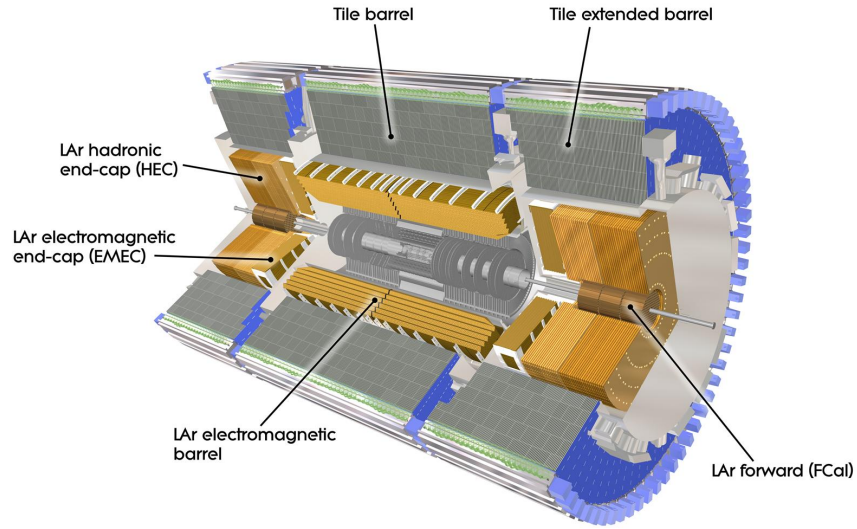


Figure 2.15: Cut-away view of the ATLAS calorimeter system that measures the energies and positions of charged and neutral particles through interleaved absorber and active layers out to $|\eta| < 4.9$ [43, 108].

2.2.5.1 The Electromagnetic Calorimeter (ECAL)

Within the region $|\eta| < 3.2$, the electromagnetic calorimeter (ECAL) [43, 109] is used to measure the energy deposited by electrons, photons, and jets using lead as the passive material and liquid argon as the active material. Electromagnetic showers, resulting from the electromagnetic interaction, are characterized by the radiation length (X_0), representing the average distance over which the energy of a high-energy electron diminishes to $1/e$ of its original value. The electromagnetic calorimeters in ATLAS are designed with a minimum depth equivalent to $22 X_0$. The ECAL is partitioned into a barrel ($|\eta| < 1.475$) and two end-caps ($1.35 < |\eta| < 3.2$) as illustrated in Figure 2.15. The width of the active LAr gaps is 2 mm in the barrel and ranges from 1.2 mm to 2.7 mm in the endcap. The calorimeter is segmented into three longitudinal layers for $|\eta| < 2.5$. The first layer, approximately $4-5 X_0$ thick, is finely segmented in the η direction to provide $\gamma - \pi^0$ separation and photon direction measurement, with a cell size of 0.003125 in the barrel region. The second layer, which collects most of the shower energy, has a granularity of $\Delta\eta \times \Delta\phi = 0.025 \times 0.025$ for $|\eta| < 2.5$. The final layer corrects for leakage behind the electromagnetic calorimeter. Together, these layers correspond to more than $22 X_0$ [110]. The barrel calorimeter is situated within barrel cryostats, enveloping the ID and accommodating the solenoid magnet. Meanwhile, two end-cap cryostats contain both the end-cap electromagnetic calorimeter and the end-cap hadronic calorime-

ter. In the region of $|\eta| < 1.8$, a pre-sampler detector is used to correct for the energy lost by electrons and photons upstream of the calorimeter. The pre-sampler consists of an active LAr layer of thickness 1.1 cm (0.5 cm) in the barrel (end-cap) region.

2.2.5.2 The Hadronic Calorimeter (HCAL)

Surrounding the ECAL, the hadronic calorimeter (HCAL) [43, 111] is used to measure the energy of hadronic showers. The hadronic counterpart to the electromagnetic radiation length, X_0 , is the hadronic interaction length, λ_I , which is characterized as the average distance between hadronic interactions and is usually significantly larger than the radiation length. The HCAL is divided into a barrel and two end-caps calorimeter covering $1.5 < \eta < 3.2$. The end-caps, positioned in the high radiation forward region, feature intrinsically radiation hard LAr as the active material, complemented by copper and tungsten serving as passive materials. In contrast, the barrel section features a scintillating tile calorimeter divided into a central barrel and two extended barrels. This sampling calorimeter is thicker compared to the ECAL, designed to cater the longer and wider hadronic showers compared to EM showers. The barrels are constructed with iron absorbers and polystyrene scintillators serving as the active material. The depth of the ATLAS hadronic calorimeters is $\approx 10\lambda_I$, providing good containment of the hadronic showers. The tile calorimeter has a granularity of $\Delta\eta \times \Delta\phi = 0.1 \times 0.1$.

2.2.5.3 The Forward Calorimeter (FCAL)

The ATLAS forward calorimeters (FCAL) [112] are located inside the endcap cryostats, along with the electromagnetic endcap calorimeter (EMEC) and the hadronic endcap calorimeter (HEC) (see Figure 2.15). The FCAL covers the very forward regions with a pseudorapidity range of $3.2 < \eta < 4.9$, an area characterized by exceptionally high radiation levels due to its proximity to the beam axis, where particle energies and densities are extremely high. The two main motivations for the FCAL are to enhance the reconstruction of missing E_T , which is crucial for many physics analyses such as SUSY searches, and to facilitate the identification and measurement of forward jets, including those produced in vector boson fusion processes [113]. The FCAL consists of three layers. The layer closest to the IP, FCAL1, is a Copper-LAr calorimeter designed for electromagnetic calorimetry. FCAL2 and FCAL3 are hadronic Tungsten-LAr calorimeters. Behind FCAL3, a passive layer of brass absorbs hadronic shower remnants that punch through. Figure 2.16 illustrates this arrangement.

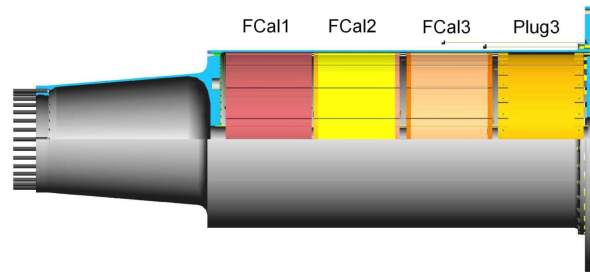


Figure 2.16: Cut-away view of the ATLAS forward calorimeter (FCAL). Particles from the IP first traverse the electromagnetic FCAL1 module (Cu/LAr-calorimeter), followed by the hadronic FCAL2 and FCAL3 modules (W/LAr-calorimeter). Figure taken from [113].

Originally, the FCALs were planned to be placed outside the endcaps, 15 m away from the IP. However, further studies favored the current placement inside the endcap cryostat, 5 m from the IP, for several reasons. This location provides a smooth transition from the other calorimeters, reducing energy losses and improving the reconstruction of jets, electrons, and missing E_T . Additionally, it

offers shielding for the muon system [113].

2.2.5.4 Energy Resolution of ATLAS Calorimetry Systems

The general parametrization of the energy resolution of a calorimeter is given by:

$$\frac{\sigma_E}{E} = \frac{a}{\sqrt{E}} \oplus \frac{b}{E} \oplus c \quad (2.2.9)$$

The first term, $\frac{a}{\sqrt{E}}$, is referred to as the stochastic term, capturing fluctuations associated with Poisson statistics, such as shower or sampling fluctuations. The second term $\frac{b}{E}$ represents the noise term, accounting for electronic noise in the detector readout. Lastly, the constant term c encompasses instrumental effects, including inefficiencies in signal collection. For the ATLAS ECAL, the typical energy resolution is given by $\frac{\sigma_E}{E} \approx \frac{10\%}{\sqrt{E}} \oplus 0.7\%$. In the case of HCAL, the energy resolution is comparatively worse due to the complexity of hadronic showers, and it is described by $\frac{\sigma_E}{E} \approx \frac{50\%}{\sqrt{E}} \oplus 3\%$ and the FCAL energy resolution is given by $\frac{\sigma_E}{E} \approx \frac{94\%}{\sqrt{E}} \oplus 7.5\%$. Here, E is measured in GeV [114].

2.2.6 The Muon Spectrometer (MS)

The Muon Spectrometer (MS) [115] constitutes the outermost layer of the ATLAS detector, serving as a high-resolution spectrometer with independent triggering and momentum measurement capabilities across a broad spectrum of transverse momentum, pseudorapidity, and azimuthal angle. Muon tracking is achieved by measuring the deflection of particles within a magnetic field produced by superconducting toroidal magnets featuring a magnetic field strength ranging from 2.0 to 6.0 Tm. As minimum ionizing particles, muons are not stopped within the calorimeter system, requiring a large detector to get tracking information. The muon system, as depicted in Figure 2.17 comprises four distinct gas detectors: Monitored Drift Tube chambers (MDT) [116], Cathode Strip Chambers (CSC) [117], Resistive Plate Chambers (RPC) [118], and Thin Gap Chambers (TGC) [119] to perform precision tracking and provide fast triggering information.

The MS comprises a barrel with three concentric, roughly cylindrical stations and two endcaps, each featuring three discs positioned perpendicular to the beam axis, known as inner, middle, and outer "wheels." Figure 2.17 illustrates the schematic of the MS, consisting of three stations of precision chambers, each comprising layers of MDTs, covering the region $|\eta| < 2.7$, except for the innermost station in the endcaps with $|\eta| < 1.3$, where the detectors used in Run 1 and Run 2 have been replaced with the New Small Wheels (NSWs) [120], detailed below. The muon trigger system spans the range $|\eta| < 2.4$, employing RPCs in the barrel and TGCs in the endcap regions.

The majority of the barrel detectors of the MS remain unchanged from the original Run 1 configuration described above. The Phase-1 upgrade of the ATLAS detector focussed on upgrading the inner wheels, often referred to as the "Small Wheels" within the barrel. Positioned between the calorimeters and the endcap toroid cryostats, within the barrel toroids, the Small Wheels have undergone a complete replacement with the New Small Wheels (NSW) occupying the same positions and offering tracking capabilities over the identical polar angle range, $1.3 < |\eta| < 2.7$. The NSWs employ two innovative gas detector technologies: micromegas (MM) [121] and small-strip thin-gap chambers (sTGC) [122] provide fast and precise muon-tracking capabilities. Furthermore, the NSWs allow for improved p_T resolution in the trigger and increased background rejection, allowing for a low muon p_T threshold and manageable Level-1 trigger rate, thus maintaining the acceptance for many interesting physics processes.

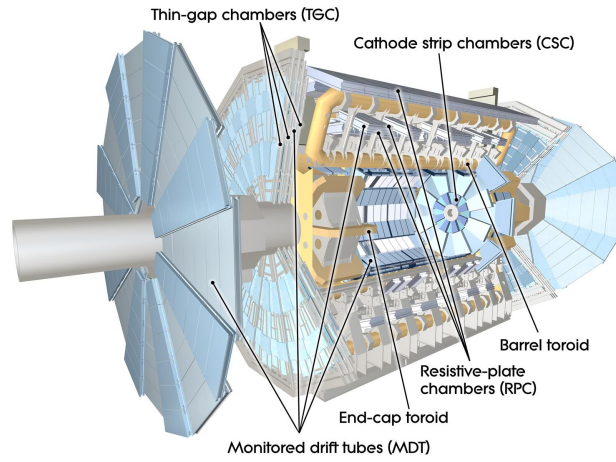


Figure 2.17: Cut-away view of the ATLAS Muon system before the installation of NSW (New Small Wheels) [123].

2.2.7 Trigger and Data Acquisition System (TDAQ)

The ATLAS detector is designed to monitor up to 1.7 billion proton-proton collisions per second, resulting in a combined data volume exceeding 60 million megabytes per second [124]. However, only a fraction of these events will contain interesting characteristics conducive to new discoveries. The ATLAS Trigger and Data Acquisition system [125] ensures optimal data-taking conditions and selects the most interesting collision events for further offline processing thereby reducing the rate of recorded data from the collision rate of 40 MHz to 1 kHz, a rate at which the data can be saved in permanent storage. The ATLAS TDAQ consists of a hardware-based Level-1 (L1) trigger and a software-based high-level trigger (HLT).

The L1 trigger employs coarse granularity information from the calorimeters and muon spectrometer to identify physics objects, such as high- p_T muons, electrons, photons, jets and large missing and total transverse energy, which can indicate interesting physics processes with Higgs bosons, vector bosons and top quarks. The decision to retain data from an event is made in less than $2.5 \mu\text{s}$ after the event's occurrence and throughout this period, the event data is temporarily stored in storage buffers. The L1 trigger effectively reduces the data rate to 100 kHz and selects the regions in $\eta - \phi$ space where the aforementioned interesting physics objects have been found, known as Regions of Interest (RoI), which are subsequently forwarded to the high level trigger (HLT), which has the capability to accept up to 10^5 events per second. The HLT reduces the trigger rate further down to 1 kHz by combining the RoI data with the complete detector information from all detector sub-systems and then performs a full offline like event reconstruction. Trigger algorithms are then employed to either select or reject the event and the selected events are further stored for offline physics analysis.

Silicon Tracking Detectors

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In modern particle physics experiments, tracking detectors (see Section 2.2.4) play a pivotal role in reconstructing the properties of particles resulting from collisions and elucidating the underlying interaction processes. Positioned closest to the IP, tracking detectors provide essential measurements for determining particle trajectories, which contain crucial information on particle properties, including momentum and charge. Furthermore, these tracking systems precisely determine the direction and origin of particles as well as the decay products of long-lived particles, facilitating the identification of those associated to a single interaction. This capability is essential in high-luminosity collider experiments like ATLAS, where hundreds of interactions occur within a single detector readout cycle and must be analyzed.

Semiconductor tracking detectors, primarily utilizing silicon sensors, are the preferred choice for the majority of current HEP experiments. Silicon sensors are solid-state ionization chambers, where incident charged particles generate electron-hole (e-h) pairs. The charge carriers drift towards the electrodes under the influence of an electric field, inducing current at the electrodes,

which is then amplified, shaped, and read out by the front-end (FE) electronics. Compared to gaseous tracking detectors, silicon's high material density ($\rho = 2.33\text{g/cm}^3$) and low mean ionization energy (3.6 eV) result in the generation of a large number of charge carriers. A Minimum Ionizing Particle (MIP) passing through a silicon sensor will, on average, generate ≈ 73 e-h pairs per micron of the silicon [126]. This results in a sufficiently large energy deposit of ≈ 22 keV in a typical sensor with a thickness of 300 μm . Additionally, the high charge carrier mobility ($\mu_e = 1350\text{cm}^2/\text{Vs}$, $\mu_h = 480\text{cm}^2/\text{Vs}$ at 300 K) in silicon resulting in a comparatively short collection time and fast readout, typically $\mathcal{O}(10\text{ ns})$ is particularly significant at the LHC, where the time between collisions is as low as 25 ns.

Silicon sensors achieve position sensitivity through the segmentation of the implants and electrodes. Design options include strip-like configurations, providing one-dimensional position measurement, or pixel-like arrangements, offering two coordinates for the point of incidence. Modern devices can achieve spatial resolutions of 10 μm or lower. The trajectory of the traversing particle is reconstructed by combining measurements from multiple detector layers.

The high particle flux typical of the radiation-rich environments in LHC experiments causes severe damage to the silicon sensor material. While silicon sensors at the ATLAS detectors are designed to withstand such high radiation fluxes, significant changes in the detector properties are observed.

This chapter offers a conceptual overview of the silicon tracking detectors utilized in the ATLAS detector. Given that tracking detectors are specifically designed for the detection of charged particles, the chapter begins with a discussion on the interaction of charged particles with matter, as elaborated in Section 3.1. Section 3.2 introduces the principles of silicon sensors, followed by an exploration of the basic macroscopic properties of silicon detectors in Section 3.3. A concise discussion on the front-end (FE) electronics for detector readout is provided in Section 3.4. Finally, Section 3.5 provides an overview of the effects of radiation damage, covering the physical processes of damage and resulting changes in detector properties. Extensive reviews on silicon detectors are available in the literature, such as [127–129].

3.1 Interaction of Charged Particles with Matter

The interaction of high energy particles with matter results in macroscopic effects such as the reduction of the particle's energy and the deflection of the primary particle. While the energy loss enables particle detection through tracking detectors, as discussed in subsequent sections, it also presents challenges in accurately measuring the particle's trajectory and momentum, further hindered by the deflection of particles as they traverse through matter.

This section offers an overview of the important effects associated with the passage of charged particles through matter. The interactions of neutral particles are not discussed herein. More comprehensive and detailed reviews of particle interactions with matter can be found in [25, 130], among others.

3.1.1 Interaction Processes

Charged particles interact with matter either by interacting with the nucleus of a nearby atom or by interacting with an electron in the atomic shell. The interaction cross-sections vary significantly depending on the charge, energy, mass of the particle and the type of material it traverses. The most dominant processes include Ionization and Excitation of atoms (Section 3.1.2.1), Bremsstrahlung (Section 3.1.2.2), and Multiple Coulomb Scattering (Section 3.1.2.3). Additional effects contributing to energy loss include inelastic scattering processes and pair production via virtual photons, particularly at very high energies. However, these effects are significantly weaker by orders of

magnitudes and are therefore disregarded in the following sections. Furthermore, highly energetic and heavy incident particles can cause substantial momentum transfers to the nucleus, resulting in significant damage to the detector material. The mechanisms and effects of this damage are discussed in detail in Section 3.5.

3.1.2 Energy Loss

The interaction processes mentioned in Section 3.1.1 result in statistical energy losses for the incident particle, with varying dependencies on momentum and material type. Figure 3.1a depicts the mean energy loss as a function of $\beta\gamma$ for a muon traversing copper, with $\beta = v/c$ and the relativistic Lorentz factor $\gamma = 1/\sqrt{1 - \beta^2}$. Figure 3.1b illustrates the energy losses from ionization, bremsstrahlung, and other scattering processes for electrons and positrons in lead, indicating that different processes dominate the energy loss at different energy regimes, a topic further discussed in the following sections.

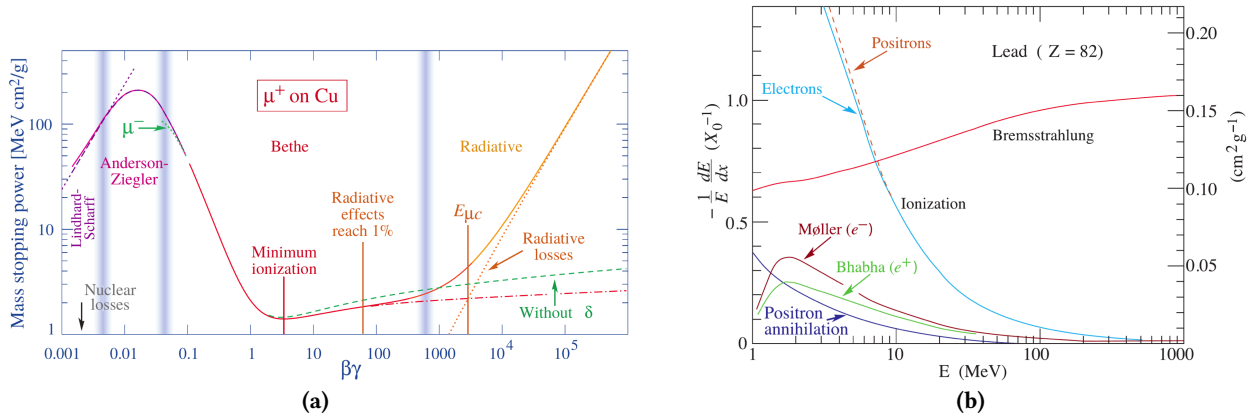


Figure 3.1: (a) Mass stopping power ($\langle dE/dx \rangle$) for positive muons in copper as a function of $\beta\gamma$. The central region is parametrized by the Bethe-Bloch formula. Particles near the minimum of the distribution, referred to as MIPs, are highlighted. Solid curves represent the total stopping power, with nuclear losses dominating at low energies and radiative losses dominating at higher energies (b) Energy loss in lead from various processes for electrons and positrons in the MeV range. The bremsstrahlung losses increase notably faster with rising energies compared to other processes. Figures taken from [25].

3.1.2.1 Ionization and Excitation

The incident high energetic particle can transfer a small amount of energy to an electron in the atomic shell through a scattering process, potentially resulting in either the excitation of the electron to a higher energy level or ionization, contingent upon the transferred energy. In the case of excitation, a radiative relaxation typically follows, resulting in the emission of low-energy photons through luminescence, while ionization, on the other hand, generates free charge carriers in the material and is the most significant process for particle detection.

The Bethe-Bloch formula describes the mean energy loss of heavy charged particles ($m > m_e$, where m_e corresponds to the mass of electron) due to ionization and excitation, over a wide range of velocities or momenta ($0.1 < \beta\gamma < 1000$), covering a significant portion of the regime relevant to HEP experiments. The mean energy loss per unit path length is given by:

$$\left\langle \frac{dE}{dX} \right\rangle = -Kz^2 \frac{Z}{A} \frac{1}{\beta^2} \left(\frac{1}{2} \ln \left(\frac{2m_e c^2 \gamma^2 \beta^2 T_{max}}{I} \right) - \beta^2 - \frac{\delta(\beta\gamma)}{2} - \frac{C}{Z} \right) \quad (3.1.1)$$

Here, K represents an aggregate constant typically expressed as $K = \frac{4\pi N_A e^2}{m_e c^2}$, with a value of approximately $0.307 \text{ MeV cm}^2/\text{g}$. z is the charge of the incident particle in electrons, Z and A denote the atomic and mass numbers of the absorbing material, respectively, $m_e c^2$ is the rest mass energy of the electron, I represents the mean excitation energy of the atoms, T_{max} denotes the maximum kinetic energy that can be transferred to an electron in a single collision, and δ describes density corrections to the energy loss due to polarization, which become pertinent at high energies. The final term, C/Z , accounts for shell corrections due to atomic binding energies, which become notably significant at lower energies. The resulting energy loss is denoted in units of $[dE/dX] = 1 \text{ MeV (g/cm}^2\text{)}$, given that the path dX is defined as surface density, where $dX = \rho \cdot dl$. Here, ρ represents the material density, and dl corresponds to the actual path length.

Figure 3.1a depicts the mean energy loss of a muon traversing through copper. At low energies, Equation 3.1.1 is predominantly governed by the term $1/\beta^2$, resulting in a decrease in stopping power as incident particle energy rises. As a particle's velocity approaches approximately $\beta \approx 0.96$ (corresponding to $\beta\gamma \approx 3.5$), a minimum is observed, as depicted in Figure 3.1a. At higher energies, the logarithmic term in Equation 3.1.1 leads to a gradual increase in the mean stopping power, which is counterbalanced by the density correction. Particles with mean energy loss rates close to the minimum of the Bethe-Bloch curve (see Figure 3.1a) are referred to as minimum ionizing particles (MIPs), as they lose only a minimal amount of kinetic energy while traversing the material. The average stopping power for a MIP in silicon is given by:

$$\left\langle \frac{dE}{dX} \right\rangle_{MIP} \approx -1.5 \frac{\text{MeV}}{\text{gcm}^2} \quad (3.1.2)$$

While the Bethe-Bloch equation gives the average energy loss of particles, the actual energy loss of a MIP traversing a material is probabilistic and can be described by Landau distributions, examples of which are shown in Figure 3.2 for different thicknesses of silicon. The Landau distribution [131] features a Gaussian-like shape at its core and a prominent long tail towards higher energy losses. The tail entries correspond to losses caused by delta electrons. These electrons, from the atomic shell, acquire significant momentum through interaction with the traversing particle. Consequently, the electrons can escape the crystal lattice, propagate through the material, and induce further ionization.

At LHC, hadrons and muons are typically MIPs with $\beta\gamma$ between 1 and 10. Consequently, the detector response is often characterized by the energy loss of MIPs, which provides a standardized reference for calibration and comparison. The electron energy deposition, however, is more complex due to their significantly larger $\beta\gamma$ values. As a result, the Bethe-Bloch equation in eq. (3.1.1) does not accurately describe their energy loss, given that processes such as Bremsstrahlung, introduced in Section 3.1.2.2, predominantly govern the energy loss of electrons.

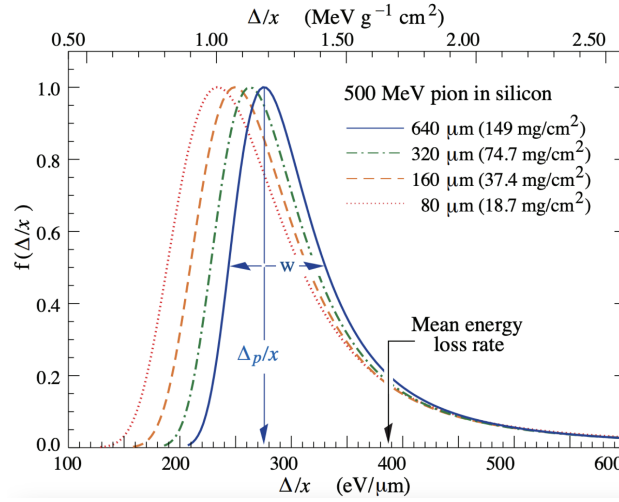


Figure 3.2: Landau distributions depicting the interaction of a 500 MeV pions with varying thicknesses of silicon, normalized to unity at the most probable value Δ_p/x . The width w is the full width at half maximum. Figure taken from [25].

3.1.2.2 Bremsstrahlung

Bremsstrahlung radiation is emitted when an incident charged particle undergoes acceleration, deceleration, or deflection due to interaction with the Coulomb field of another particle or atomic nuclei, resulting in energy loss via the emission of photons. The bremsstrahlung photons, characterized by significantly higher energy levels than those emitted during atomic relaxation after excitation, are the dominant source of energy loss at high energies as illustrated in Figure 3.1a.

The mean energy loss from bremsstrahlung can be determined by Equation 3.1.3:

$$\left\langle \frac{dE}{dX} \right\rangle_{MIP} = -\frac{E}{X_0} \quad (3.1.3)$$

The bremsstrahlung energy loss, as described in Equation 3.1.3, shows a linear dependence on the particle energy. Here X_0 is the material dependent radiation length, defined as the path length at which the incident particle retains a fraction of $1/e$ of its initial energy.

The intensity of bremsstrahlung radiation is directly proportional to the square of the atomic number of the target, the energy of the incident particle, and inversely proportional to the square of the particle mass. Consequently, lighter particles like electrons and positrons, when bombarding targets with high atomic numbers, are more effective in producing bremsstrahlung radiation compared to heavier particles. The total bremsstrahlung power for electrons and positrons is predominant already at energies above 10 MeV as depicted in Figure 3.1b.

3.1.2.3 Multiple Coulomb Scattering

In addition to the radiative effects, the interaction between the incident charged particles and the electric field of nuclei results in small deflections in the trajectory of the incident particle at each nucleus encountered. While traversing the sensor material medium, the particle undergoes numerous random deflections, cumulatively resulting in an effective deflection known as multiple coulomb scattering, as illustrated in Figure 3.3a. The probability for large deflections increases with the amount and density of material traversed.

The multiple scattering angle follows a distribution with Gaussian central core complemented by

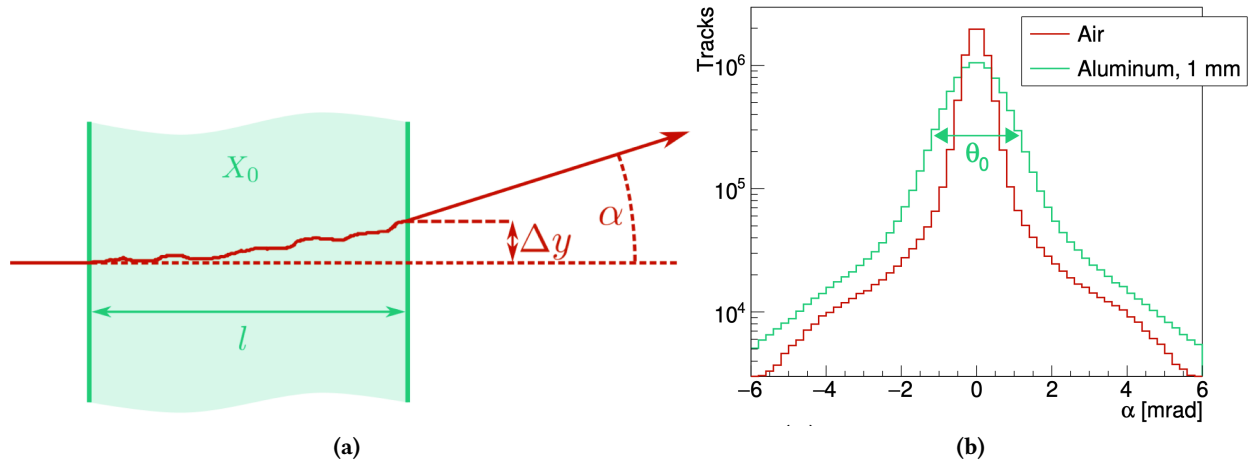


Figure 3.3: (a) Multiple Coulomb scattering of charged particles off atomic nuclei resulting in an effective deflection angle α and a lateral displacement Δy (b) The distribution of deflection angles with a Gaussian core and pronounced tails for an incidence positron at 2 GeV. Figures taken from [132].

more pronounced tails at larger angles as illustrated in Figure 3.3b with an RMS value given by Equation 3.1.4:

$$\theta_0 = \frac{13.6 \text{ MeV}}{\beta pc} z \sqrt{\frac{l}{X_0}} [1 + 0.038 \ln(\frac{l}{X_0})] \quad (3.1.4)$$

Here, l is the path length inside a material of the radiation length X_0 and p is the particle momentum. The particle deflection, as depicted in Figure 3.3a, results in a lateral displacement of the particle, similar to the deflection angle, and can be calculated as:

$$\sigma_y = \frac{l}{\sqrt{3}} \theta_0 \quad (3.1.5)$$

Multiple scattering significantly impacts the tracking performance of the detectors in HEP experiments, as the particle deflection deteriorates both spatial and momentum resolution. Consequently, the characteristics of this process are studied using high energy particles and the materials employed in the detectors, aiming to accurately model multiple scattering for the reconstruction and simulation of particle physics processes [133, 134].

3.2 Silicon Sensors for High Energy Physics

Semiconductor materials, with silicon notably standing out as the most prevalent in modern technology and widely utilized across various industrial sectors, play a pivotal role in HEP experiments at LHC. Silicon-based detectors are used in tracking systems due to their ability to provide fast and accurate positional information and energy resolution of a passing charged particle. The core of the current ATLAS ID (see Section ??)- the IBL, Pixel and SCT subsystems comprise silicon detectors while the new ATLAS ITk detector (see Section 5.4), presently under development for the high luminosity operations of the LHC, will feature an all-silicon tracker. The following section provides a brief introduction to the properties of semiconductors and outlines how silicon can be utilized in tracking detectors.

3.2.1 Properties of Semiconductors

Solid state materials are categorized into three distinct types—metals, semiconductors, and insulators—based on their electronic band structure. In isolated atoms, electrons occupy discrete energy levels within atomic shells, while within a crystal lattice, the atomic orbitals of the constituents overlap, forming continuous energy bands that encompass a wide range of possible energy levels for the electrons. Distinct gaps emerge between these energy bands, defining the forbidden energy levels for the electrons. This energy band model can be used to describe the electrical properties of the material.

The Fermi-Dirac distribution describes the probability of electrons occupying an energy level E and is given by:

$$f(E) = \frac{1}{e^{(E-E_F)/k_B T} + 1} \quad (3.2.1)$$

Here, k_B represents the Boltzmann constant, T denotes the absolute temperature, and E_F denotes the Fermi energy, at which the occupancy probability is :

$$f(E = E_F) = \frac{1}{2}$$

At $T = 0$ K, all energy states with $E \leq E_F$ ($E > E_F$) are occupied (empty), while at higher temperatures, some electrons occupy excited states above the Fermi energy. In the energy band model, the valence band represents the highest band completely filled with electrons at $T = 0$ K, while the next higher energy band, the conduction band, is only partially filled with electrons. The electrons can move freely within the crystal lattice due to the available energy states in the conduction band, thereby contributing to the material's conductivity.

The position of the valence and conduction bands, with respect to each other and to the Fermi level, determines a material's electrical properties. Figure 3.4 illustrates the three different band configurations for conductors, semiconductors, and insulators. A material is classified as a conductor if its Fermi energy lies within the conduction band or if there is an overlap between the valence and conduction bands. On the other hand, insulators feature a Fermi energy above the valence band, with an energy gap between the two bands too large for electron excitation, even at high temperatures. Semiconductor materials, at $T = 0$ K, behave like insulators with the Fermi level positioned above the valence band. The band gap (E_G) of these materials are significantly smaller than insulators, enabling the thermally excited electrons to transition to the conduction band. This thermal excitation results in free electrons in the conduction band and electron vacancies or holes in the valence band with a positive charge. These thermally excited electrons and holes are referred to as intrinsic charge carriers, and the pure material is termed an intrinsic semiconductor. The movement of electrons in the conduction band and holes in the valence band contribute to the electrical conduction in semiconductor materials.

The band gap size is a material-dependent parameter and significantly influences the material's properties. Silicon with a band gap of $E_G = 1.12$ eV at room temperature has an inherent low probability for thermal excitation. Nevertheless, an external excitation is possible with comparatively little energy, which is beneficial for detecting excitation caused by external energy deposits from traversing charged particles. An energy deposition of $\Delta E = 3.6$ eV is required to excite an electron from the valence band to the conduction band in silicon. The electron-hole pair creation energy in silicon is more than the band gap energy as additional momentum transfer to the lattice is required since silicon has an indirect band gap, with the valence and the conduction bands located at different wave vectors. For comparison, germanium, belonging to the 14th group of the periodic

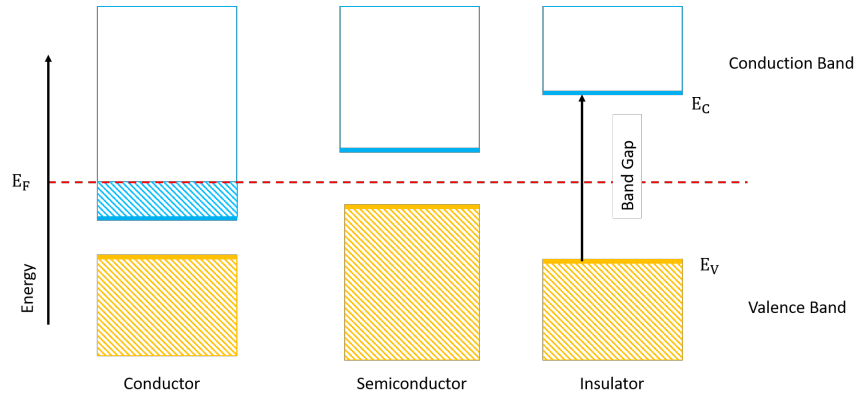


Figure 3.4: Fermi energy (E_F) and band configurations across conductors, semiconductors, and insulators in the energy band model. Conductors have Fermi energy within the conduction band, while semiconductors and insulators have it below. For electrical conductivity, electrons must occupy the conduction band, as shown by the hatched area in conductors. While conductors contain free charge carriers even at $T = 0$ K, in semiconductors, the small energy band gap between the valence and conduction bands allows electrons to transit via thermal excitation.

table like silicon, with a relatively smaller band gap of approximately $E_G = 0.66$ eV at room temperature, has a low mean ionization energy, rendering it suitable for spectrometers requiring high energy resolution. However, the small band gap also leads to a high density of free charge carriers at room temperature, necessitating cooling with liquid nitrogen to reduce thermal noise. Consequently, germanium detectors are impractical for tracking detectors, whereas silicon detectors can be effectively utilized at room temperature.

3.2.2 Extrinsic Semiconductors

Intrinsic semiconductors are seldom utilized in semiconductor device production due to their low electrical conductivity [135]. To enhance the conductivity, the properties of intrinsic semiconductors are modified by introducing artificial impurities into the lattice in a controlled manner. This process, known as doping, involves replacing silicon atoms with impurity elements. The impurity materials create additional energy levels within the band gap, altering the electrical conductivity.

Doping silicon (a group-IV element) with a group-V element, such as phosphorus, introduces an additional weakly bound valence electron. This extra electron occupies a discrete energy level known as the donor level (E_D), which is close to the conduction band, as illustrated in Figure 3.5. This loosely bound donor electron can easily be excited into the conduction band, while the phosphorus atom itself becomes a positively charged donor ion. This process is termed n-doping, resulting in the silicon being classified as n-type silicon, where electrons are the majority charge carriers. Similarly, shallow acceptor states (E_A), as depicted in Figure 3.5, are created by introducing a group-III element, such as boron, into the silicon crystal lattice. As boron has one fewer valence electron than the surrounding silicon atoms, it creates a vacancy, or "hole," in the valence band that can be occupied by valence band electrons. This process is referred to as p-doping, resulting in holes being the majority carriers, and the silicon is classified as p-type silicon.

A semiconductor is classified as extrinsic if the carrier concentration due to doping significantly surpasses the intrinsic carrier concentration of the undoped material. The intrinsic carrier concentration (n_i) is a fundamental property of a pure (undoped) semiconductor, defined as the number of charge carriers (electrons and holes) present at thermal equilibrium, and is given by :

$$n_i = \sqrt{N_c N_v} \exp\left(-\frac{E_g}{2kT}\right) \quad (3.2.2)$$

Here, N_c represents the effective density of states in the conduction band, N_v denotes the effective density of states in the valence band, E_g is the bandgap energy, k is the Boltzmann constant, and T is the absolute temperature. The intrinsic charge carrier concentration of silicon at room temperature is approximately $\mathcal{O}(10^{10})\text{cm}^{-3}$ while the extrinsic carrier concentration ranges from 10^{14} to 10^{19}cm^{-3} for typical doping levels.

In addition to doping bulk silicon material, precise implantations of p- or n-type can be produced, facilitating the introduction of segmentations into the silicon sensor material, as outlined in Section 3.2.5. Various doping technologies are commercially available, enabling the creation of diverse doping profiles and concentrations, thus allowing the sensor design to be tailored to different requirements.

Henceforth, implant dopings are designated as n+ and p+, highlighting their higher dopant concentration, while bulk doping is referred to as n and p, respectively.

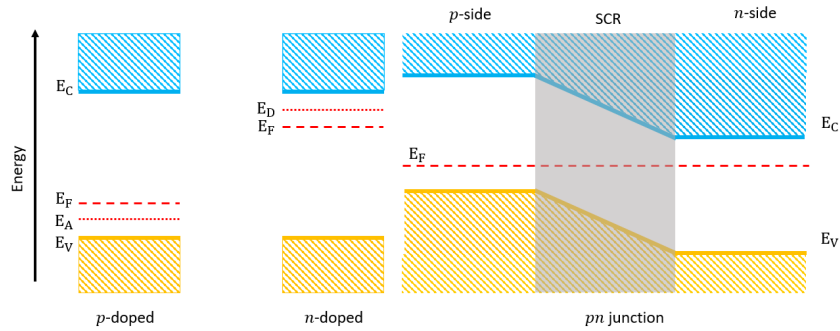


Figure 3.5: Band structure and energy levels of n-doped and p-doped silicon. Dopant-induced acceptor (E_A , left) and donor (E_D , center) energy levels modify the Fermi energy E_F of the material. Upon junction formation (right), a shared Fermi level emerges, leading to the creation of a space-charge region (SCR).

3.2.3 The pn-Junction

In intrinsic silicon with a thickness of $300\text{ }\mu\text{m}$, the number of free charge carriers is approximately 10^9 . In contrast, the expected signal from an incident charged particle is around 10^4 , as discussed in Section 3.3. To separate the signal from this noise contribution, reducing the number of free charge carriers is crucial, and this is achieved by combining p- and n-type silicon in a pn-junction and operating the junction in reverse bias mode. The subsequent sections present the analysis of a simplified 1D abrupt pn-junction model.

Figure 3.5 illustrates the isolated p- and n-type silicon materials with Fermi energies modified by the acceptor E_A and donor levels E_D as well as the joined pn-junction. By joining n-type and p-type silicon, a gradient of charge carrier concentration between the differently doped regions forms, resulting in free charge carriers drifting through the material via diffusion to level out the different Fermi energies. Since the donor and acceptor ions are immobile, an electric field builds up as the charge carriers diffuse, counteracting the diffusion process until an equilibrium is achieved. This results in a bending of the band structure, as depicted in Figure 3.5.

The charge carriers near the junction recombine with majority carriers of the opposite type, resulting in the formation of a space-charge region (SCR) devoid of free charge carriers, as illustrated in Figure 3.5. The SCR, while electrically neutral, comprises a negatively charged area at the p-doped side and a positively charged area on the n-doped side of the junction, with one side potentially having a significantly larger thickness depending on the relative doping concentrations. The electrostatic potential within the pn-junction termed the built-in voltage (U_{bi}), is determined by a twofold integration of Poisson's equation :

$$\frac{d^2\Phi}{dx^2} = -\frac{\rho(x)}{\epsilon_r\epsilon_0}, \quad (3.2.3)$$

where $\rho(x)$ represents the charge density and ϵ_0 and ϵ_r denotes the permittivities of vacuum and silicon, respectively. Integrating Equation 3.2.3 yields the electrostatic potential given by :

$$\Phi(x) = \begin{cases} -\frac{N_A}{2\epsilon_r\epsilon_0}(x + d_p)^2 & \text{for } -d_p < x < 0 \text{ (p-doped region)} \\ \frac{N_D}{2\epsilon_r\epsilon_0}(x - d_n)^2 & \text{for } 0 < x < d_n \text{ (n-doped region)} \end{cases} \quad (3.2.4)$$

Here, d_n and d_p denotes the thickness of the SCR in the n-doped and p-doped material, respectively. N_A and N_D represents the individual doping concentrations of acceptor and donor atoms, respectively. The built-in voltage between the boundaries of the SCR is calculated from Equation 3.2.4 as :

$$U_{bi} = \frac{1}{2\epsilon_r\epsilon_0} \cdot |N_{eff}|^2 \cdot d^2 \quad (3.2.5)$$

Here, $d = d_p + d_n$ is the total thickness of the depleted SCR and N_{eff} denotes the effective doping concentration, defined as :

$$N_{eff} = N_D - N_A \quad (3.2.6)$$

The width of the SCR varies with the external applied voltages U_{bias} and can be determined by inverting Equation 3.2.5. Subsequently, the thickness d can be derived from this calculation as :

$$d(U_{bias}) = \sqrt{\frac{2\epsilon_r\epsilon_0}{|N_{eff}|} \cdot (U_{bias} + U_{bi})} \quad (3.2.7)$$

The built-in voltage (U_{bi}) typically ranges in the range of 0.6 to 0.8 eV, resulting in an SCR spanning only a few microns. However, by applying an external voltage (U_{bias}), the thickness of the depleted region can be increased or decreased depending on the polarity of U_{bias} as indicated by Equation 3.2.7. A voltage that reduces the thickness of the SCR is referred to as forward bias, while the polarity that increases the thickness is termed reverse bias, representing the standard operational mode for semiconductor sensors.

3.2.4 Depletion Voltage, Capacitance, and Leakage Current

The voltage at which the entire sensor volume is depleted of free charge carriers, known as the depletion voltage U_{dep} , is obtained from Equation 3.2.7 by neglecting the small built-in voltage. Assuming the total sensor thickness is denoted by D , the full depletion voltage is given by :

$$U_{dep} = \frac{|N_{eff}| \cdot D^2}{2\epsilon_r\epsilon_0} \quad (3.2.8)$$

A silicon sensor biased in reverse can be described as a parallel plate capacitor with the capacitance depending upon the width of the SCR:

$$C \propto \frac{\epsilon_r \epsilon_0}{d(U_{bias})} \propto \begin{cases} \sqrt{\frac{\epsilon_r \epsilon_0 |N_{eff}|}{2 \cdot U_{bias}}} & \text{for } U_{bias} \leq U_{dep} \\ \frac{\epsilon_r \epsilon_0}{D} & \text{for } U_{bias} > U_{dep} \end{cases} \quad (3.2.9)$$

The proportionality in Equation 3.2.9 represents the surface area of the pn-junction. At full depletion, the bulk capacitance C is directly correlated with the sensor thickness, as illustrated by Equation 3.2.9. Hence, the capacitance can serve as a metric for determining the depletion voltage of the sensor. Once full depletion is attained, the capacitance ceases to increase with higher bias voltage, and the full depletion voltage U_{dep} can be determined from the kink point of the curve $\frac{1}{C^2}$ versus U_{bias} .

When the bias voltage exceeds U_{dep} , an additional electric field develops inside the silicon sensor. This field attracts thermally excited electrons in the conduction band toward the electrodes, effectively removing them from the sensor volume. This movement of charge carriers constitutes the leakage current (or reverse current), which can significantly impact the sensor's noise and power consumption. In an ideal pn-junction, the leakage current is primarily due to the diffusion of thermally generated charge carriers. However, in practical devices, impurities and radiation-induced defects (as discussed in Section 3.5) introduce additional energy levels close to the band gap center, which significantly increase the leakage current. Moreover, since the density of free charge carriers in the conduction band is temperature-dependent, the leakage current also scales with temperature. To estimate the leakage current at different temperatures, the current measured at temperature T_1 can be used to calculate the current at any other temperature T_2 using:

$$I(T_2) = I(T_1) \cdot \left(\frac{T_2}{T_1}\right)^2 e^{-\frac{E_{eff}}{2k_B} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)} \quad (3.2.10)$$

Here, E_{eff} is the effective band gap with a value of 1.21 eV in silicon [136]. Operating the sensor at lower temperature thus leads to a reduced leakage current.

3.2.5 Sensor Segmentation

The pn-junctions in silicon sensor designs for HEP applications, discussed in Section 3.2.4, typically feature a bulk with a typical thickness ranging from 50 μm to 500 μm , allowing for sufficient charge carrier generation, while the implant layer is typically only a few microns thick. The position of the traversing particle is measured by segmenting the implants on the top side into strips or pixels, creating multiple independent pn-junctions with the sensor bulk. The distance between the centers of the pixel or strip implants is referred to as the pitch. A fine segmentation allows for precise position measurement. Since each electrode is read out independently, the collected charge carriers, which drift towards the surface, can be accurately assigned to the specific volume where they were generated. This high precision in position measurement is crucial for accurately tracking the particle's traversal through the sensor.

Figure 3.6 depicts a typical n-in-p silicon sensor, featuring a p-type silicon bulk with n^+ implants at the sensor surface. The high doping concentration of the n^+ implants introduces a large number of free electrons, which is sufficient to neutralize the majority of holes in the p-type bulk, thereby depleting the bulk region of free charge carriers. The backplane is typically processed with a high doping concentration, in this case with p^+ doping, to confine the SCR. The electric field is highest at the transition region between the bulk and the implant within the pn-junction formed. Once the sensor is fully depleted, electrons drift to the implant side and are collected therein, while holes

drift towards the backplane. The implant side is additionally coated with a layer of silicon dioxide (SiO_2) for isolation between the pixels or strips, as shown in Figure 3.6. Metal pads in strip or pixelated form are further placed atop each implant to facilitate charge readout.

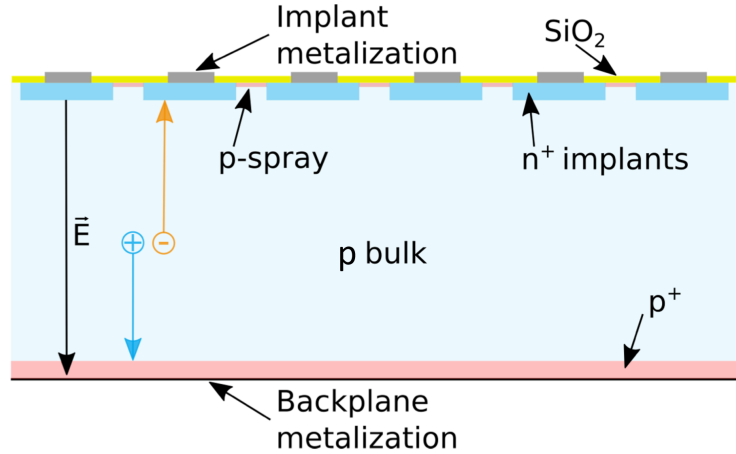


Figure 3.6: Visual representation depicting sensor segmentation aimed at achieving high-resolution estimation of particle traversal, exemplified here with n-in-p sensors. Adapted from [132]. This configuration is intended for use in the ATLAS ITk pixel detector.

In n-in-p technology, where n^+ doped implants are used for charge collection and the sensor is reverse-biased, positive ions can accumulate at the Si-SiO₂ interface. This accumulation may form a layer of electrons that bridges the gap between the n^+ implants and the surrounding material, effectively short-circuiting the n^+ implants and creating a conduction channel. Consequently, e-h pairs generated by a charged particle can spread across multiple pixels or strips, degrading spatial resolution. This issue can be mitigated using techniques such as p-spray, p-stop, or a combination of both. P-stop involves placing small p^+ implants between the n^+ implants, while p-spray adds a thin, homogeneous p^+ layer between the implants. These techniques create high electric field regions that repel electrons and prevent accumulation near the n^+ implants, thereby ensuring proper charge collection by directing the electric field towards the collecting electrodes. Additionally, guard ring implants (p^+ regions) at the sensor's edge help shape the electric field around the perimeter to prevent breakdowns caused by high electric fields near the edge, ensuring stability and uniformity across the entire sensor. The ATLAS ITk pixel modules utilize n-in-p technology for HL-LHC operations. Further details on the pixel modules employed in the ITk detector can be found in Section 5.4.

In hybrid silicon detectors (see Section 5.4.3.1), the signal processing electronics are housed on a separate readout chip, providing benefits such as the modular design of the sensor and readout and decoupling the readout electronics from the bias voltage, which can exceed 100V, thereby reducing the risk of damaging the electronics. However, routing the signal to the readout chip requires wire bonds for strip detectors and bump bonds for pixel detectors. Bump bonds are small solder balls that establish electrical connections between the sensor's metal layer and the readout chip. Alternative detector designs integrate the readout electronics into the sensor volume or silicon dioxide layer, as seen in monolithic active pixel sensors (MAPS) [137, 138], which are beyond the scope of this thesis.

3.3 Signal Formation

When a charged particle passes through a reverse-biased silicon sensor, it ionizes the silicon, generating charge carriers that drift in the electric field, producing a signal in the readout electrodes. This section provides an overview of the signal formation process in silicon detectors, including

the mechanisms of charge carrier generation and collection, parametrizations of carrier mobility, and an introduction to Lorentz drift. These topics are crucial for understanding the simulation of irradiated silicon sensors presented in this thesis.

3.3.1 Charge Carrier Generation

The passage of a high energetic charged particle through an active sensor volume leads to energy deposition, as discussed in Section 3.1, exciting electrons from the valence band to the conduction band, creating free charge carriers. With an ionization energy (E_e) of 3.6 eV in silicon, the number of electron-hole pairs created by a particle with energy loss E_{loss} is given by:

$$N_{eh} \approx \frac{E_{\text{loss}}}{E_e} \quad (3.3.1)$$

The mean energy loss for a MIP in silicon is approximately 3.8 MeV/cm (see Equation 3.1.2), resulting in a mean number of electron-hole pairs per unit length of around $10^2/\mu\text{m}$. The energy loss, however, follows a Landau distribution, depicted in Figure 3.2, with the MPV lower than the mean, yielding a most probable number of generated charge carriers of approximately $76/\mu\text{m}$. For typical silicon sensors with thicknesses ranging from tens to hundreds of micrometers, this results in $\mathcal{O}(10^4)$ charge carriers per traversing particle.

3.3.2 Charge Carrier Mobility

As a charged particle traverses the silicon sensors, it generates electron-hole pairs that drift under the influence of an electric field. The velocity of these ionization charges is determined by their mobility μ , which is expressed as:

$$\mu = \frac{v_D}{E} \quad (3.3.2)$$

Here, v_D is the drift velocity of the charge carriers and E is the electric field. The mobility of charge carriers in silicon depends on various operational parameters, including the electric field (as indicated by Equation 3.3.2), sensor temperature, and material properties such as crystal orientation. When the electric field strength is low, the charge carrier mobility is relatively constant and independent of the field. However, as the field strength increases, the mobility becomes inversely proportional to the electric field, causing the carrier velocity to approach a constant value, known as the saturation velocity (v_s). The critical electric field (E_c) marks the transition point between these two distinct regimes. Various parametrizations have been developed to model the charge carrier mobility in silicon detectors, using parameters derived from measurements in such detectors, and are used for interpreting drift property measurements as well as for simulating silicon detectors [132].

In the simulation studies presented in Section 6.2, the charge carrier mobility is parameterized using the Canali model [139]. The Canali parameterization, equivalent to the Jacoboni-Canali model [140] (the most widely used in Silicon, previously employed as the default mobility model in ATLAS Run 1 though with a slightly mis-transcribed electron mobility value), describes charge carrier mobility as a function of electric field E , with a corrected value for electron mobility. The charge carrier mobility is parameterized as:

$$\mu(E) = \frac{v_m}{E_c} \frac{1}{\left(1 + \left(\frac{E}{E_c}\right)^\beta\right)^{\frac{1}{\beta}}} \quad (3.3.3)$$

where v_m , E_c and β are phenomenological parameters, defined for electrons and holes respectively. The temperature dependence of these parameters is considered by scaling them relative to a reference parameter value:

$$A = A_{ref} \cdot T^\gamma \quad (3.3.4)$$

Here, A_{ref} is the reference parameter value, T is the temperature in Kelvin and γ is the temperature scaling parameter. The parameter values for electrons and holes are as follows:

$$\begin{aligned} v_{m,e} &= 1.43 \times 10^9 \text{ cm s}^{-1} \cdot T^{-0.87} \\ E_{c,e} &= 1.01 \text{ V cm}^{-1} \cdot T^{1.55} \\ \beta_e &= 2.57 \times 10^{-2} \cdot T^{0.66} \\ v_{m,h} &= 1.62 \times 10^8 \text{ cm s}^{-1} \cdot T^{-0.52} \\ E_{c,h} &= 1.24 \text{ V cm}^{-1} \cdot T^{1.68} \\ \beta_h &= 0.46 \times 10^{-2} \cdot T^{0.17} \end{aligned} \quad (3.3.5)$$

In Equation 3.3.5, $v_{m,e}$ represents the corrected electron velocity according to the Canali parameterization, while the values of all other parameters adhere to the Jacoboni-Canali model for charge carrier mobility in silicon.

3.3.3 Charge Carrier Collection

The charge carriers generated by the incident particle drift toward the sensor implants due to the applied electric field, inducing a signal on the readout electrodes, as discussed in Section 3.3. This induced signal is calculated using the Shockley-Ramo (SR) theorem [141, 142], which describes the current i induced on an electrode by a moving point charge q as follows:

$$i(t) = q \mathbf{v}_D \cdot \mathbf{E}_w(\mathbf{r}) \quad (3.3.6)$$

Here, $\mathbf{v}_D$ represents the instantaneous velocity vector of the charge q , and $\mathbf{E}_w(\mathbf{r})$ denotes the electric field at the position $\mathbf{r}$ of the charge q . This field $\mathbf{E}_w$, known as the Ramo field or weighting field, is computed under the conditions where the selected electrode is at unit potential, all other electrodes are at zero potential, and all other charges are removed. The total instantaneous current $I(t)$ is then determined by summing the induced currents from all such moving charges, and is given by :

$$I(t) = \sum i(t) = \sum q \mathbf{E}_w(\mathbf{r}) \cdot \mathbf{v}_D \quad (3.3.7)$$

The drift velocity, $\mathbf{v}_D$, of the charge carrier varies based on the position dependent electric field $\mathbf{E}$, leading to different velocities for carriers within the sensor based on their position and the mobility μ , differing for electrons and holes. The drift velocity is calculated as:

$$\mathbf{v}_D = q\mu(\mathbf{E})\mathbf{E}, \quad (3.3.8)$$

where q denotes the sign of the charge carriers. The mobility depends on the electric field, as indicated in Equation 3.3.8, and is further discussed in Section 3.3.2. The electron mobility is typically in the order of $10^3 \text{ cm}^2/\text{Vs}$ at moderate electric field strengths. For instance, with an example electric field of $|E| = 5 \text{ kV/cm}$, electron velocities reach around $|v_D| = 50 \text{ } \mu\text{m/ns}$. Consequently,

electrons take few nanoseconds to be collected in a silicon sensor with a thickness of a few hundred micrometers. Holes, however, exhibit significantly lower mobility, approximately one-third that of electrons, resulting in longer collection times and reduced currents. The fast charge collection makes silicon sensors well-suited for use as tracking detectors in particle physics. At the LHC, with a time interval of 25 ns between collisions, the signal can be completely read out, and the sensor can be cleared of charge carriers before the subsequent particle interaction generates new carriers.

A carrier completing its trajectory from the initial position $\mathbf{r}_i$ where it was generated, to the final electrode position $\mathbf{r}_f$ induces the total charge Q as dictated by the Ramo theorem :

$$Q = -q(V_w(\mathbf{r}_f) - V_w(\mathbf{r}_i)) \quad (3.3.9)$$

Here, $V_w(\mathbf{r})$ represents the weighting (or Ramo) potential evaluated at the position $\mathbf{r}$. The weighting field, as indicated in Equation 3.3.10, is the negative gradient of the weighting potential:

$$\mathbf{E}_w = -\nabla V_w \quad (3.3.10)$$

Charge carriers generated at position $\mathbf{r}_i$ and drifting towards the collecting electrodes may become trapped (see Section 3.5.3.3) before reaching the final electrode position $\mathbf{r}_f$. Despite not reaching the electrode, these trapped carriers still contribute to the induced signal. The charge Q induced on the electrode by a carrier that is trapped en route is determined using the formula in Equation 3.3.9. Both trapped electrons and holes lead to a reduction in the final signal amplitude. A detailed discussion on carrier trapping is provided in Section 3.5.3.3.

In addition to the directed drift of charge carriers toward the electrodes under the influence of an electric field, the carriers also undergo diffusion. Diffusion is a stochastic process characterized by the random, undirected movement of carriers, leading to the broadening of the charge cloud. The diffusion width, which quantifies this broadening, is defined as the mean square displacement of a charge carrier projected onto one dimension over a time interval t . This relationship is described by Einstein's diffusion equation [143]:

$$\sigma = \sqrt{2Dt} \quad (3.3.11)$$

with the diffusion constant, D , calculated from the sensor temperature T and the charge carrier mobility μ , defined as :

$$D = \frac{k_B T}{e} \mu \quad (3.3.12)$$

In silicon sensors with drift times on the order of nanoseconds, the diffusion length is typically a few micrometers, which is generally smaller than the pixel pitch used in HEP applications. Therefore, while diffusion contributes to the distribution of charge across pixels improving the estimation of the charge cloud's central position, it is primarily the drift that predominantly influences sensor performance and accuracy in position measurements.

The FE readout electronics (see Section 3.4) in silicon sensors typically integrate the induced current for each pixel to determine the collected charge Q . Ideally, all charge carriers generated would be collected at the electrodes. However, factors such as charge trapping (see Section 3.5.3.3) in silicon lattice impurities, electron-hole recombination, or charge trapping in regions of low electric field within the sensor bulk can lead to some generated charges not reaching the electrodes. The charge collection efficiency is defined as :

$$CCE = \frac{Q}{Q_i} \quad (3.3.13)$$

where Q_i represents the initial charge generated in the sensor by a passing high-energy charged particle. The CCE is a critical parameter for silicon sensors, as a low CCE can lead to deterioration of position resolution and hit detection efficiency. Therefore, the CCE of an irradiated planar sensor is carefully simulated and studied in Section 6.2.

In silicon sensors, the spatial resolution is a critical factor for determining the accuracy of particle position measurements. The resolution quantifies how well the detector can pinpoint the location of the charge carriers generated by an incident particle within its active volume. If a particle generates charge that is collected entirely within a single pixel, the most accurate estimate of the particle's position is the center of that pixel. The residual distribution describes the difference between the true position of the particle and the estimated position based on the pixel hit. When a particle hits a single pixel, the residuals from multiple events are distributed according to a box function, where the width of this function is equal to the pixel pitch d_x . The spatial resolution of the sensor is quantified by the root mean square (RMS) of this box distribution, calculated as:

$$\sigma = \frac{d_x}{\sqrt{12}} \quad (3.3.14)$$

Here, σ represents the spatial resolution of the sensor, and d_x is the pixel pitch. This equation reflects the spread of the charge cloud within a single pixel and serves as an important indicator of the sensor's ability to resolve the position of incident particles. When charge is collected by multiple pixels, forming a cluster, the particle position can be estimated more precisely by calculating the center of gravity of adjacent pixels that have registered charge. Charge sharing can occur through various mechanisms, including diffusion of charge carriers, inclined particle incidence generating charge carriers beneath multiple pixels or via Lorentz angle deflection (see Section 3.3.4).

3.3.4 Lorentz Angle

The charge carriers in silicon sensors drift along the electric field lines with minimal lateral displacement due to diffusion. In the presence of a non-parallel magnetic field, however, the charge carriers are deflected, resulting in an inclined drift path relative to the electric field lines. The drift velocity for a charge carrier under these conditions is estimated using [144]:

$$\mathbf{v}_D = \mu(E) \frac{q\mathbf{E} + \mu_H \mathbf{E} \times \mathbf{B} + q\mu_H^2 (\mathbf{E} \cdot \mathbf{B}) \mathbf{B}}{1 + \mu_H^2 |\mathbf{B}|^2} \quad (3.3.15)$$

Here, q represents the charge carrier's sign, while $\mathbf{E}$ and $\mathbf{B}$ denote the electric and magnetic field vectors, respectively. The Hall mobility μ_H , along with the Hall factor r_H , is defined as:

$$\mu_H = r_H \mu \quad (3.3.16)$$

The Lorentz angle, defined as the angle between the drift velocities with and without a magnetic field, when $\mathbf{B} \perp \mathbf{E}$, is given as:

$$\tan(\theta_L) = r_H \mu(E) B = \mu_H B \quad (3.3.17)$$

Figure 3.7a depicts the drift paths of electrons in a silicon sensor under a 2 T magnetic field perpendicular to a linear electric field, simulated using the Allpix-Squared simulation framework introduced in Section 6.2.2.2. The deflection caused by the Lorentz angle results in charge sharing, enhancing position resolution beyond single-pixel resolution (refer to Equation 3.3.14) as discussed in 3.3.3.

In an ideal setting with constant electric and magnetic fields across the sensor volume, absence of diffusion, and only one type of charge carrier contributing to the signal, the cluster size is exclusively dictated by geometric factors. Assuming normal incidence, the charge carriers generated by the incident particle drift towards the electrodes at the Lorentz angle θ_L , as defined in Equation 3.3.17. Charge carriers generated at the backside of the sensor experience the largest lateral drift Δx (where x is aligned with $\mathbf{E} \times \mathbf{B}$), extending the cluster from the endpoint of this drift to where the primary particle crosses the electrodes, as depicted in Figure 3.7a. Thus, the mean cluster size n_x can be calculated from drift angle θ_L , sensor thickness w , and pixel pitch d_x as :

$$\langle n_x \rangle \approx 1 + \frac{\Delta x}{d_x} = 1 + |\tan(\theta_L)| \frac{w}{d_x} \quad (3.3.18)$$

Equation 3.3.18 represents the average cluster size for numerous particles traversing the sensor at normal incidence randomly, resulting in a floating-point number, while the size of an individual cluster is always an integer value.

In the context of the simplified model outlined above, Equation 3.3.18 indicates that the Lorentz angle can be determined from the average cluster size. Figure 3.7b depicts the Allpix-Squared simulation of the mean transverse cluster size against the incident particle angle in a silicon sensor with an unirradiated detector, where the angle corresponding to the minimum cluster size provides the measurement of the Lorentz angle. The measured Lorentz angle from the simulation study is 0.265 rad.

There is often some confusion regarding the term "Lorentz angle." While it is inherently defined as the drift angle of charge carriers in silicon sensors, it's also commonly used to describe the angle formed by the average lateral drift distance of the charge carriers and the sensor thickness, as given by:

$$\tan(\theta_L) = \frac{\Delta x}{w} \quad (3.3.19)$$

In HEP experiments, the definition stemming from the lateral deflection in Equation 3.3.19 - a proxy for the average lorentz angle - is of greater interest, as it governs the charge sharing among multiple pixels and, consequently, the sensor resolution. Therefore, within the context of this thesis, the definition of the Lorentz angle aligns with Equation 3.3.19.

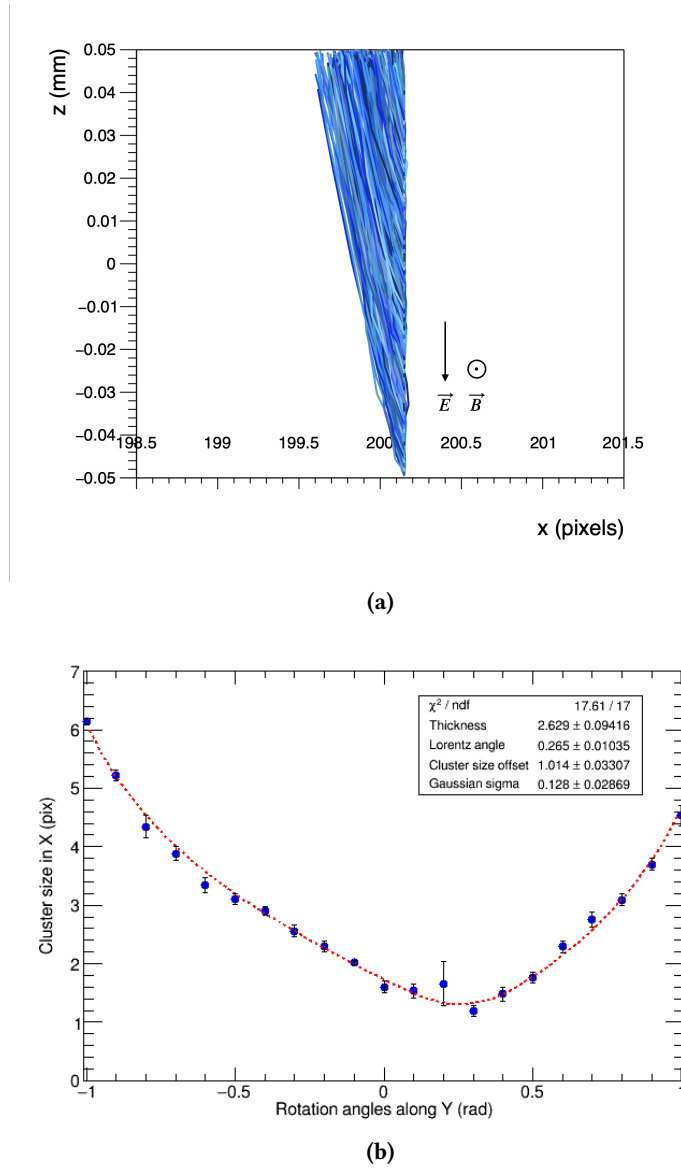


Figure 3.7: (a) Enhanced caption: Allpix-Squared simulation depicting electron drift within a silicon sensor for normal incident particles. The electric field varies linearly with sensor depth (z), while the magnetic field remains constant, aligned along the y -axis (b) Enhanced caption: Allpix-Squared simulation illustrating the mean transverse cluster size variation with rotation angle. The distribution is fitted using a convolution of Landau-Gaussian functions to determine the Lorentz angle, identified as the angle corresponding to the minimum cluster size.

3.4 Front-End (FE) Electronics and Detector Readout

The front-end (FE) electronics process the charge collected at individual pixel implants to extract hit information essential for particle tracking. In hybrid pixel detectors, the pixel implants are usually DC-coupled to the sensor readout pads, and bump bonds connect the pixel cells of the FE electronics to the sensor pads. Due to the high number of readout channels, zero suppression [145] becomes necessary to handle the limited readout bandwidth. Zero suppression is a technique used to improve data processing by eliminating signals below a certain threshold, which helps in discriminating signals from noise within the pixel cell electronics.

Figure 3.8 illustrates the typical building blocks of pixel detector FE electronics. The charge collected in the sensor is first directed to the preamplifier and the shaper circuits. Subsequently, the comparator discriminates between signal and noise for zero suppression. Typically, the threshold of the comparator is configurable, enabling adaptation for different signal-to-noise conditions and

helps mitigate aging effects such as radiation damage and reduced CCE in the sensor.

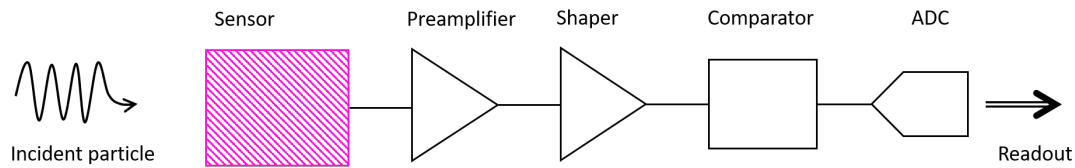


Figure 3.8: Typical elements of pixel front-end electronics: The induced signal by an incident particle in the sensor is amplified and shaped by the preamplifier and shaper. Signal discrimination by the comparator precedes digitization via the ADC for readout. Adapted from [129].

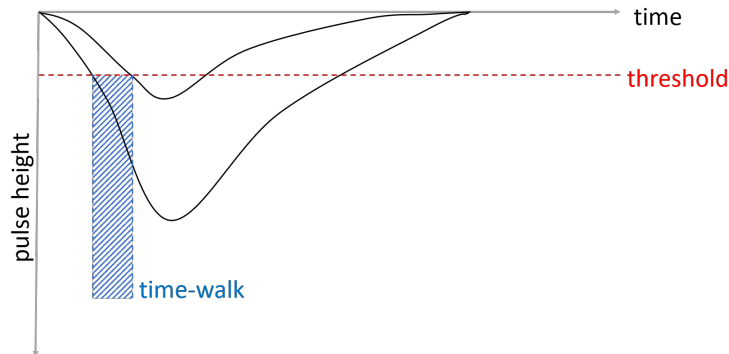


Figure 3.9: Time walk phenomena occur within the comparator, where smaller pulses reach the threshold later than larger ones. The discrepancy in sampling times defines the time walk characteristic of the comparator.

Two distinct thresholds can be defined: the absolute threshold, which defines the input charge signal with a 50% likelihood of firing the discriminator and triggering the comparator to read out the pixels, and the in-time threshold, denoting the minimum input signal that can be detected in the correct bunch crossing [146]. Small-amplitude signals are sensitive to the Time-Walk effects, a phenomenon that occurs when the time for preamplifier signals to cross a fixed threshold varies with pulse height as sketched in Figure 3.9. Lower pulse heights result in delayed signal crossing, leading to delayed hit detection by the pixel. Time-Walk is one of the limiting factors for the time resolution of the pixel chip. A parameter known as overdrive can be introduced, defined as the difference between the in-time and absolute thresholds. Section 6.1.4 extensively discusses Time-Walk effects and their implementation in the ATLAS software framework, Athena, to model the behavior of RD53—type readout chips (see Section 5.4.3.2) in MC simulations.

Once the input signal surpasses the charge threshold, it is encoded digitally by an Analog-to-Digital Converter (ADC) for digitization. The digitized charge data is then read out alongside the pixel address information and timing information. This readout mode is referred to as charge sensitive since it samples the entire pulse height of the signal, allowing for the utilization of additional information regarding charge sharing among neighboring pixel cells. For applications requiring fast timing, the binary mode can be selected, wherein only the information regarding the surpassed threshold is transmitted (hit or no-hit). This method is commonly employed in high-speed devices or FE electronics with extremely small pixel pitches that cannot accommodate the additional components required for buffering and pulse height sampling.

Random fluctuations in electric signals, known as electronic noise, poses a significant challenge for FE electronics, degrading the accuracy of pulse height sampling and, if substantial, may trigger noise hits by crossing the charge threshold, thereby limiting the minimum achievable threshold. Key sources of noise in FE electronics include stray capacitances from nearby electrical components and electronic noise from the amplification process. Therefore, it is crucial to carefully route supply voltage lines to improve the analog performance of the device [147].

Section 2.2.4.1 provides an overview of the FEI4 readout chip used in the existing ATLAS pixel detectors, while detailed discussions on the planned readout chip for the ATLAS ITk pixel detector is elaborated in Section 5.4.3.2.

3.5 Radiation Damage

Silicon detectors play a pivotal role in the modern HEP experiments. At hadron colliders, where collision rates and track densities are high, the ATLAS and CMS pixel detector layers closest to the IP can be exposed to a particle fluence of several 10^{11} per square centimeter per hour [128]. This high flux of particles causes damage to both the sensor and the electronics, altering the performance of the detector. Thus, it is vital to understand the mechanism of radiation damage and its impacts to accurately simulate charged particle interactions with the detector and reconstruct their trajectories, discussed further in Section 6.2. This section offers an overview of radiation damage mechanisms in silicon sensors and the impact on detector performances. Additional detailed information can be found in [148, 149].

3.5.1 Sensor Damage Mechanisms

The primary cause of sensor damage is the transfer of energy and momentum from highly energetic hadrons to the atoms within the sensor material. Radiation-induced effects are typically categorized into two types: bulk and surface damage. Bulk damage is caused by the displacement of crystal atoms, while surface damage includes all effects in the dielectrics and the interface region. The predominant surface effect is the rise in oxide charge, which saturates around several kilograys¹ to approximately 10^{12}cm^{-2} while bulk damage within the sensor results in an increase in leakage current, a change in operational voltage, and a reduction in signal amplitude.

Surface damage occurs due to ionization within the silicon dioxide layer. In this insulator layer, free-charge carriers tend to separate and drift under small electric fields, depending on the sensor configuration. As a result, a significant number of holes can become trapped near the SiO_2 -Si interface, leading to the formation of a negative space charge beneath the SiO_2 layer. This charge accumulation can impact inter-pixel capacitance and resistance, potentially affecting cross-talk between pixels and increasing noise levels. Surface damage studies are beyond the scope of this thesis and are not considered in the following sections. Comprehensive studies on surface damage effects can be found in [150, 151].

The bulk damage becomes significant at higher hadron fluences, typically in the range of 10^{14} - 10^{16}cm^{-2} , where highly energetic particles create various types of lattice defects in the sensor bulk, as illustrated in Figure 3.10a. When an incident particle transfers momentum to a silicon atom, it can dislodge the atom from the crystal lattice, creating what is known as a vacancy (V). This dislodged silicon atom, the primary knock-on atom (PKA), can propagate through the lattice, generating more defects if the momentum transfer is high. Alternatively, if the momentum transfer is low or at the end of its track, the PKA becomes trapped between lattice atoms, forming an interstitial (I); the interstitial and the vacancy (V) together constitute a Frenkel pair, as illustrated in Figure 3.10a. Additionally, dopant atoms or atoms from other parts of the sensor may become displaced, introducing impurities into the lattice structure or between lattice atoms. Common impurities include carbon (C) and oxygen (O) atoms, either naturally present in silicon due to manufacturing or intentionally added. Oxygen atoms can also form complexes, such as vacancy-oxygen (VO) complexes, or combine with other interstitials, like carbon atoms (CO), as depicted in Figure 3.10a.

¹The Gray (Gy) is a unit of absorbed radiation dose, defined as the absorption of one joule of ionizing radiation energy per kilogram of material, 1 Gy = 1 J/kg.

When a PKA acquires significant momentum, it is more prone to inducing numerous defects within a confined space, termed cluster defects. Conversely, isolated defects without neighboring defects are termed point defects. The predominant type and structure of bulk damage vary considerably based on the radiation type. Neutral particles, such as neutrons prevalent in the LHC environment induces a significant number of cluster defects due to nuclear interactions, imparting substantial momentum to the PKA. On the other hand, charged particles like pions and protons occasionally induce cluster defects but are more inclined to produce point defects. Neutrons with kinetic energies above 185 eV can create Frenkel pairs, while those exceeding 35 keV can generate clusters [149]. Figure 3.10b depicts MC simulation representing the recoil of an atom with a primary energy E_R of 50 keV, which is the average energy transferred to a lattice atom by a 1 MeV neutron [149].

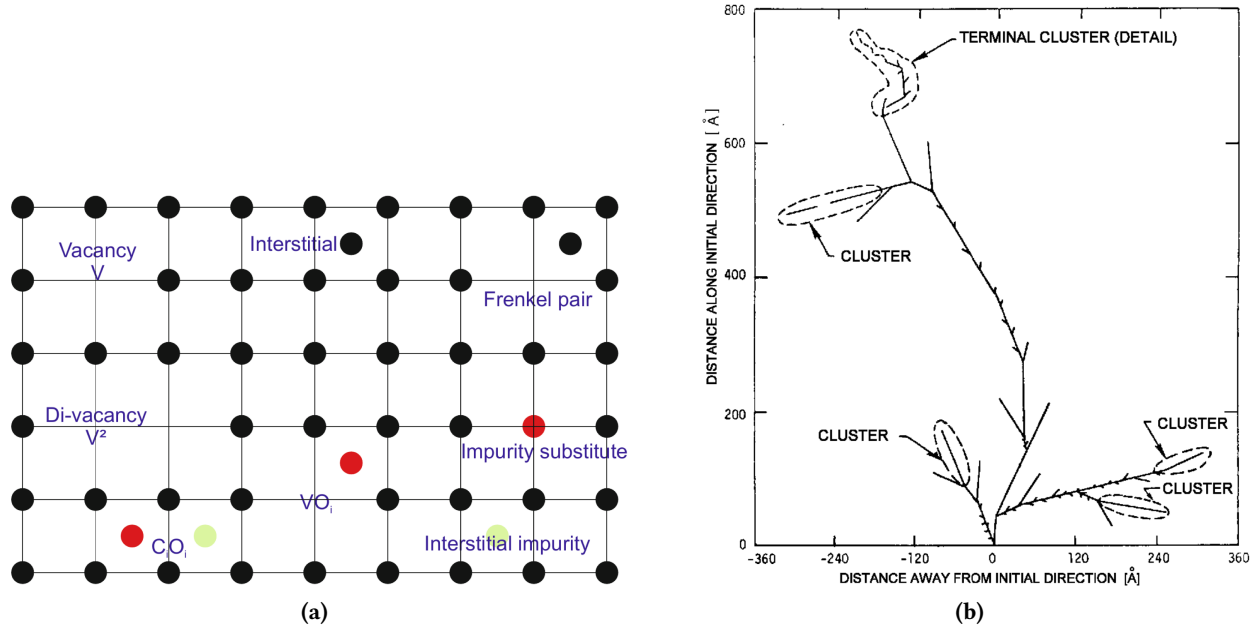


Figure 3.10: (a) Various lattice defects in silicon crystals created by the incident particle interactions. High momentum transfer can displace a nucleus from the lattice (vacancy), relocate it to a distant position between lattice atoms (interstitial), or position it near the original vacancy (Frenkel pair). Additionally, impurities from other sensor regions may be introduced into the silicon bulk, indicated by their chemical element symbols [128]. (b) Monte Carlo simulation of a recoil-atom track with a primary energy E_R of 50 keV. From [152].

3.5.2 The Non-Ionizing Energy Loss (NIEL) Scaling Hypothesis

The bulk damage in the silicon sensor depends upon the energy and type of primary particles involved in the irradiation process, as discussed in Section 3.5.1. Even though the behavior of charged particles differs from that of neutral particles, the main impacts of radiation damage, as described in Section 3.5.3, can be compared by normalizing the fluences the sensor receives. In HEP sensor development, the non-ionizing energy loss (NIEL) scaling hypothesis is widely used for this normalization. NIEL quantifies all the energy deposited in the crystal that has not been utilized for the fully reversible process of ionization.

According to the NIEL hypothesis, the fluence from irradiation with any particle type and energy is scaled to the fluence of 1 MeV neutrons, which causes equivalent damage. Damage functions $D(E)$ specific to each particle describe the displacement cross-section as a function of particle energy, as shown in Figure 3.11 for various particles and normalized to the value for 1 MeV neutrons. For an arbitrary particle type with a fluence spectrum $\phi_i(E)$, the hardness factor, a parameter used to compare the relative damage potential of different types of particles or radiation compared to a standard reference, usually neutrons with an energy of 1 MeV, is defined as:

$$k_i = \frac{\int D_i(E) \phi_i(E) dE}{D_n(E = 1 \text{ MeV}) \int \phi_i(E) dE} \quad (3.5.1)$$

Here, i denotes the particle type and D_n represents the damage function for neutrons. The hardness factor is used to convert the fluence of various types of radiation into a neutron equivalent fluence. For mono-energetic particle beam irradiation, Equation 3.5.1 simplifies to the ratio of the respective particle's damage function and the neutron damage function at 1 MeV:

$$k_{i,mono} = \frac{D_i(E)}{D_n(E = 1 \text{ MeV})} \quad (3.5.2)$$

This allows the total received particle fluence $\Phi_i = \int \phi_i(E) dE$ to be scaled to what is referred to as the neutron equivalent fluence using :

$$\Phi_{eq} = k_i \Phi_i \quad (3.5.3)$$

In this thesis, all fluences are expressed in units of 1 MeV neutron equivalent fluence, n_{eq}/cm^2 .

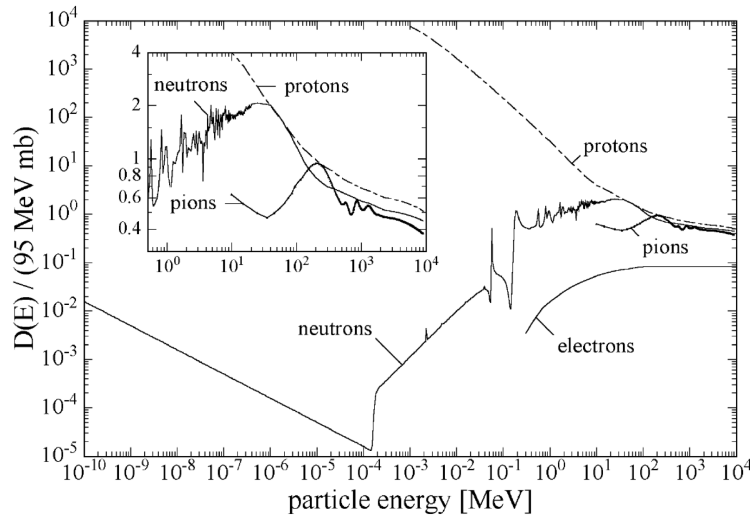


Figure 3.11: Damage functions $D(E)$ for various particles over a broad energy range, normalized to the value for 1 MeV neutrons. The inset provides a detailed view of the damage functions at energies above 1 MeV. Figure taken from [149].

3.5.3 Impact of Radiation Damage on Detector Performance

The primary defects created by irradiation, silicon vacancies and interstitials, can move within the crystal lattice, potentially undergoing annealing (see Section 3.5.3.4) when they meet and can interact with existing defects to form secondary point defects, which could have stable electrical properties different from the primary defects. These defects generate energy levels within the band gap, which are detectable through spectroscopic methods and can be charged, potentially impacting the space charge in the depletion zone depending on their energy level positions.

Various techniques have identified numerous defects that have a significant impact on silicon diodes. Some of these defects are charged at ambient temperatures, directly affecting the effective doping concentration N_{eff} . The electrical characteristics of these defects, such as energy level E_a and capture cross-section σ , are illustrated in Figure 3.12 [153].

Radiation-induced defects created through macroscopic mechanisms outlined in Section 3.5.1 significantly influence the macroscopic properties of silicon detectors. These defects function as generation centers, increasing leakage current, become charged, resulting in shifts in operational voltage, and act as trapping centers for fluences over $10^{14} n_{eq}/cm^2$, ultimately reducing the signal amplitude. The subsequent section presents an overview of the aforementioned macroscopic effects.

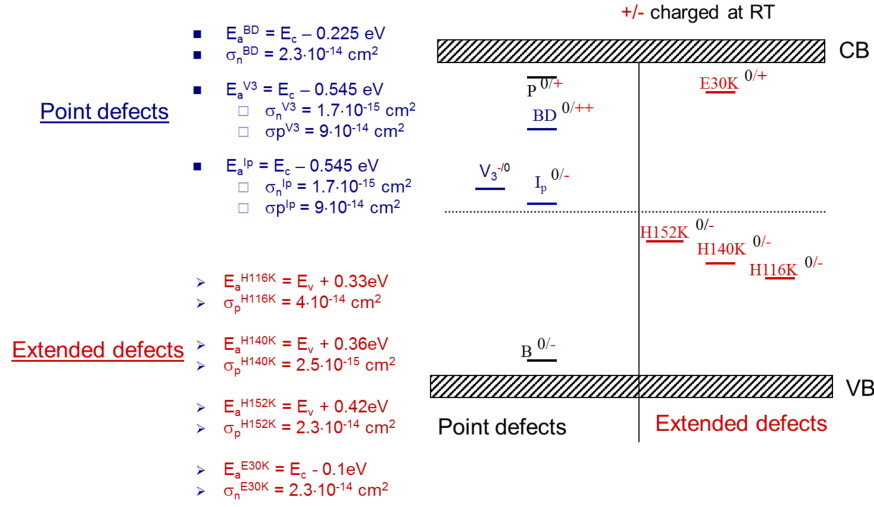


Figure 3.12: Radiation induced defects in silicon influencing the effective doping concentration N_{eff} and the leakage current. P (phosphorus) and B (boron) denote the doping impurities used to fabricate the silicon pn-junctions. CB and VB stand for conduction and valence bands, respectively [153].

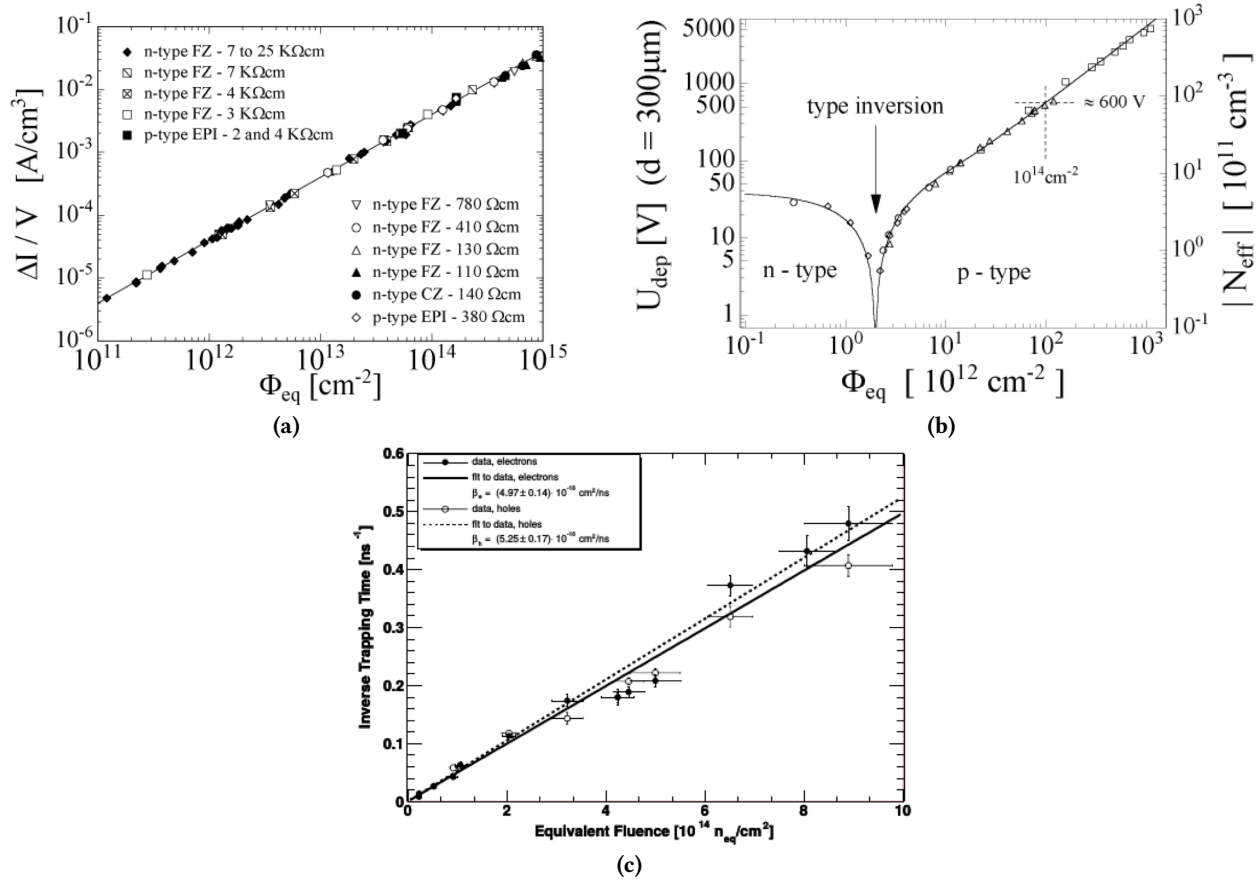


Figure 3.13: The dependency of various sensor properties on fluence. The leakage current (a) and trapping probability (c) exhibit a proportionate increase with fluence. For the effective space charge concentration and the depletion voltage in an initially n-doped sensor bulk (b), a type inversion to a p-type occurs, followed by an asymptotically linear increase. Images sourced from [149] (a,b) with data sourced from [154] (b), and [155] (c).

3.5.3.1 Leakage Current

The new energy levels within the band gap, resulting from crystal defects, act as generation-recombination centers, causing a reduction in the generation lifetime τ_g , and consequently, an increase in the leakage current I_{leak} within the volume. While at moderate fluences, this current remains below detection thresholds; it notably escalates detector power consumption. It has been observed that the leakage current has a linear dependence on the neutron equivalent fluence Φ_{eq} over a broad fluence range and particle type:

$$I_{\text{leak}}(\Phi_{eq}) = I_{\text{leak},0} + \alpha V \Phi_{eq} \quad (3.5.4)$$

Here, V represents the sensor volume, $I_{\text{leak},0}$ denotes the initial leakage current, and α is the proportionality constant, known as the current-related damage rate. It quantifies the rate of increase of leakage current ΔI per unit of fluence Φ and per unit of volume V :

$$\alpha = \frac{\Delta I}{V \Phi} \quad (3.5.5)$$

The typical value of α post-irradiation is on the order of 10^{-17} A/cm at 20 °C . Following a standard annealing duration of 80 minutes at a temperature of 60 °C, a measured value of $\alpha = (3.99 \pm 0.03) \times 10^{-17}$ A/cm is consistently observed across different sensor types at an operational temperature of 20 °C, as depicted in Figure 3.13a [149].

Equation 3.2.10 illustrates how leakage current scales with temperature. For unirradiated silicon sensors, the leakage current typically ranges from $\mathcal{O}(1 - 10)$ nA/cm² at 20 °C for sensors approximately 300 μm thick. In contrast, for irradiated sensors subjected to a fluence of about 10^{13} n_{eq}/cm² and with similar thickness, the leakage current can increase to the order of $\mathcal{O}(10 - 100)$ nA/cm². Coupled with high bias voltages, this leads to significant power dissipation and consequent heat generation. Excessive power dissipation and current increases at higher temperatures can trigger a thermal runaway effect. Thus, adequate cooling infrastructure is crucial for detectors operating in highly radiative environments. Figure 3.14 illustrates the distribution of leakage current at the end of Run 2 as a function of z , η and the radial distances for the silicon-based parts of the ATLAS inner detector.

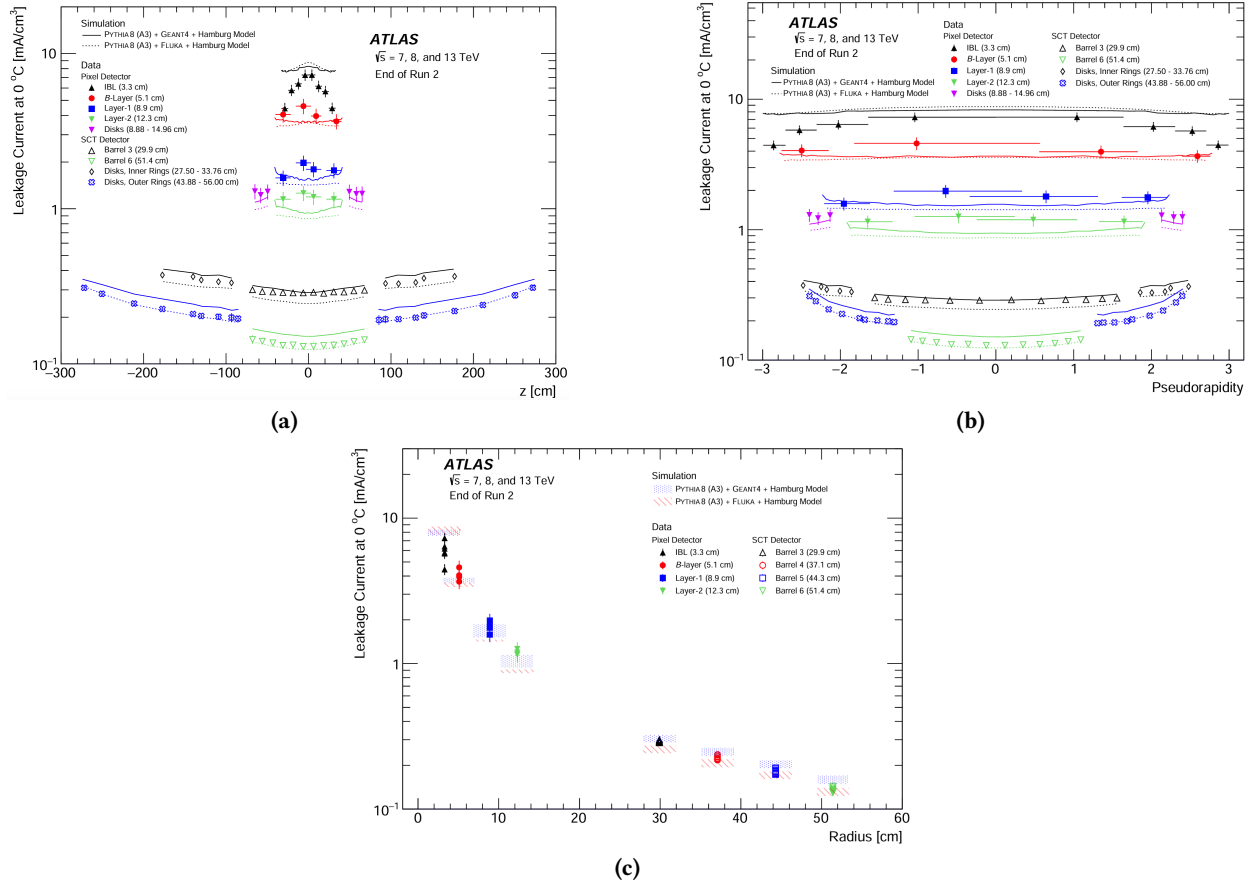


Figure 3.14: Leakage current at the end of Run 2 as a function of (a) z , (b) pseudorapidity η , and (c) radius for the silicon-based components of the ATLAS ID. The leakage current values are symmetric with respect to z and η by design. Radial positions, indicated in parentheses, correspond to the distances of the sensors from the geometric center of ATLAS. For the IBL, error bars primarily reflect the residual dependence of leakage current on high voltage beyond full depletion. For the outer pixel detector layers, uncertainties are mainly due to power supply variations, temperature fluctuations, and luminosity effects. For the SCT, uncertainties arise from sensor temperature variations, luminosity, and the RMS spread across modules. Note that uncertainties related to silicon damage factors, relevant for simulation and the Hamburg Model, are not included. Figures adapted from [156].

3.5.3.2 Operational Voltage Shifts

The radiation damage mechanisms presented in Section 3.5.1 result in changes in space charge, consequently altering the required operational voltage of detectors. Original dopants like Phosphorus or Boron may be trapped in new defect complexes, thus losing their original role in the doping process. These new defect complexes may have different charge states within the space-charge region from the original dopants [127]. The evolution of acceptors and donors with fluence can be explained by the removal of acceptors or donors via the formation of defect complexes containing acceptors/donors, and by creating acceptors and donors via forming defect complexes with positive/negative charge states in the space-charge region. Consequently, the effective doping concentration N_{eff} (Refer to Equation 3.2.6) is expected to vary accordingly with fluence :

$$N_{\text{eff}} = N_{d,0}e^{-c_d\Phi} - N_{a,0}e^{-c_a\Phi} + b_d\Phi - b_a\Phi \quad (3.5.6)$$

Here, $N_{d,0}$ and $N_{a,0}$ represent the donor and acceptor concentrations before irradiation, respectively, while c_d , c_a , b_d , and b_a are constants to be determined experimentally [127].

The depletion voltage of the sensor is determined by the absolute effective space charge concentration $|N_{\text{eff}}|$, as described in Equation 3.2.8. In Equation 3.5.6, N_{eff} is inherently negative for p-type

silicon due to an excess of acceptors, while it is positive for n-type silicon. Radiation-induced bulk defects primarily act as acceptors, increasing the absolute effective space charge concentration and, consequently, the depletion voltage in p-type silicon. However, in n-type silicon, $|N_{\text{eff}}|$ (refer to Equation 3.2.6) initially decreases until it reaches a point where the number of acceptor sites equals the number of donors in the semiconductor. Further irradiation then leads to a rise in $|N_{\text{eff}}|$ and thus the depletion voltage, causing the material to exhibit characteristics similar to p-type silicon — a phenomenon known as type inversion. This inversion typically occurs at a fluence of approximately $2 - 5 \times 10^{13} n_{\text{eq}}/\text{cm}^2$. For the current ATLAS n^+ -in-n pixel sensors, type inversion has already been observed at around $3 \times 10^{13} n_{\text{eq}}/\text{cm}^2$. The evolution of the depletion voltage for a sensor initially comprising n-type bulk material is depicted in Figure 3.13b, with the right axis showing the corresponding $|N_{\text{eff}}|$ determined via Equation 3.2.8.

Once the fluence required for type inversion is reached (a threshold quickly achieved in pixel detectors at the LHC), the depletion voltage increases almost proportionally with fluence as illustrated in Figure 3.15. The depletion voltage can quickly escalate to several hundreds of volts and as long as a bias voltage can be supplied to accommodate the escalating depletion voltage and the sensor remains fully depleted, it continues to function effectively. However, the bias voltage is constrained by the sensor's breakdown voltage².

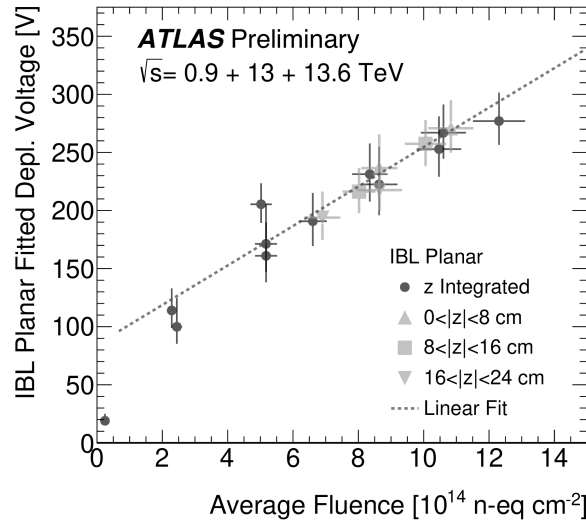


Figure 3.15: Depletion voltage fitted values for IBL planar sensors as a function of average fluence. The data are extracted from cluster charge fits versus applied bias voltage in dedicated high-voltage scans, typically conducted at the beginning and end of each annual run from 2016 to 2023. The black filled points represent results from fits on data integrated along the entire length of the IBL modules (longitudinal coordinate z). These are compared to data collected at the end of the 2018 and 2022 runs, with integrated luminosities of 154 fb^{-1} and 194 fb^{-1} , respectively, shown by the grey triangles and squares for three symmetric sections in z . These sections correspond to varying average fluence values received by the IBL sensors. The dotted line represents a linear fit across the range of fluence values, indicating that the depletion voltage scales linearly with fluence after accounting for the non-linear effects observed due to silicon type inversion. Figure taken from [157].

Additionally, in the current ATLAS pixel detector, with n^+ -in-n pixel sensors, an initial pn-junction forms between the n-type bulk and the p^+ backplane. This causes the depletion region to grow from the backside, where the pixels are interconnected until the entire bulk is depleted, as depicted in Figure 3.16a. When type inversion occurs, the pn-junction shifts to the pixel side (n^+), isolating the pixels and allowing operation even if the bulk cannot be fully depleted, as shown in Figure 3.16b. This spatial shift of the pn-junction toward the n^+ implants creates an electric field from the implant side, which is advantageous for this type of sensor as the highest electric field is present at

²The breakdown voltage of a silicon sensor is the voltage at which the electric field becomes strong enough to cause a sudden increase in current due to avalanche breakdown. This voltage can be affected by radiation damage, which increases the sensor's leakage current and reduces its breakdown voltage over time.

the junction (close to the implants). Thus, with an under-depleted sensor, no undepleted region is situated at the implants, preventing the collection of electrons. Furthermore, the new ITk pixel detector employs n^+ -in-p sensors, as the p-bulk does not experience type inversion at high irradiation doses, thereby enabling prolonged operation of the detector under the demanding conditions of the HL-LHC, particularly in the inner layers of the ITk detector. A comprehensive discussion on the ITk pixel detector is provided in Section 5.4.

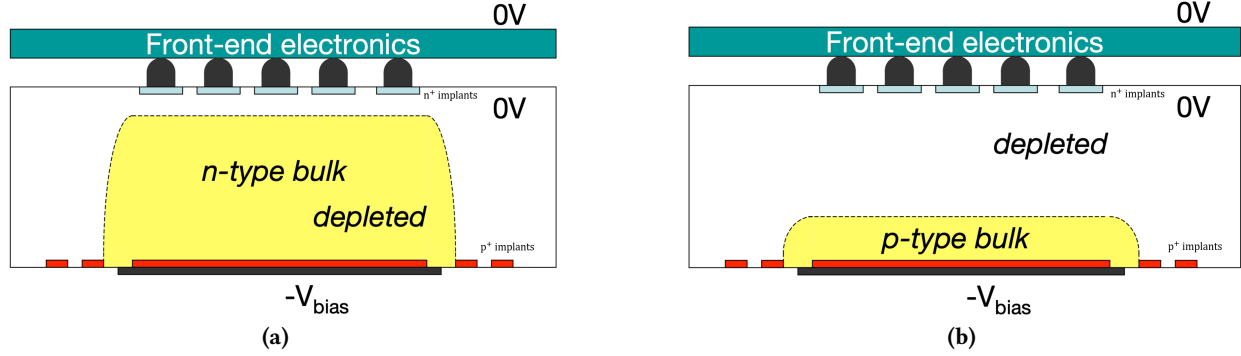


Figure 3.16: Comparison of depletion zones in n^+ -in-n pixel sensors before (a) and after (b) type inversion. Before type inversion the electrical field grows from the backside and reaches the pixel implants at full depletion. After type inversion the depletion zone grows from the pixel side and allows operation even if the bulk is not fully depleted.

Figures taken from [158]

The modified effective space charge concentration due to irradiation (see Equation 3.5.6) also leads to a deviation from the linear electric field profile observed in unirradiated sensors. Experimental measurements and simulations indicate a double-junction model, characterized by two peaks in the electric field profile as a function of the sensor depth [159–161]. The double-peak phenomenon (see Figure 3.17) can be qualitatively explained by defects being populated by carriers drifting under reverse bias voltage. In an n^+ -in-p detector, electrons move towards the n^+ implants under reverse bias, while holes move towards the p^+ backside. Consequently, the probability of encountering a negatively charged defect near the n^+ electrode is higher than that of encountering a positively charged one; conversely, the opposite is true for defects near the p^+ electrode. The resulting altered electric field significantly influences charge carrier drift and charge collection, a topic extensively examined in Section 6.2.

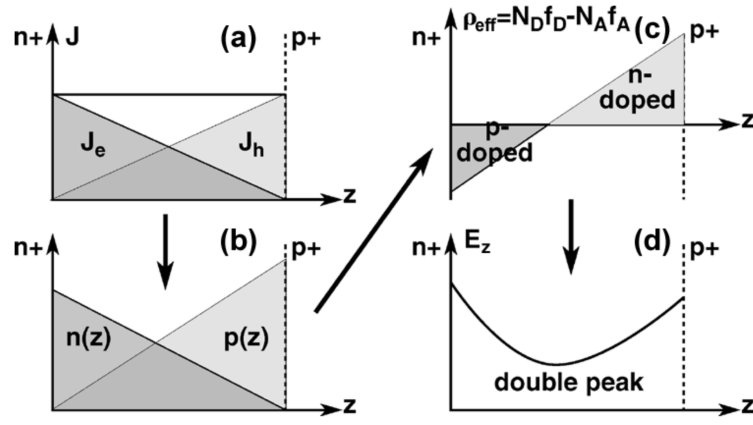


Figure 3.17: A schematic explanation of the double peak formation in an electric field for a reverse biased irradiated device. (a) Uniform current density in reverse-biased junction. Holes flow to backplane, increasing density from n^+ implant. Electrons move to n^+ implant, increasing the current density as distance decreases (b) Distribution of carrier densities across the junction (c) The trapping of the mobile carriers produces a net positive space charge density near the backplane and a net negative space charge density near the implant. Positive space charge corresponds to n-type doping and negative space charge corresponds to p-type doping resulting in the formation of p-n junctions at both sides of the detector (d) The resulting z -component of electric field from simultaneous solution of Poisson's and the continuity equations [159].

3.5.3.3 Trapping

Radiation-induced defects in the sensor bulk act as trapping centers within the energy band gap. The drifting electrons and holes generated by high-energy charged particles within the active sensor volume can transition from the conduction and valence bands into these energy levels within the band gap. These trapping sites temporarily trap the charge carriers before releasing them. If the de-trapping time surpasses the integration time (usually tens of nanoseconds), the trapped charges cease to contribute to the induced signal after being trapped, thereby reducing the collected signal in the detector.

The distance a charge carrier drifts before being trapped, L_{drift} , equals the effective trapping time, τ_{eff} , multiplied by the drift velocity, v_{drift} , as expressed in Equation 3.5.7 :

$$L_{drift} = \tau_{eff} v_{drift} \quad (3.5.7)$$

The charge capture probability is determined by the inverse of the effective trapping time constant, τ_{eff} , and is directly proportional to the irradiation fluence, Φ_{eq} , as expressed by Equation 3.5.8 and illustrated in Figure 3.13c.

$$\frac{1}{\tau_{eff}} = \beta \Phi_{eq} \quad (3.5.8)$$

Here, β is denoted as the trapping-related damage constant, which varies based on the type of charge carrier and the particle type (neutron or charged hadrons) used for irradiation [162]. The measured β values range between $4 - 6 \times 10^{-16} \text{ cm}^2/\text{ns}$ for electrons and $6 - 8 \times 10^{-16} \text{ cm}^2/\text{ns}$ for holes [162]. Larger β values for holes compared to electrons indicate more severe trapping for holes. Moreover, with the hole mobility approximately one-third of electron mobility, holes move slower and are more prone to trapping. Consequently, modern silicon detectors featuring n-in-n and n-in-p sensor configurations that collect electrons are favored over configurations that collect holes, like p-in-n.

The trapping probability allows conclusions to be drawn regarding the number of trapped charge

carriers over the collection time τ_c , and consequently, about the resulting collected charge Q , which can also be expressed as a function of irradiation fluence, as shown by Equation 3.5.9 :

$$Q(\Phi_{eq}) \approx Q_0 e^{\frac{-t_c}{\tau_{eff}}} = Q_0 e^{-t_c \beta \Phi_{eq}} \quad (3.5.9)$$

Here, Q_0 represents the full collected charge, i.e., the signal before irradiation. At fluences exceeding $10^{15} n_{eq} cm^2$, the trapping time reduces to less than 2 ns in the saturation regime of carrier velocity, indicating that the drift distance L_{drift} is less than 200 μm , which aligns with the typical thickness of a pixel sensor in the current ATLAS detector. Consequently, trapping is the primary factor limiting the Charge Collection Efficiency (CCE, see Equation 3.3.13) at the HL-LHC due to radiation damage, and it is extensively examined in Section 6.2.

3.5.3.4 Annealing of Defects

Radiation defects introduced in silicon bulk are not stable in time, as they can freely traverse the lattice, interacting with other defects or impurities, leading to recombination or the formation of new defect structures in the bulk. These processes alter the electrical properties of the bulk and consequently impact the macroscopic properties mentioned in Section 3.5.3; this phenomenon is referred to as annealing. At temperatures below 0°, annealing effects are minimal and typically negligible. At room temperature, annealing progresses slowly and may continue over the course of several years. However, at elevated temperatures, the annealing process accelerates significantly. The annealing process has the following impact on the aforementioned properties, as empirically observed in [149, 162]:

Annealing results in a decrease in the leakage current. The variation of current-related damage rate (α , see Equation 3.5.4) over time for various annealing temperatures is depicted in Figure 3.18a, illustrating ongoing changes lasting up to approximately a year at around room temperature.

The effective space charge concentration, N_{eff} , varies over annealing time, as shown in Figure 3.18b for an annealing temperature of 60°. The distribution is modeled as a combination of a constant and two exponential functions, all dependent on fluence. Unlike the leakage current, the distribution of N_{eff} displays two phases with opposite slopes: an initial decrease, leading to a reduction in the depletion voltage (see Equation 3.2.8), known as short-term or beneficial annealing followed by a rapid increase termed reverse annealing.

The trapping time constants for the charge carriers, described in Equation 3.5.8, are found to be influenced by annealing time, as depicted in Figure 3.18c at an annealing temperature of 60°. The distribution illustrates that the trapping probability increases for holes and decreases for electrons for annealing durations of up to 200 hours.

The results indicate that annealing initially enhances the performance of silicon sensors post-irradiation, leading to reduced leakage current, lower depletion voltage, and decreased trapping probability for electrons. This effect persists throughout the entire beneficial annealing phase and is utilized in high-energy physics detectors by allowing the detector to warm up to room temperature over several days. Monitoring this process closely is essential to prevent entering the reverse annealing regime [132].

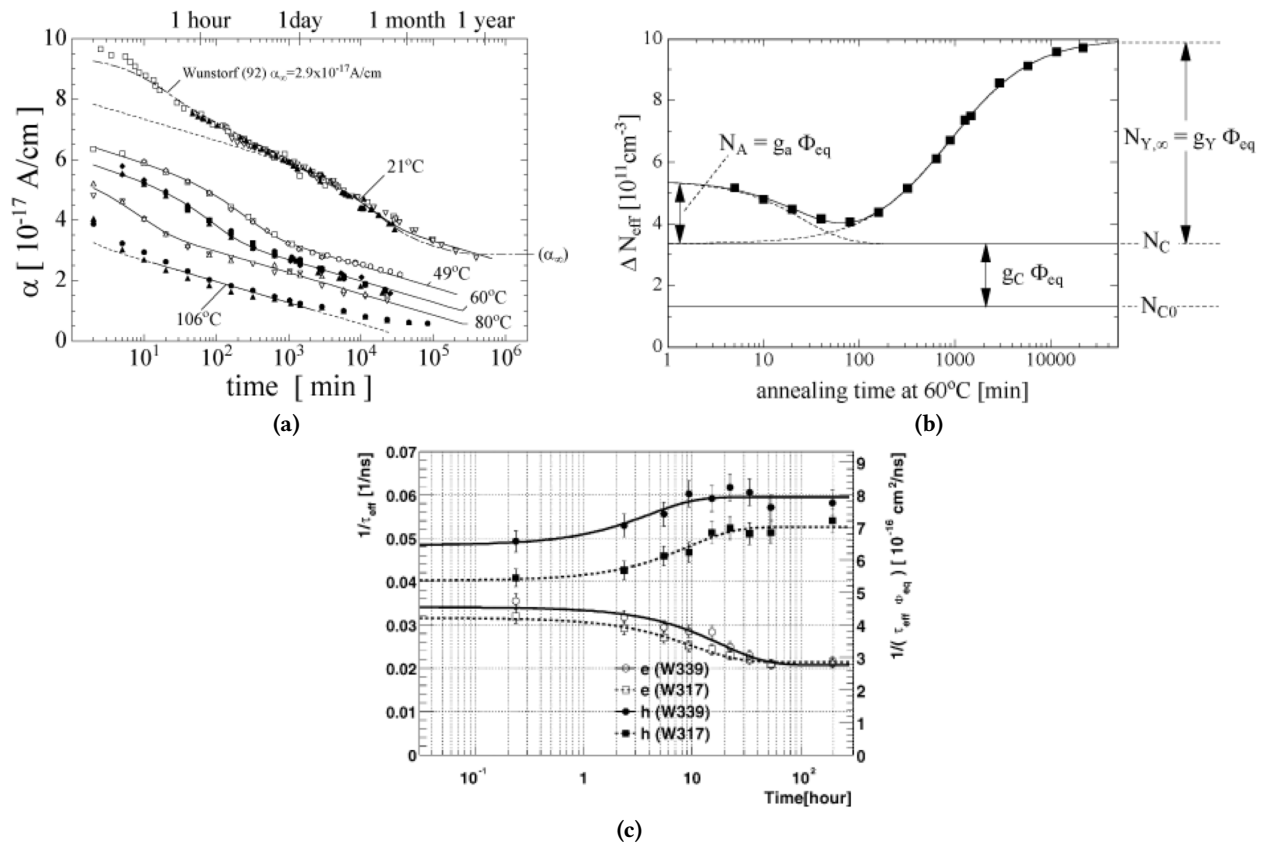


Figure 3.18: Annealing effects on different sensor characteristics The current-related damage rate is depicted for various annealing temperatures (a). For the effective space charge concentration (b) and the trapping probability (c), annealing was conducted at a temperature of 60°. Figures taken from [149] (a,b) and [162] (c).

Measurement of the $H \rightarrow \gamma\gamma$ fiducial inclusive cross-sections

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The following chapter outlines the first measurement of the Higgs boson’s production cross-section in the di-photon decay channel, utilizing the early Run 3 dataset collected by the ATLAS detector in 2022, comprising 31.4fb^{-1} of pp collision data at $\sqrt{s} = 13.6$ TeV. Expanding on similar measurements carried out by both ATLAS and CMS collaborations across di-photon [163–166], four-lepton [167–170], and ATLAS combined [171, 172] decay channels at $\sqrt{s} = 8$ TeV and $\sqrt{s} = 13$ TeV datasets, this analysis closely follows the $pp \rightarrow H \rightarrow \gamma\gamma$ Run 2 analysis from 2015 to 2018, with notable differences, including the migration to Release 22 of Athena, utilizing the Run 3 data, and a focused effort on evaluating the inclusive fiducial cross-section.

The chapter is structured as follows: Section 4.1 outlines the motivation and strategy behind the measurements. Section 4.2 introduces the collision and simulated data samples. Section 4.3 details

the analysis chain for the $H \rightarrow \gamma\gamma$ fiducial cross-section measurement, covering event selection and reconstruction, signal and background modeling, investigation of systematic uncertainties, statistical analysis results, and subsequent cross-checks. Section 4.3.5.1 briefly addresses the fiducial cross-section measurement in $H \rightarrow ZZ^* \rightarrow 4l$ and the combined total cross-section result for $\sigma(pp \rightarrow H)$ across these channels. Further details can be found in the cited publication [27, 173].

4.1 Introduction

Following the discovery of the Higgs boson (referred to as H hereafter) by the ATLAS [3] and CMS [4] collaborations at the LHC in 2012, the primary objective of the LHC experiments has been to measure its properties and determine if it confirms to predictions from the SM or involve new phenomena beyond its framework. The first of these studies focused on measuring the signal strength, representing the ratio of total production rate over the SM expectation [174]. Subsequent studies focused on quantifying the Higgs boson production, decay rates, and coupling strengths relative to the SM expectations within the κ -framework [175]. The studies above are performed under the presumption that the kinematics governing Higgs boson production and decay are the same as those expected for the SM Higgs boson.

During Run 2, the Higgs studies were broadened with the development of a simplified template cross-section (STXS) framework [176], dividing Higgs boson production modes into distinct kinematic regions of the phase space. These kinematic bins, defined using the SM as a template and depending on properties like the Higgs boson p_T or the number of accompanying particle-level jets, disentangle the theoretical interpretation (SM or BSM) from the measurement, thereby reducing the theory dependence of the results on the SM prediction. Additionally, the STXS bins can be further subdivided into finer categories, systematically enhancing sensitivity and minimizing residual theoretical uncertainty, while also being defined independently of the Higgs boson decay mode, thereby facilitating the combination of measurements across different decay channels. The measurement of Higgs boson properties using the STXS framework falls outside the scope of this thesis and will not be addressed further. Extensive studies on this topic can be found in the cited literature [177, 178].

The studies presented in this chapter employ a distinct approach centered on measuring the fiducial cross-sections, which involves selecting quantities for measurement largely independent of specific models, as elaborated in subsequent sections. These quantities typically pertain to inclusive (discussed herein) and differential [179, 180] Higgs boson production cross-sections within a fiducial region closely matched to the detector-level selection. The measurements, also detailed in [27, 173], utilize the early Run 3 dataset of LHC proton-proton collisions recorded with the ATLAS detector.

4.1.1 Motivation

The fiducial inclusive cross-section measurements offer an alternative framework for measuring the properties of the Higgs boson. In this framework, the Higgs boson cross-sections are measured in regions of the phase space termed fiducial volumes, defined by selections that closely resemble the experimental selection. The advantages of conducting measurements in the fiducial volumes are manifold:

1. The approach eliminates the need for extrapolating to the full phase space, thereby removing additional theoretical uncertainties typically associated with such extrapolations. Furthermore, unlike the STXS method, the fiducial regions of these cross-sections encompass require-

ments on the final state particles from Higgs boson decay, further minimizing extrapolation and associated theoretical uncertainties.

2. The model-dependence of the signal efficiencies within the fiducial volumes can be reduced to be smaller than the overall experimental uncertainty, thus minimizing the impact of theoretical variations on the signal efficiency [181].
3. The approach facilitates model-independent measurements allowing for comparison with various current theoretical frameworks and any subsequent models developed post-measurement, without necessitating a re-analysis of the data.

The cross-section measurements for $pp \rightarrow H \rightarrow \gamma\gamma$ presented in this thesis are performed within a defined fiducial region characterized by two isolated photons with an absolute pseudorapidity of $|\eta| < 1.37$ or $1.52 < |\eta| < 2.37$, with the leading (subleading) photon satisfying $p_T/m_{\gamma\gamma} > 0.35$ (0.25), where p_T represents the transverse momentum of the photon and $m_{\gamma\gamma}$ denotes the diphoton invariant mass. The results discussed in this thesis assume a value of the Higgs boson mass of 125.09 ± 0.24 GeV [182].

4.1.2 Strategy

The strategy employed for measuring the fiducial inclusive cross-sections, as depicted in Figure 4.1, is as follows:

- The data and simulated samples utilized in the measurement are described in detail in Section 4.2.
- An event selection, closely adhering to the definition of the fiducial region, is implemented, with both the event selection criteria and the definition of the fiducial region outlined in Section 4.3.1.
- Following the event selection process, the primary differentiating factor between the Higgs signal and the background is the di-photon invariant mass ($m_{\gamma\gamma}$). The analysis entails studying the $m_{\gamma\gamma}$ distributions for both signal and background, where analytic parameterizations of their shapes and associated uncertainties are determined, as elaborated in Section 4.3.2.
- The Higgs boson signal cross-section yield is determined by fitting the distribution of di-photon invariant mass distribution in the data using the signal and background parameterizations established earlier. Comprehensive details of this fitting procedure are outlined in Section 4.3.4.
- The measurements are compared with various theoretical predictions, as elaborated in Section 4.3.5.
- A summary of the uncertainties associated with the various stages of the measurement is provided in Sections 4.3.3.1, 4.3.3.2, and 4.3.3.3.

A similar strategy was employed in previous Higgs boson cross-section measurements at both $\sqrt{s} = 8$ TeV and $\sqrt{s} = 13$ TeV [163, 183]. The analysis follows a "blind-analysis" approach, optimizing and validating the analysis chain before examining the data in the signal region. The signal region comprises events that pass all the selection criteria and have reconstructed di-photon invariant masses within a narrow window around the Higgs boson mass. Optimization and validation utilize simulation samples and data in control regions, including events with photon candidates failing some selection criteria (enriched in "reducible" background where at least one photon candidate originates from the misidentification of a hadronic jet) or events passing all selection criteria but with di-photon invariant masses in a "sideband" region away from the Higgs boson mass value (enriched in "irreducible" background).

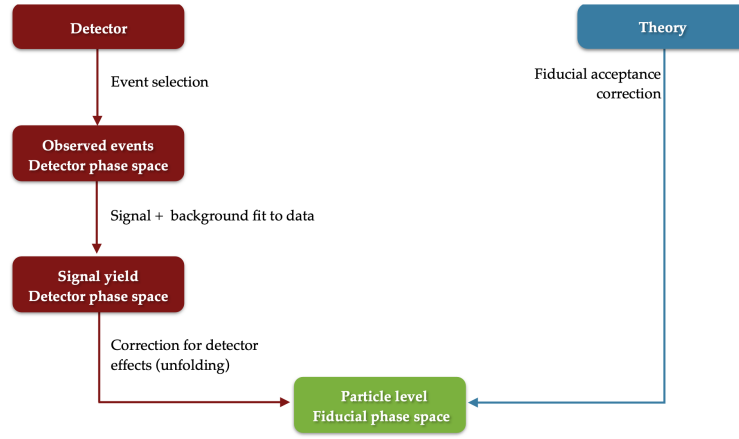


Figure 4.1: Schematic representation of the analysis strategy. Processing stages of quantities measured by the detector are depicted in dark red, while stages involving quantities predicted by theory are illustrated in blue. The comparison of measured quantities at the particle-level fiducial volume to theory is represented in green. Adapted from [184].

4.2 Data and Simulation Samples

The analysis utilizes data and simulation samples reconstructed using Athena release 22. The input comprises HIGG1D1 derivations generated with AthDerivation [185], which involves a preliminary selection that is less strict than the final selection, requiring events to pass basic diphoton and single photon triggers and include at least two offline photon candidates. All samples are analyzed using the HGamCore analysis framework [186] to produce Mini xAODs (MxAODs), during which particle candidates are calibrated and data and simulation corrections, along with weights, are computed, applied, or saved in the MxAOD. A preselection is performed requiring the following criteria:

- Data events must pass the good runs lists requirement to ensure good data quality.
- Data events must satisfy detector quality flags, rejecting events with data integrity errors in the calorimeters and incomplete events where some detector information is missing.
- The event must contain at least one primary vertex candidate.
- There must be at least two photon candidates passing loose identification requirements based on their shower shapes in the electromagnetic calorimeter and the leakage in the hadronic calorimeter, while also avoiding regions of the calorimeter with cells connected to dead high-voltage lines.

4.2.1 Data Samples

The measurement presented in this chapter is based on pp collision data collected with the ATLAS detector in the year 2022. The dataset corresponds to an integrated luminosity of $31.4 \pm 0.7 \text{ fb}^{-1}$. The uncertainty in the integrated luminosity for data recorded in 2022 is 2.2% [187], determined using the van der Meer beam separation scans as discussed in [188], with primary luminosity measurements conducted using the LUCID-2 detector [189], supplemented by measurements from the inner detector and calorimeters. The mean number of interactions per bunch crossing, averaged over all colliding bunch pairs, is $\langle \mu \rangle = 41.2$. Data selection is carried out solely if all relevant detector components for this analysis are verified to be in optimal operating condition.

Only events that pass single- or di-photon triggers [190] are used in this measurement. The single-photon trigger requires a photon candidate with at least 140 GeV of transverse energy (E_T), and

this photon must meet loose identification criteria based on its calorimeter shower shape. The di-photon trigger necessitates two photon candidates with E_T of at least 25 GeV and 35 GeV, respectively, and both must satisfy medium identification requirements. On average, these trigger requirements achieve 99.4% efficiency for events that meet the reconstruction-level criteria outlined in Section 4.3.1. The efficiency is primarily driven by the di-photon trigger, while the single-photon trigger contributes to the recovery of less than 0.1% of the relevant events [27].

4.2.2 Simulated Samples

Simulated event samples are used to estimate the expected signal yield, model the signal diphoton invariant mass for fitting the data to extract the signal and background yields, and compute the correction factors to unfold the detector-level yields to the particle-level yields. Furthermore, the simulated samples are used to determine the relative fractions of various background types and in constructing background-only templates. These templates are essential for selecting an appropriate analytic function to model the diphoton invariant mass distribution of the background and to estimate the corresponding systematic uncertainty on the signal yield determined from signal + background fit to the data.

4.2.2.1 Higgs Boson Signal Simulation

At the LHC, Higgs bosons are predominantly generated via gluon-gluon fusion (ggF), vector-boson fusion (VBF, with $V = W, Z$ bosons), and associated production with a vector boson (VH), as well as top or bottom-quark pairs ($t\bar{t}H$, $b\bar{b}H$), as discussed in detail in Section 1.3. The hard scattering process resulting in the production of the Higgs boson is generated using POWHEG v2 [191–195] MC generator with PDF4LHC21 family of PDFs. All generated samples assume a Higgs boson mass of 125.0 GeV and width set to 4.07 MeV [27]. $H \rightarrow \gamma\gamma$ decays, as well as the effects of parton showering (PS), hadronisation and the underlying event (UE), are simulated by interfacing the output of the $pp \rightarrow H + X$ event generation with Pythia 8.2 [196] using parameter values determined by the A14 tune [197]. The stable particles generated from these simulations (refer Section 4.3.1.4) undergo simulation of the interactions with ATLAS detector using GEANT4 [198], with subsequent execution of the same reconstruction algorithms employed for the collision data. The samples are normalized to the most accurate theoretical cross-section predictions [199], which are extrapolated to the new LHC center-of-mass energy of 13.6 TeV, based on cross-section values available at various center-of-mass energies ranging from 6 to 15 TeV in 0.5 TeV increments [200].

The specifics of event generation for the various production modes, as summarized in Table 4.1, are as follows:

- The matrix elements for the ggF signal sample is computed at next-to-leading (NLO) accuracy with up to one extra jet by following the MiNLO approach [201, 202]. The ggF sample is normalised to a next-to-next-to-next-to-leading-order (N³LO) QCD calculation with NLO electroweak corrections. The ggF sample comprises approximately 4M events.
- VBF events are generated using POWHEG-BOX at NLO accuracy in QCD. The VBF sample is normalized to an approximate next-to-next-to-leading-order (NNLO) QCD cross-section with NLO electroweak corrections [203–205]. The VBF sample includes approximately 1.8M events.
- VH samples generated with POWHEG-BOX include both quark-initiated ($q\bar{q} \rightarrow VH$) and gluon-initiated ($gg \rightarrow ZH$) events. The samples are generated with NLO accuracy in QCD for quark-initiated production and leading-order (LO) accuracy for gluon-initiated production. The VH samples are normalized to cross-sections calculated at NNLO in QCD with NLO electroweak corrections for quark-initiated production, and at NLO and next-to-leading-logarithm

(NLL) accuracy in QCD for gluon-initiated production [206–210]. The VH sample comprises approximately 560k events.

- The $t\bar{t}H$ samples are generated using POWHEG-BOX at NLO accuracy in QCD. These samples are then normalized to a cross-section calculation at NLO accuracy in QCD with electroweak NLO correction [211–213]. The $t\bar{t}H$ samples comprise approximately 500k events.

The $b\bar{b}H$ and tH samples are not generated for this analysis; however, the corresponding cross-sections are considered in the calculation of the expected number of signal events. Given the comparable acceptance of ggF and $b\bar{b}H$ events, the ggF cross-section is scaled to account for this contribution, with the $b\bar{b}H$ contribution representing approximately 1% of the total ggF + $b\bar{b}H$ production [27]. Summing up all the production modes, the total predicted SM Higgs boson cross-section at 13.6 TeV is 59.8 ± 2.6 pb [27]. Additionally, the predicted SM branching ratio for the decay $H \rightarrow \gamma\gamma$ is $(2.27 \pm 0.07) \times 10^{-3}$ [199] for a Higgs boson mass of 125.09 GeV.

4.2.2.2 Background Simulation

The background samples, comprising non-resonant prompt diphoton production ($\gamma\gamma$) within a mass range of $90 < m_{\gamma\gamma} < 175$ GeV, are generated using MadGraph5_aMC@NLO [214] with matrix elements (ME) accuracy up to NLO including up to two partons. The NNPDF3.0 PDF set [215] is utilized for the computation of the matrix element and similar to the signal samples, parton showering, hadronization, and underlying event are modeled using Pythia 8.2 with the A14 tune as detailed in Table 4.1. Furthermore, all generated background events are passed through a simulation of the ATLAS detector response using Geant4. The simulated background sample comprises approximately 835 million events.

Process	Generator	Showering	PDF set	σ [pb] $\sqrt{s} = 13.6$ TeV
ggF + $b\bar{b}H$	POWHEG Box v2 + MiNLO	PYTHIA 8.2	PDF4LHC21	52.7 ± 2.6
VBF	POWHEG Box v2	PYTHIA 8.2	PDF4LHC21	$4.075^{+0.088}_{-0.089}$
WH	POWHEG Box v2 + MiNLO	PYTHIA 8.2	PDF4LHC21	$1.453^{+0.029}_{-0.028}$
$q\bar{q} \rightarrow ZH$	POWHEG Box v2 + MiNLO	PYTHIA 8.2	PDF4LHC21	$0.806^{+0.033}_{-0.029}$
$gg \rightarrow ZH$	POWHEG Box v2	PYTHIA 8.2	PDF4LHC21	$0.136^{+0.034}_{-0.026}$
$t\bar{t}H$	POWHEG Box v2	PYTHIA 8.2	PDF4LHC21	$0.569^{+0.040}_{-0.057}$
$\gamma\gamma, m_{\gamma\gamma} \in 90\text{--}175$ GeV	MADGRAPH5_aMC@NLO	PYTHIA 8.2	NNPDF3.0	-

Table 4.1: Simulated signal and background event samples. The last column reports the total cross-sections used to normalise the signal samples reported for $m_H = 125.09$ GeV [27].

4.2.2.3 Pileup Simulation

The impact of pileup (see Section 2.1.4) is simulated by overlaying the hard-scatter signal and background events with a set of simulated inelastic pp events generated by EPOS 2.0.1.4 [216] and Pythia 8.2. The events generated with EPOS utilize the EPOS LHC tune, while the Pythia 8.2 events use the NNPDF2.3 [217] LO set of PDFs and parameter values set according to the A3 tune [218]. Pythia 8.2 simulates events containing at least one high transverse momentum jet, isolated photon, or lepton from the decay of b-hadrons, while EPOS simulates all other events in the sample. These events are generated independently, and a filter is applied to EPOS-generated events to veto events simulated by Pythia 8.2 [219]. Additionally, dedicated weights are employed to ensure that these samples adequately describe the mean number of interactions per bunch crossing observed in the 2022 collision data.

4.3 The $H \rightarrow \gamma\gamma$ Measurement

The following sections provide an overview of the various steps involved in the analysis chain for measuring the fiducial inclusive cross-section in the $H \rightarrow \gamma\gamma$ decay channel using the early Run 3 2022 dataset.

4.3.1 Event Reconstruction and Selection

In the cross-section measurement outlined within this section, events are chosen through a multi-step procedure. Firstly, the reconstructed photon candidates must satisfy a set of pre-selection criteria as described in Section 4.3.1.1. Next, the surviving candidates are ranked based on their transverse energy E_T . The candidates with the two highest E_T are then used to build a di-photon system to determine the primary vertex of the event (see Section 4.3.1.2). Lastly, a final set of requirements is applied to the di-photon system, which defines the fiducial region as detailed in Section 4.3.1.4.

4.3.1.1 Photon Reconstruction, Identification and Pre-Selection

The set of pre-selection criteria applied on the reconstructed photon candidates described herein were optimized for the Run 2 $H \rightarrow \gamma\gamma$ measurements. Photons are reconstructed using a dynamic clustering algorithm [220, 221], wherein variable-sized topological clusters are constructed based on the signal in electromagnetic calorimeter cells. Tracks reconstructed in the inner detector are assessed based on their matching quality to the reconstructed calorimeter energy cluster. Photon candidates with no matching track are categorized as unconverted photons, while those with a matching track but lacking innermost pixel-layer hits or with two matching tracks are classified as converted photons. All photon candidates must fall within the acceptance region of the finely-segmented first layer of the electromagnetic calorimeter, defined to have $|\eta| < 2.37$, and outside the transition region between the barrel and end-cap calorimeters, specified as $1.37 < |\eta| < 1.52$. This selection criterion excludes areas where the transverse segmentation of the first layer of the LAr calorimeter is too coarse for effective discrimination between prompt photons and π^0 particles. The photon candidates are calibrated using the method outlined in [221].

This reconstruction procedure effectively reconstructs prompt photons from Higgs decay and similar objects, such as di-photon decays of neutral hadrons within jets. An identification algorithm based on calorimeter shower shape information [222] is employed to reduce the contribution from these other objects, with the loose working point serving as the initial identification pre-selection requirement [221]. The algorithm relies on the shape of the shower in the second layer of the electromagnetic calorimeter and the energy deposition in the hadronic calorimeter. This method has a nominal prompt photon efficiency exceeding 98%.

An additional pre-selection criterion preserves events with at least two photon candidates, each possessing $E_T > 25$ GeV, and constructs a di-photon system. If, in an event, more than two-photon candidates satisfy these three pre-selection requirements, the two candidates with the highest E_T are used to build the di-photon system to identify the diphoton primary vertex.

4.3.1.2 Primary Vertex Selection

The primary vertex (PV) of an event is determined using a neural-network (NN) algorithm [223], trained to differentiate between the hard-scatter vertex of ggF events and vertices resulting from pile-up interactions. The algorithm utilizes information about all the reconstructed vertices in the event and the following input quantities:

- The scalar sum, $\sum p_T$, the total transverse momentum of the tracks associated with each reconstructed vertex.
- The sum, $\sum p_T^2$, the squared total transverse momentum of the tracks associated with each reconstructed vertex.
- The difference in azimuthal angle, $\Delta\phi$, between the vector sum of the track momenta and the transverse momentum vector of the di-photon system.
- The pointing, determined by the primary vertex variable, $\frac{z_{common} - z_{vertex}}{\sigma_z}$, uses the flight direction of the photons as determined by the measurement utilizing the longitudinal segmentation of the calorimeter and the conversion point or hits detected in the precision tracking devices. z_{vertex} is the position of the primary vertex in the z-direction (beam direction), z_{common} is the weighted mean of z-positions of extrapolated photon trajectories and σ_z is the associated error of extrapolation.

The implementation of this neural network yields on average vertex selection efficiency of 71.4% for the ggF process, in contrast to an efficiency of 52.2% when relying solely on the largest $\sum p_T^2$ of its associated tracks (referred to as the hardest vertex), a method typically adopted as the default in ATLAS. This efficiency is estimated using the simulated Run 3 $H \rightarrow \gamma\gamma$ samples, requiring a z-axis distance of less than 0.3 mm between the particle-level (true) PV and the reconstructed PV. The di-photon vertex selection efficiency is validated using $Z \rightarrow e^+e^-$ decays in both data and simulated events. Figure 4.2 illustrates the efficiency of selecting the correct primary vertex in MC simulated with $H \rightarrow \gamma\gamma$, alongside a comparison with $Z \rightarrow e^+e^-$ decays in both data and MC (with electron tracks removed).

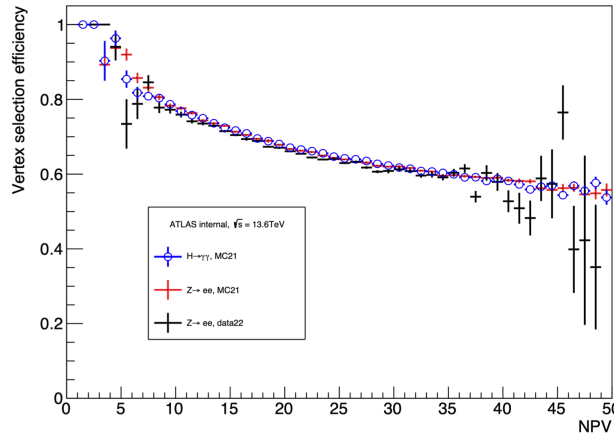


Figure 4.2: Efficiencies for selecting the correct primary vertex within a 0.3 mm range using the NN-algorithm as a function of the number of primary vertices for $H \rightarrow \gamma\gamma$ events and $Z \rightarrow e^+e^-$ events, both in data and simulation.

4.3.1.3 Detector-level Event Selection

The full event selection applies additional criteria to the two leading p_T photons that constitute the di-photon system after the preselection described in Section 4.3.1.1, ensuring that the final detector-level selection closely resembles the fiducial selection applied at the particle level, except for the photon identification requirements. The following provides a summary of the complete event selection:

- The two photon candidates with the highest p_T are matched to the di-photon trigger, featuring a 2-part trigger system with a minimum L1 energy threshold of 20 GeV and HLT p_T thresholds of 35 and 25 GeV. These two photon candidates are selected to reconstruct the Higgs boson candidate.

- The two selected photons must satisfy stricter identification criteria defined by the tight working point [224]. The efficiency of the tight working point requirement varies with the E_T of the photon candidate, ranging from 84% (85%) at $E_T = 25$ GeV to 94% (98%) at $E_T = 100$ GeV for unconverted (converted) photon candidates. This working point utilizes the same information as the loose working point employed for pre-selection but imposes stricter criteria while integrating data from the finely segmented first layer of the electromagnetic calorimeter. Furthermore, photons with pseudorapidity $|\eta| > 2.37$, or within the transition region between the barrel and endcap sections of the LAr calorimeter ($1.37 < |\eta| < 1.52$) are excluded by this selection where the transverse segmentation of the first layer of the LAr calorimeter is coarse and does not facilitate prompt photon/ π^0 discrimination.
- The two selected photons must also satisfy the "FixedCutLoose" isolation criteria, aimed at isolating them from significant activity in the inner detector or calorimeters to mitigate hadronic background contamination. Track-based isolation is determined by calculating the scalar sum of the p_T of all tracks with at least 1 GeV momentum, located within a cone of $\Delta R = 0.2$ around the photon candidate, and consistent with originating from the selected PV. Track isolation requirements are met if the sum of p_T is below 5% of the photon candidate's E_T . Calorimeter-based isolation is defined as the scalar sum of the E_T of all positive energy topological clusters within a $\Delta R = 0.2$ cone, excluding the energy of the photon candidate itself. Calorimeter isolation is deemed satisfactory if the resulting sum of E_T is less than 6.5% of the photon candidate's E_T .
- The leading (sub-leading) photons are required to have $p_T/m_{\gamma\gamma} > 0.35$ (0.25), respectively.
- The di-photon invariant mass must be in the range $105 < m_{\gamma\gamma} < 160$ GeV.

The total number of events selected in the full Run 3 data is 307,996, with the event cutflow for data presented in Table 4.2.

Selection step	Data 2022		ggF		SM $\gamma\gamma$	
	Events	rel. eff.	Fraction of yields	rel. eff.	Fraction of yields	rel. eff.
xAOD	3165860000	4.9%	100.0%	100.0%	100.0%	100.0%
DAOD	156635000	100.0%	100.0%	100.0%	73.2%	73.2%
No duplicates	156635000	97.5%	99.8%	99.8%	73.2%	100.0%
GRL	152702000	89.6%	99.8%	100.0%	73.2%	100.0%
Pass trigger	136773000	100.0%	57.4%	57.5%	55.6%	76.0%
Detector DQ	136764000	100.0%	57.4%	100.0%	55.6%	100.0%
Has PV	136764000	10.9%	57.4%	100.0%	55.6%	100.0%
2 loose photons	14865800	100.0%	50.7%	88.3%	46.6%	83.7%
dead HV cell veto	14865800	70.1%	50.7%	100.0%	46.6%	100.0%
Trigger match	10427900	34.3%	49.2%	97.1%	40.5%	87.0%
tight ID	3581030	42.0%	43.2%	87.8%	33.9%	83.6%
isolation	1502710	86.6%	38.7%	89.5%	26.9%	79.5%
photon $p_T/m_{\gamma\gamma}$ cuts	1301130	23.7%	35.9%	93.0%	23.4%	86.9%
$m_{\gamma\gamma} \in [105, 160]$ GeV	307996	23.7%	35.9%	100.0%	13.6%	57.9%
Events per fb^{-1}	9814 $\pm$ 99					

Table 4.2: Selection cutflow in the data, ggF MC and background MC.

4.3.1.4 Particle-level Event Selection

The cross-section is measured within a fiducial region defined at the particle level, based on event generation information, to enable comparison with results from other experiments or theoretical predictions. Thus, in order to minimize the model dependence stemming from extrapolation between the phase space regions defined by kinematic and isolation criteria, as well as detector acceptance, fiducial measurements are conducted within a phase space volume closely resembling that selected by detector-level criteria outlined in Section 4.3.1.3.

The fiducial volume and observables are defined based on the stable particles that pass through the

detector. Stable particles are those with a lifetime of $c\tau_0 > 10$ mm, excluding those created by the GEANT simulation of the detector response [225]. Each particle is identified by a PdgId number in the Monte Carlo Numbering Scheme of the Particle Data Group [126]. Particles created by pileup collisions are not considered. The applied particle-level selection criteria are as follows:

Photons At the particle level, photons are identified by $\text{PdgId} = 22$. They must not originate during hadronization, indicated by their parent having $|\text{PdgId}| < 111$. If the parent is a τ lepton ($|\text{PdgId}| = 15$) or another photon, representing a final-state radiative emission, the PdgId of the grandparent is examined, and so forth.

Kinematic photon preselection Kinematic selections of $p_T > 25$ GeV and $|\eta| < 1.37$ or $1.52 < |\eta| < 2.37$ are applied to the selected photons.

Di-photon system The two photons with the highest p_T are defined as the Higgs candidate system. These photons are selected after the application of the kinematic photon cuts.

Isolated photons Particle-level photon isolation is applied to minimize the model dependence of the correction for detector effects, described further in Section 4.3.3.3. The isolation energy, E_T^{iso} , of a photon is computed as the transverse energy, E_T , of the four-vector sum of all charged particles with $p_T > 1$ GeV within a cone of $\Delta R = 0.2$ around the photon. If at least one of the two selected photons fails the criterion $E_T^{\text{iso}} < 0.05p_T$, the event is discarded.

Final kinematic photon selection The invariant mass of the di-photon system, $m_{\gamma\gamma}$, is required to fall within the range $m_{\gamma\gamma} \in [105, 160]$ GeV. Additionally, the leading (subleading) photons are required to satisfy $p_T/m_{\gamma\gamma} > 0.35$ (0.25).

The number of expected events at the particle level is obtained by multiplying the theoretical fiducial cross-section, σ , with the luminosity of the dataset, $\mathcal{L}$. The anticipated number of particle-level events categorized by production mode is tabulated in Table 4.3. The average signal acceptance for this di-photon fiducial region is calculated to be 49.73% relative to the full phase space. Based on SM values for the production cross-section, acceptance, and di-photon branching fraction, a total of 2117 signal events are anticipated within the fiducial region.

Process	Events	Composition	Acceptance wrt inclusive phase space
ggF	1874	88%	50%
VBF	146	6.9%	50%
W^+H	26	1.2%	42%
W^-H	19	0.89%	47%
$q\bar{q} \rightarrow ZH$	30	1.4%	45%
$gg \rightarrow ZH$	5.3	0.25%	55%
$t\bar{t}H$	21	0.99%	52%
Total	2121		

Table 4.3: Expected number of particle level events in the fiducial volume in 31.4fb^{-1} of data. The composition column indicates the percentage of total events that are attributed to each specific Higgs production process.

4.3.2 Signal and Background Modelling

The $H \rightarrow \gamma\gamma$ cross-section measurement presented in this thesis is determined through an analytical fit to the di-photon mass spectrum, as elaborated upon in Section 4.3.4. The analytic function used to model the signal distribution is primarily derived from simulation, after applying the relevant calibrations, as outlined in Section 4.3.2.1. Additionally, the parameters of the functional

form utilized for the background distribution are determined from a fit to the data, as discussed in Section 4.3.2.2. The systematic uncertainties associated with the signal and background modeling are incorporated into the fit through nuisance parameters, as elucidated in Sections 4.3.3.1 and 4.3.3.2, respectively. The measured signal yields are corrected to the particle level using a single correction factor derived from MC simulation (see Section 4.3.3.3), which accounts for detector effects as well as out-of-acceptance signal contributions.

4.3.2.1 Signal Modelling

The $m_{\gamma\gamma}$ distribution is expected to be resonant for the signal process $pp \rightarrow H \rightarrow \gamma\gamma$. In the absence of interference from the background process $pp \rightarrow \gamma\gamma$, this distribution is anticipated to follow a Breit-Wigner curve with a peak at the Higgs mass m_H , which has a narrow width of around 4 MeV in the Standard Model. However, the measured photon energies have a finite resolution, which causes the observed distributions in data to be smeared. Therefore, a double-sided Crystal Ball function (DSCB), illustrated in Figure 4.3a, is used to model the $m_{\gamma\gamma}$ distribution by fitting it to the MC simulation with $m_H = 125$ GeV. The analytic form of this function is given by Equation 4.3.1.

$$CB(m_{\gamma\gamma}) = N \times \begin{cases} e^{-\frac{t^2}{2}}, & \text{if } -\alpha_{\text{low}} \leq t \leq \alpha_{\text{high}} \\ e^{-\frac{\alpha_{\text{low}}^2}{2}} \left[\frac{1}{R_{\text{low}}} (R_{\text{low}} - \alpha_{\text{low}} - t) \right]^{-n_{\text{low}}}, & \text{if } t \leq -\alpha_{\text{low}} \\ e^{-\frac{\alpha_{\text{high}}^2}{2}} \left[\frac{1}{R_{\text{high}}} (R_{\text{high}} - \alpha_{\text{high}} - t) \right]^{-n_{\text{high}}}, & \text{if } t \geq \alpha_{\text{high}} \end{cases} \quad (4.3.1)$$

Here, $t = \frac{m_{\gamma\gamma} - \mu_{CB}}{\sigma_{CB}}$, $R_{\text{low}} = \frac{\alpha_{\text{low}}}{n_{\text{low}}}$, and $R_{\text{high}} = \frac{\alpha_{\text{high}}}{n_{\text{high}}}$. N represents the normalization parameter, σ_{CB} signifies the width of the Gaussian distribution, α_{low} and α_{high} denote the positions of the transitions from the Gaussian core to the power-law tails on the low and high mass sides, and n_{low} and n_{high} represent the exponents of the low and high mass tails.

The six parameters defining the DSCB shape are determined via a fit to the simulated signal samples and are held fixed in the fit to the data. The overall normalization, represented by the parameter N , is determined within the fit to the data. Given that the signal samples are generated at a Higgs boson mass of 125.0 GeV, the mean value of the central Gaussian is shifted by 90 MeV to simulate a signal at 125.09 GeV. Shifts in μ_{CB} are still permitted, with uncertainties considered as nuisance parameters in the fit, as described in Section 4.3.3.1.

The shape parameters are consistent across all processes (ggH, VBF, VH, ttH) and a fit to the sum of all processes, normalized to their expected SM yield is performed for the inclusive region. The parameterization results for the inclusive bin are illustrated in Figure 4.3b, with the fitted parameters of the signal parameterization outlined below:

$$\begin{aligned} \mu - 125 &= 0.5632 \pm 0.00023 \text{ GeV} \\ \sigma &= 1.7280 \pm 0.0026 \text{ GeV} \\ \alpha_{\text{low}} &= 1.6426 \pm 0.0080 \\ \alpha_{\text{high}} &= 1.5313 \pm 0.0054 \\ n_{\text{low}} &= 5.1274 \pm 0.0842 \\ n_{\text{high}} &= 18.33 \pm 0.0063 \end{aligned} \quad (4.3.2)$$

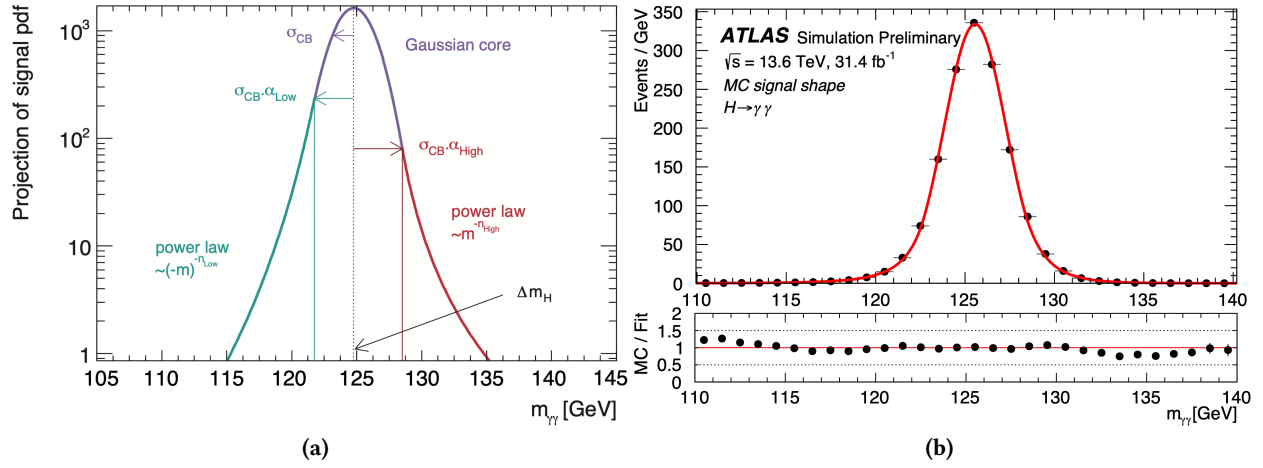


Figure 4.3: (a) Example of a double-sided crystal ball function (b) Fit of the double-sided Crystal Ball function to the simulated signal events normalised to the SM prediction.

4.3.2.2 Background Modelling

To accurately estimate the Higgs boson signal yield, it is essential to precisely determine the background within the selected dataset. The primary backgrounds influencing this analysis can be classified into irreducible and reducible components. The irreducible component arises from non-resonant prompt photon pairs generated in processes like $q\bar{q} \rightarrow \gamma\gamma$, $qg \rightarrow \gamma\gamma$, or $gg \rightarrow \gamma\gamma$. These photons are predominantly indistinguishable from those originating from Higgs boson decay, hence termed "irreducible". Conversely, the reducible component originates from events featuring γ -jet and jet-jet final states, where hadronic jets are misidentified as photons. The photon identification and isolation criteria, outlined in Section 4.3.1.3, discard the majority of these events. Consequently, the reducible component of the background post-selection is minor, and the jet-jet component of the reducible background is negligible, as illustrated in Figure 4.4.

The relative contribution of each background component is measured in data using a 2-dimensional double-sideband method ($2 \times 2D$), detailed in [226, 227]. The $2 \times 2D$ side-band method calculates the background fraction in the signal region by utilizing the yields in data from the background-enriched control regions (CR), populated by events in which at least one of the two photon candidates fails either the tight identification or isolation requirements, or both. The fractions attributed to the $\gamma\gamma$, γj , and $j j$ background sources following the inclusive di-photon selection are $73.0 \pm 1.9\%$, $23.6 \pm 1.5\%$, and $3.4 \pm 0.4\%$, respectively, as illustrated in Figure 4.4. These fractions are solely used to construct the background-only templates (see Section 4.3.2.2) for studying various background models to be used in the signal + background fit (see Section 4.3.2.3) and are not used to fix the fit parameters.

The $m_{\gamma\gamma}$ backgrounds, characterized by smoothly falling distributions, can be effectively described by an empirically chosen functional form, which can result in an increase or decrease in the measured signal events. Therefore, the selection of the empirical function ensures the minimization of this bias, as discussed in Section 4.3.2.2. Various functional forms assessed for parametrizing the diphoton mass spectrum background are discussed in Section 4.3.2.2, with the procedures for obtaining these templates detailed in Section 4.3.2.2.

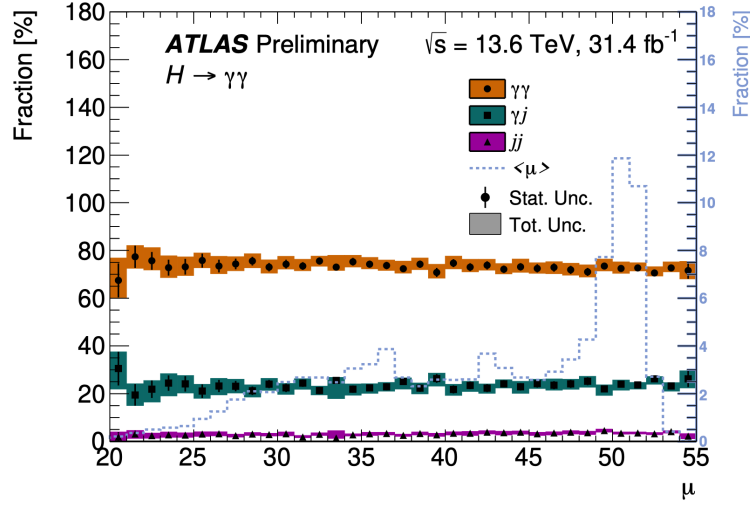


Figure 4.4: Fractional composition of the different background components determined using two-dimensional double-sideband method as a function of the number of interactions per bunch crossing μ . The dashed histogram shows the distribution of the number of interactions per bunch crossing in the 2022 data.

Functional Form

Several functional forms were explored for parametrizing the background $m_{\gamma\gamma}$ spectrum, including exponentials of first (Exp), second (ExpPoly2), and third (ExpPoly3) degree polynomials, Bernstein polynomials of degree 3 (Bern3), 4 (Bern4), and 5 (Bern5), as well as power law functions of first (Pow) order. Previous studies [228] have shown that the preferred function for modeling the background distribution in most cases is ExpPoly2, characterized by the functional form presented in Equation 4.3.3:

$$\mathcal{B}(m_{\gamma\gamma}; \alpha^{\text{bkg}}) = N(\alpha^{\text{bkg}}) \cdot \exp\left(-\frac{m_{\gamma\gamma}}{\alpha_1^{\text{bkg}}} - \frac{m_{\gamma\gamma}^2}{\alpha_2^{\text{bkg}}}\right) \quad (4.3.3)$$

Here, α_1^{bkg} , α_2^{bkg} are nuisance parameters and $N(\alpha^{\text{bkg}})$ normalises the function to unity.

Selecting an inappropriate analytical function to describe the background may result in an underestimation or overestimation of the number of background events under the signal peak, thereby biasing the measured signal events in the signal+background fit to the data. This bias is termed the spurious signal and is discussed in detail in Section 4.3.2.2.

Background templates

A background template for the diphoton invariant mass is created by combining the $\gamma\gamma$, γj , and $j j$ components based on the measured fractions. While the $\gamma\gamma$ component is directly derived from the simulated background samples after applying the event selection outlined in Section 4.3.1, generating large samples of γj and $j j$ events that satisfy the analysis selections is computationally challenging due to their large cross-sections and the high jet-rejection performance of the ATLAS photon identification algorithms. Consequently, the shape of the sum of γj and $j j$ components is derived from data control samples defined by inverting the identification and/or isolation requirements of one or both photons while retaining the other nominal event selection requirements. The ratio of the $m_{\gamma\gamma}$ distribution of the γj and $j j$ components to that of the simulated $\gamma\gamma$ sample is observed to be well-described by a simple linear function of $m_{\gamma\gamma}$. Consequently, a linear fit to the ratio of these distributions is employed to derive an $m_{\gamma\gamma}$ -dependent weight. This weight is then applied to the $\gamma\gamma$ sample to generate a template encompassing the γj and $j j$ components. The two

templates, $\gamma\gamma$ and CR ($\gamma j + jj$) are combined with the measured relative fractions to obtain the total background shape. To further improve the accuracy of the background modeling, a second-order polynomial in $m_{\gamma\gamma}$ is fitted to the ratio of the $\gamma\gamma + \text{CR}$ template to the data in the side-bands (excluding the 120 – 130 GeV mass region). Subsequently, this fitted polynomial is utilized to refine the shape of the background template.

A second template for background modeling studies is generated via the implementation of a normalizing flow (NF) technique [229], utilizing a generative machine learning (ML) model to mimic the detector's response to photons. Alongside utilizing the MadGraph $\gamma\gamma$ full simulation sample as the baseline background for this analysis, the same sample is processed with TRUTH information, and the detector response is simulated using the NF method. The NF method offers significant speed advantages over the standard full Geant4 simulation. The alternative template is generated using the equivalent of approximately 3.5 ab^{-1} of integrated luminosity, compared to the 1.3 ab^{-1} obtained from the Geant4-based sample.

The NF-smeared sample includes the kinematic distributions of the two photons with detector resolution, but does not include the identification and isolation quantities for these photons as they are part of the ML model's learning process. Since photon identification and isolation efficiencies vary across different photon p_T and η regions, the NF-smeared samples are re-weighted with the photon p_T - η distribution after applying the ID/ISO selections to the full simulation samples. The procedure described for the Geant4-based sample is also applied to the NF sample, to take into account the non-prompt photon component and the data side-bands mass shape when creating the second background template. Further details on the R&D of an alternative normalizing flow method for $H \rightarrow \gamma\gamma$ background modeling can be found in [229, 230].

Spurious Signal

The spurious signal method quantifies the bias in the signal yield resulting from the chosen background parameterization by fitting a background-only MC simulation, as detailed in Section 4.2.2.2, with a signal + background parameterization. In an ideal scenario, where the chosen analytical function (see Section 4.3.2.2) perfectly describes the background template, the average number of fitted spurious signals would be zero. The objective is to identify a background function that minimizes the occurrence of spurious signals while limiting the number of degrees of freedom in the model to prevent excessive inflation of the statistical uncertainty on the signal yield. The selected function must satisfy the following requirements on the number of spurious signal events (N_{sp}) and its statistical uncertainty (Δ_{sp}):

- $N_{\text{sp}} \pm 2\Delta_{\text{sp}}$ constitutes less than 20% of the background uncertainty, an estimation of the statistical uncertainty on the signal δS .
- $N_{\text{sp}} \pm 2\Delta_{\text{sp}}$ is less than 10% of the expected signal events N_{ref} .

The spurious signal is calculated as the maximum signal within the mass range of 123-127 GeV, divided into bins of 0.5 GeV width. If multiple functions meet the aforementioned criteria, the one with the fewest degrees of freedom is selected. If there are two functions with the same degree of freedom, the one with the lower uncertainty in the spurious signal is chosen. An additional loose goodness-of-fit test requires that the chi-squared probability be higher than 1%, ensuring that the selected functions reasonably describe the data in the side-bands.

The main challenge in estimating the spurious signal stems from the statistical fluctuations present in the background template. These statistical fluctuations, particularly in bins with low Monte Carlo statistics, can potentially generate spurious signals and lead to the failure of the tested model to meet one of the two aforementioned criteria. To address this issue, the MC simulated sample used to construct the background template must be significantly larger, on the order of $\mathcal{O}(100)$ times

the data size. This ensures smooth $m_{\gamma\gamma}$ distributions even in bins with a low number of events. Moreover, the envelope of $2\Delta_{sp}$ established around the spurious signal mitigates the impact of fluctuations, preventing the rejection of a background model when statistical power is insufficient. The spurious signal is computed using the two background templates, the MadGraph full-simulation and the MadGraph normalizing-flow template, described in Section 4.3.2.2 and the largest value is selected. The function selected by this procedure is an exponential of a second-order polynomial (ExpPoly2, see Section 4.3.2.2) in $m_{\gamma\gamma}$, with an associated spurious signal uncertainty corresponding to 6.2% of the expected SM signal yield.

4.3.2.3 Fit Methodology

The fiducial cross-section is determined through an unbinned maximum likelihood fit to the reconstructed di-photon invariant mass spectrum within the range of 105-160 GeV. The systematic uncertainties outlined in Section 4.3.3 are incorporated into the fit as nuisance parameters, constrained by additional Gaussian or log-normal likelihood terms, as described in Section 4.3.4. The probability density functions for the signal and background are characterized by analytic functions described in Sections 4.3.2.1 and 4.3.2.2, respectively. In the likelihood shown in Equation 4.3.7, the signal yield ν^{sig} is parameterized in terms of the fiducial cross-section as follows:

$$\nu^{sig} = \sigma_{fid} \times \mathcal{L} \times \mathcal{C}_{\mathcal{F}}, \quad (4.3.4)$$

Here, σ_{fid} is the fiducial cross-section, the parameter of interest in the fit, and is defined as the product of the total production cross-section σ_{tot} , the di-photon branching ratio $\mathcal{B}_{\gamma\gamma}$, and the acceptance $\mathcal{A}$:

$$\sigma_{fid} = \sigma_{tot} \times \mathcal{B}_{\gamma\gamma} \times \mathcal{A}, \quad (4.3.5)$$

The signal acceptance $\mathcal{A}$ is the fraction of signal events that pass the particle-level (fiducial) selection described in Section 4.3.1.4. The other terms in Equation 4.3.4 include $\mathcal{L}$, the integrated luminosity, and $\mathcal{C}_{\mathcal{F}}$, the correction factor. The correction factor is defined as the ratio of the number of signal events selected at the reconstruction level to the number of signal events selected at the particle level after applying the selection criteria described in Section 4.3.1. This factor is computed inclusively, assuming the ratio of the different Higgs boson production modes follows the SM prediction (see Appendix A.1.2). The value of $\mathcal{C}_{\mathcal{F}}$, derived from the simulated signal samples, is 71.6%. The dependence on the production mode is minimal, varying between 71.5% for ggF and 72.4% for VBF, and this variation is incorporated into the systematic uncertainties 4.3.3.

4.3.3 Systematic Uncertainties

The following section outlines the different sources of systematic uncertainty that affect the measurement of the fiducial $H \rightarrow \gamma\gamma$ cross-section. Based on Equation 1, the fiducial cross-section is given by:

$$\sigma_{fid} = \frac{\nu^{sig}}{\mathcal{C}_{\mathcal{F}} \cdot \mathcal{L}_{int}} \quad (4.3.6)$$

The various sources of uncertainties can thus be categorized as follows:

- Uncertainties impacting the signal yield ν^{sig} . These pertain to systematic uncertainties associated with the signal and background models, as discussed in Sections 4.3.3.1. The methodology

for incorporating these uncertainties into the signal extraction fit is detailed in Section 4.3.4.

- Uncertainties affecting the correction factor $\mathcal{C}_{\mathcal{F}}$ and the luminosity $\mathcal{L}_{\text{int}}$. The Luminosity uncertainty, described in Section 4.2.1, is evaluated to be of 2.2% [187]. The experimental and theoretical uncertainties on the correction factors are discussed in Section 4.3.3.3.

4.3.3.1 Systematic Uncertainties on the $m_{\gamma\gamma}$ Signal Modelling

Uncertainties affecting the peak position (μ_{CB}) or width of the signal peak (σ_{CB}) of the DSCB function (see Section 4.3.2.1) will impact the cross-section measurement, as the fiducial cross-section is determined from fitting the DSCB function to the $m_{\gamma\gamma}$ spectrum. The main sources of uncertainties in the signal di-photon invariant mass shape stem from the photon energy scale and resolution. The photon energy scale (PES) uncertainty influences μ_{CB} , causing a shift in the peak position, illustrated in Figure 4.5a, while the photon energy resolution (PER) uncertainty impacts σ_{CB} , either broadening or narrowing the signal width, as depicted in Figure 4.5a. The shifts induced by these uncertainties are regarded as systematic variations, with each variation corresponding to a nuisance parameter in the signal plus background fit. The impact of nuisance parameters on μ_{CB} and σ_{CB} is determined by calculating the relative shift in these parameters when fitting the signal model to the $m_{\gamma\gamma}$ distribution of signal MC events after recalculating the di-photon invariant mass using modified photon energies, while keeping all other fit parameters fixed at their nominal values. Additional uncertainties, including the uncertainty on the measured Higgs boson mass (125.09 ± 0.24 GeV [182]), variations in conditions between Run 2 and Run 3, and modifications to the MC simulation, are considered as additional nuisance parameters [27]. Tables 4.4a and 4.4b present the total uncertainties (ϵ^{PES} and ϵ^{PER} , respectively) for the fiducial bin, combining all the energy scale and resolution variations into single uncertainties each.

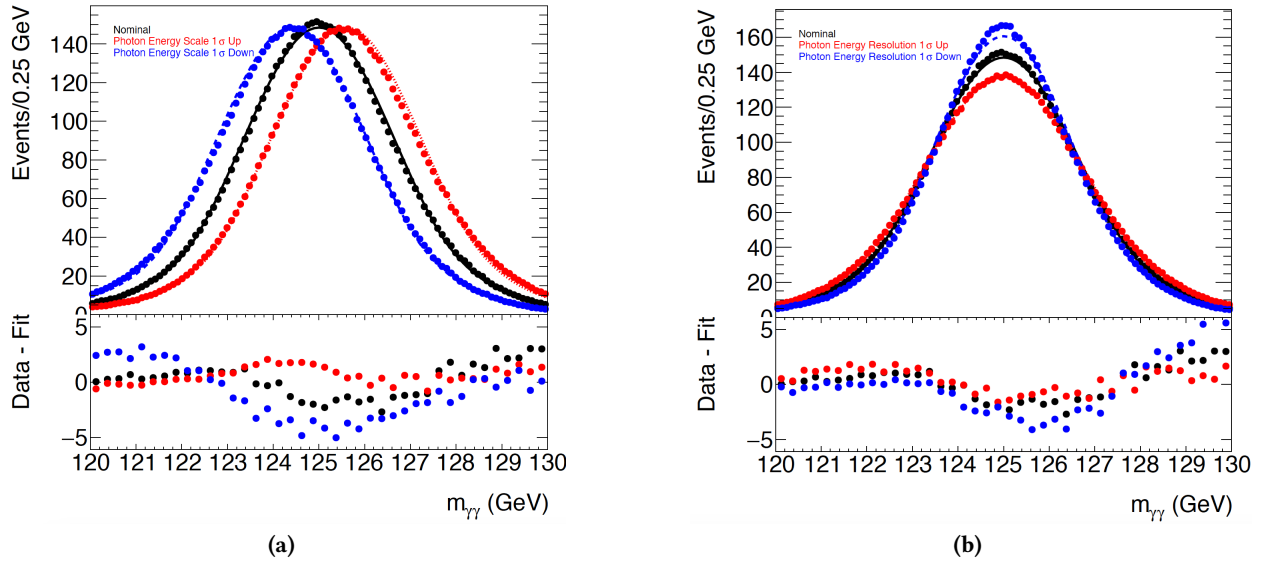


Figure 4.5: The effect of varying the total (a) the photon energy scale and (b) the photon energy resolution on the Higgs boson signal shape [184].

Variable	Inclusive Bin
inclusive up	2.4
inclusive down	2.4

(a)

Variable	Inclusive Bin
inclusive up	11.2
inclusive down	8.3

(b)

Table 4.4: Total relative error (in units of 10^{-3}) on the signal $m_{\gamma\gamma}$ peak position resulting from various (a) PES and (b) PER variations incorporated into the fit for the fiducial bin.

The PES uncertainty has a modest impact of under 0.24% on the peak position, with an additional 0.4% uncertainty accounting for changes in detector simulation between Run 2 and Run 3, while the photon energy resolution uncertainty, the largest contributor to signal shape uncertainty, results in a total error of approximately 11.2% on the peak width. To avoid over-constraining the nuisance parameters, the total energy scale and resolution uncertainties are divided into multiple components. The baseline decorrelation scheme, provided by the EGamma calibration and CP group, includes 10 PER components and 74 PES components, which are summarized in Tables 4.5, 4.6 and 4.7 for the inclusive region.

Component	Uncert
EG_RESOLUTION_MATERIALCALO_down	-0.0047492
EG_RESOLUTION_MATERIALCALO_up	0.0047828
EG_RESOLUTION_MATERIALCRYO_down	-0.0115938
EG_RESOLUTION_MATERIALCRYO_up	0.0118024
EG_RESOLUTION_MATERIALGAP_down	-0.0066636
EG_RESOLUTION_MATERIALGAP_up	0.0058511
EG_RESOLUTION_MATERIALIBL_down	-0.0105113
EG_RESOLUTION_MATERIALIBL_up	0.0119938
EG_RESOLUTION_MATERIALID_down	-0.0342210
EG_RESOLUTION_MATERIALID_up	0.0377687
EG_RESOLUTION_MATERIALPP0_down	-0.0195616
EG_RESOLUTION_MATERIALPP0_up	0.0185918
EG_RESOLUTION_OFC_down	-0.0441903
EG_RESOLUTION_OFC_up	0.0645125
EG_RESOLUTION_PILEUP_down	0.0264822
EG_RESOLUTION_PILEUP_up	-0.0200900
EG_RESOLUTION_SAMPLINGTERM_down	0.0166838
EG_RESOLUTION_SAMPLINGTERM_up	-0.0152666
EG_RESOLUTION_ZSMEARING_down	-0.0458453
EG_RESOLUTION_ZSMEARING_up	0.0748281

Table 4.5: Breakdown of PER relative errors that enter the fit for the inclusive fiducial region.

Component	Uncert
EG_SCALE_ADD_SIGNALMASS_down	-0.004000
EG_SCALE_ADD_SIGNALMASS_up	0.004000
EG_SCALE_E4SCINTILLATOR_ETABN0_down	-0.0000005
EG_SCALE_E4SCINTILLATOR_ETABN0_up	-0.0000005
EG_SCALE_E4SCINTILLATOR_ETABN1_down	0.0000035
EG_SCALE_E4SCINTILLATOR_ETABN1_up	-0.0000046
EG_SCALE_E4SCINTILLATOR_ETABN2_down	0.0000357
EG_SCALE_E4SCINTILLATOR_ETABN2_up	-0.0000364
EG_SCALE_G4_down	-0.0001397
EG_SCALE_G4_up	0.0001391
EG_SCALE_L1GAIN_down	-0.0004126
EG_SCALE_L1GAIN_up	0.0004229
EG_SCALE_L2GAIN_down	-0.0010701
EG_SCALE_L2GAIN_up	0.0010667
EG_SCALE_LARCALIB_ETABN0_down	0.0007791
EG_SCALE_LARCALIB_ETABN0_up	-0.0007800
EG_SCALE_LARCALIB_ETABN1_down	0.0002322
EG_SCALE_LARCALIB_ETABN1_up	-0.0002313
EG_SCALE_LARELECCALIB_down	-0.0000507
EG_SCALE_LARELECCALIB_up	0.0000503
EG_SCALE_LARELECUNCONV_ETABN0_down	0.0008766
EG_SCALE_LARELECUNCONV_ETABN0_up	-0.0008797
EG_SCALE_LARELECUNCONV_ETABN1_down	0.0003257
EG_SCALE_LARELECUNCONV_ETABN1_up	-0.0003232

Table 4.6: Breakdown of PES relative errors that enter the fit for the inclusive fiducial region.

Component	Uncert	Component	Uncert
EG_SCALE_LARUNCONVCALIB_ETABN0_down	-0.0003046	EG_SCALE_MATCRYO_ETABN4_down	-0.0000894
EG_SCALE_LARUNCONVCALIB_ETABN0_up	0.0003042	EG_SCALE_MATCRYO_ETABN4_up	0.0000883
EG_SCALE_LARUNCONVCALIB_ETABN1_down	-0.0000695	EG_SCALE_MATCRYO_ETABN5_down	-0.0000515
EG_SCALE_LARUNCONVCALIB_ETABN1_up	0.0000688	EG_SCALE_MATCRYO_ETABN5_up	0.0000508
EG_SCALE_MATCALO_ETABN0_down	-0.0000434	EG_SCALE_MATCRYO_ETABN6_down	-0.0000557
EG_SCALE_MATCALO_ETABN0_up	0.0000427	EG_SCALE_MATCRYO_ETABN6_up	0.0000549
EG_SCALE_MATCALO_ETABN10_down	-0.0000005	EG_SCALE_MATCRYO_ETABN7_down	-0.0001003
EG_SCALE_MATCALO_ETABN10_up	-0.0000005	EG_SCALE_MATCRYO_ETABN7_up	0.0000995
EG_SCALE_MATCALO_ETABN11_down	-0.0000005	EG_SCALE_MATCRYO_ETABN8_down	-0.0001019
EG_SCALE_MATCALO_ETABN11_up	-0.0000005	EG_SCALE_MATCRYO_ETABN8_up	0.0001019
EG_SCALE_MATCALO_ETABN1_down	-0.0000402	EG_SCALE_MATCRYO_ETABN9_down	-0.0000227
EG_SCALE_MATCALO_ETABN1_up	0.0000387	EG_SCALE_MATCRYO_ETABN9_up	0.0000217
EG_SCALE_MATCALO_ETABN2_down	-0.0000335	EG_SCALE_MATID_ETABN0_down	-0.0001804
EG_SCALE_MATCALO_ETABN2_up	0.0000323	EG_SCALE_MATID_ETABN0_up	0.0001803
EG_SCALE_MATCALO_ETABN3_down	-0.0000558	EG_SCALE_MATID_ETABN1_down	-0.0001044
EG_SCALE_MATCALO_ETABN3_up	0.0000550	EG_SCALE_MATID_ETABN1_up	0.0001035
EG_SCALE_MATCALO_ETABN4_down	-0.0000699	EG_SCALE_MATID_ETABN2_down	-0.0001381
EG_SCALE_MATCALO_ETABN4_up	0.0000691	EG_SCALE_MATID_ETABN2_up	0.0001365
EG_SCALE_MATCALO_ETABN5_down	-0.0000689	EG_SCALE_MATID_ETABN3_down	-0.0000208
EG_SCALE_MATCALO_ETABN5_up	0.0000683	EG_SCALE_MATID_ETABN3_up	0.0000200
EG_SCALE_MATCALO_ETABN6_down	-0.0000597	EG_SCALE_MATPP0_ETABN0_down	-0.0000621
EG_SCALE_MATCALO_ETABN6_up	0.0000588	EG_SCALE_MATPP0_ETABN0_up	0.0000612
EG_SCALE_MATCALO_ETABN7_down	-0.0000095	EG_SCALE_MATPP0_ETABN1_down	-0.0001821
EG_SCALE_MATCALO_ETABN7_up	0.0000087	EG_SCALE_MATPP0_ETABN1_up	0.0001815
EG_SCALE_MATCALO_ETABN8_down	-0.0000282	EG_SCALE_OFC_down	0.0000616
EG_SCALE_MATCALO_ETABN8_up	0.0000269	EG_SCALE_OFC_up	-0.0006015
EG_SCALE_MATCALO_ETABN9_down	-0.0000005	EG_SCALE_PEDESTAL_down	0.0000820
EG_SCALE_MATCALO_ETABN9_up	-0.0000005	EG_SCALE_PEDESTAL_up	-0.0000834
EG_SCALE_MATCRYO_ETABN0_down	-0.0000306	EG_SCALE_PS_BARREL_B12_down	0.0006287
EG_SCALE_MATCRYO_ETABN0_up	0.0000297	EG_SCALE_PS_BARREL_B12_up	-0.0006303
EG_SCALE_MATCRYO_ETABN10_down	-0.0000106	EG_SCALE_PS_ETABN0_down	0.0000771
EG_SCALE_MATCRYO_ETABN10_up	0.0000099	EG_SCALE_PS_ETABN0_up	-0.0000781
EG_SCALE_MATCRYO_ETABN11_down	-0.0000130	EG_SCALE_PS_ETABN1_down	0.0000593
EG_SCALE_MATCRYO_ETABN11_up	0.0000124	EG_SCALE_PS_ETABN1_up	-0.0000603
EG_SCALE_MATCRYO_ETABN1_down	-0.0000538	EG_SCALE_PS_ETABN2_down	0.0000614
EG_SCALE_MATCRYO_ETABN1_up	0.0000526	EG_SCALE_PS_ETABN2_up	-0.0000624
EG_SCALE_MATCRYO_ETABN2_down	-0.0000474	EG_SCALE_PS_ETABN3_down	0.0001010
EG_SCALE_MATCRYO_ETABN2_up	0.0000463	EG_SCALE_PS_ETABN3_up	-0.0001020
EG_SCALE_MATCRYO_ETABN3_down	-0.0000810	EG_SCALE_PS_ETABN4_down	0.0000459
EG_SCALE_MATCRYO_ETABN3_up	0.0000805	EG_SCALE_PS_ETABN4_up	-0.0000466
		EG_SCALE_PS_ETABN5_down	0.0000634
		EG_SCALE_PS_ETABN5_up	-0.0000639

(a)

(b)

Table 4.7: Continuation of Table 4.6 : breakdown of PES relative errors that enter the fit for the inclusive fiducial region.

4.3.3.2 Systematic Uncertainties on the $m_{\gamma\gamma}$ Background Modelling

The choice of analytic function used to model the background $m_{\gamma\gamma}$ distribution can influence the measured cross-section, and this effect is quantified through the spurious signal, as described in Section 4.3.2.2.

4.3.3.3 Systematic Uncertainties on the Correction Factor ($\mathcal{C}_{\mathcal{F}}$)

In particle physics, the outcome of a measurement is the result of an underlying physical process intended for measurement, potentially involving unknown physics phenomena, convoluted with the response of the detector. The finite resolution of the detector causes smearing of the quantities intended for measurement. Additionally, the detector has limited acceptance and efficiency, which may result in missing certain events if they produce particles that do not cross the active detector regions or due to reconstruction inefficiency. The measurements presented in the chapter are based on counting Higgs boson signal events in particular regions (bins) of the phase space. Consequently, the finite resolution of the detector leads to events migrating to incorrect bins. The procedure for correcting resolution migrations and detector efficiency is known as unfolding.

Unfolding is particularly challenging in particle physics because measurements include statistical fluctuations and potential background events. For the measurement of inclusive fiducial Higgs boson production cross-sections presented in this thesis, the unfolding procedure is an essential component of the analysis as it facilitates comparison of theory predictions with measured cross-sections, resulting in long-lasting measurements that can be compared to theoretical models developed long after the measurement is completed. Additionally, unfolding enables easier comparison and combination with results from other experiments, as the data are deconvoluted from detector effects.

The measured detector-level signal yields are thus corrected for detector effects through an unfolding procedure that accounts for resolution, causing migration between bins of detector-level and particle-level quantities; efficiencies, resulting in some particle-level candidates failing the detector-level selection, and out-of-fiducial events, where particle-level candidates outside the fiducial volume pass the detector-level selection. Theoretical (refer Section 4.3.3.3) and experimental uncertainties (refer Section 4.3.3.3) can affect the expected signal yield in the fiducial region by impacting the correction factor ($\mathcal{C}_{\mathcal{F}}$), with theoretical uncertainties introducing a slight model dependence to the measurement. These sources of uncertainty also affect the fiducial acceptance (see Appendix A.1.3) and are relevant when extrapolating the fiducial cross-section measurement results to the full phase space.

A detailed discussion on the formalism of unfolding is presented in [184]. For this analysis, a matrix inversion unfolding procedure is employed. R_{ij} is the response matrix element that relates the number of signal events reconstructed in a certain bin j at detector level to the number of events belonging to a certain bin i at particle level: $n_i^{\text{det}} = R_{ij} n_j^{\text{ptcl}}$. This includes both the efficiency of the selection and any extrapolation between the detector and particle level phase space regions considered. The response matrices are derived from migration matrices (or yield matrices) that tabulate the number of events at particle level and detector level in two dimensions. For the inclusive region, the migration matrix has only 2×2 bins, so the response matrix reduces to a single correction factor. This factor describes the ratio of signal events reconstructed in the signal region (n_{reco}) to the events selected at truth level in the fiducial region (n_{truth}), given by $\mathcal{C}_{\mathcal{F}} = n_{\text{reco}}/n_{\text{truth}}$. The value of $\mathcal{C}_{\mathcal{F}}$ is found to be 0.7163. Correction factors are also derived separately for each Higgs production mode, with the results summarized in Table 4.8. The migration matrix for the inclusive fiducial region is shown in Figure 4.6. The correction factors are derived by rescaling the matrices for each production mode using the Standard Model (SM) cross-section, σ_S^{SM} , for each production mode, and the total initial weights generated, N_S .

Production mode	Reco yield n_{reco}	Truth n_{truth}	Ratio $n_{\text{reco}}/n_{\text{truth}}$
ggF	1337.7	1869.9	0.7154 ± 0.0016
VBF	105.7	146.0	0.7241 ± 0.0024
ZH	21.5	29.9	0.7194 ± 0.0049
ggZH	3.9	5.3	0.7467 ± 0.0124
W^-H	13.5	18.8	0.7179 ± 0.0076
W^+H	18.8	26.2	0.7190 ± 0.0080
ttH	15.0	21.0	0.7166 ± 0.0045
Total	1516.2	2117	0.7163 ± 0.0015

Table 4.8: Yields and correction factors for different signal production modes. The uncertainty is determined from the statistical uncertainty of the simulated samples.

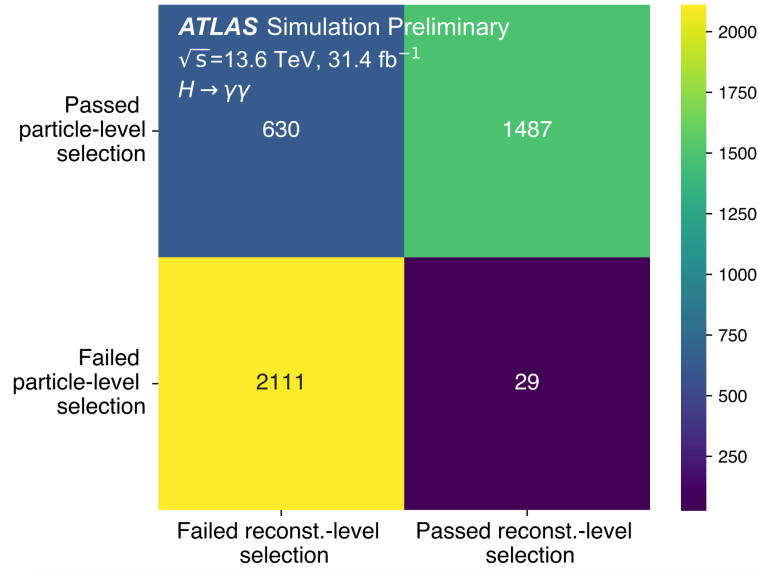


Figure 4.6: Number of MC signal events (normalised to 31.4fb^{-1}) selected or rejected by the selections applied at reconstruction (x-axis) and particle (fiducial, y-axis) level.

Unfolding Uncertainties

The fiducial cross-section measurements are intended to be as model-independent as possible, as introduced in Section 4.1.1 to allow comparison with different theoretical predictions. The unfolding procedure might introduce a model dependence since it corrects the experimentally determined yields using corrections estimated from the simulation. Model dependence may be introduced in several ways. If the phase space region sampled by the detector differs from the fiducial phase space at the particle level, the calculation of the matrix and correction factors implicitly assumes that distributions follow Standard Model expectations during extrapolation. Additionally, if the correction factors depend on the Higgs production modes, it necessitates assuming knowledge of the relative amplitudes of these modes to correct the data. Furthermore, if the correction factors rely on the modeling of Higgs kinematics and event properties predicted by the matrix element calculation, as well as the hadronization and underlying event (UE) model, an additional modeling uncertainty is introduced.

Choosing a fiducial region as close as possible to the detector acceptance, including a particle-level photon isolation requirement, minimizes the aforementioned dependencies. Any residual model dependence on correction factors is treated as a systematic uncertainty. In addition to the modeling uncertainties, the response matrices are affected by uncertainties in the experimental efficiency and resolution of the ATLAS detector.

Theoretical and experimental uncertainties in the response matrix and correction factors result in uncertainties in the measured cross-sections, which are estimated as described in the following sections.

Theoretical Uncertainties

The model dependence of the correction factors and the corresponding uncertainty is evaluated based on the following variations:

- The relative contributions of different Higgs production mechanisms are varied within their experimental bounds based on the latest combined measurements.
- Assessing the impact of underlying event modeling by comparing simulations produced with

Pythia8 and Herwig7.

- Evaluating the impact of matrix element modeling by comparing nominal samples generated with Powheg to alternative ones produced using MadGraph for the matrix element calculation.
- Dalitz events ($H \rightarrow \gamma\gamma^* \rightarrow \gamma f \bar{f}$) are currently excluded at the generator level. Consequently, while their branching ratio uncertainty previously affected the correction factors, it is not considered in the current analysis. Any uncertainty stemming from Dalitz events is addressed by the spurious signal uncertainty.

Signal composition uncertainty : The final correction factor $\mathcal{C}_{\mathcal{F}}$ is calculated by combining the $\mathcal{C}_{\mathcal{F}}$ values from all production modes of the Higgs boson, weighted by their SM cross-sections. This may introduce model dependence if the $\mathcal{C}_{\mathcal{F}}$ values vary significantly among the different production modes. A signal composition uncertainty is estimated by adjusting the Standard Model cross-sections of the different production modes by a certain relative amount, determined by the ratio between the uncertainty and the central value of the measurement of that production mode's cross-section obtained by ATLAS through the combination of several Higgs boson decay channels [231]. The methodology is elaborated in detail in Appendix A.4.3 of Ref [232]. The relative variations of the production cross-sections employed to estimate these uncertainties are:

$$\text{ggF} : \pm 6.8\%, \text{VBF} : \pm 11.7\%, \text{WH} : \begin{smallmatrix} +19.5\% \\ -18.6\% \end{smallmatrix}, \text{ttH} : \begin{smallmatrix} +20.6\% \\ -18.6\% \end{smallmatrix}$$

The impact of signal composition uncertainties on correction factor are summarized in Table 4.9 (TheorySig_SigComp_*).

Underlying event and parton shower modelling : The simulation samples used in this analysis are interfaced with showering and hadronization models as described in Section 4.2.2. These models convert inclusive parton-level cross-sections into exclusive particle-level counterparts as well as simulate the underlying events (UE), which can cause migrations in or out of the fiducial region, thus contributing to sources of uncertainty in the $\mathcal{C}_{\mathcal{F}}$ s. To estimate these uncertainties, the correction factors ($\mathcal{C}_{\mathcal{F}}$ s) are computed using two samples with the same matrix element calculation but interfaced with different hadronization models (Herwig7 or Pythia8). The impact of the alternative parton showering model on the cross-section in the inclusive region was found to be at the level of 0.5% using the Run 2 samples. Given its small magnitude, this effect is disregarded in the current iteration of the analysis.

Matrix element calculation : The matrix element uncertainty is assessed using simulated signal event samples generated with MadGraph5 instead of Powheg. The response matrix is then computed using these alternative samples, and the relative difference of each matrix element compared to the one obtained with the nominal samples is incorporated into the likelihood (see Section 4.3.4), multiplied by the corresponding nuisance parameter representing this source of uncertainty. Due to the parton shower configurations of the MadGraph5 samples (Herwig for VBF, Pythia for the others), the relative differences of the response matrices are determined concerning the Powheg+Herwig sample for VBF and the Powheg+Pythia8 sample for the others, thereby avoiding the double counting of parton shower uncertainties. Based on the Run 2 analysis samples, it was observed that the total expected yield from the MadGraph5 sample differed from the nominal Powheg sample by only -0.1% . Given the negligible magnitude of this effect, this source of uncertainty is disregarded in the current iteration of the analysis.

Additional uncertainties are considered when extrapolating the fiducial cross-section to the full phase space to derive the total cross-section. These include a 1.4% uncertainty on the acceptance (see Appendix A.1.3), mainly from missing higher-order terms in perturbative QCD, parton shower modeling, PDFs, and α_s [165, 178]. The theoretical uncertainty on the calculated $H \rightarrow \gamma\gamma$ branching ratio of 2.9% is also included.

Experimental Uncertainties

Several experimental uncertainties impact the correction factor $\mathcal{C}_{\mathcal{F}}$, including uncertainties related to the efficiency of the photon trigger, identification and isolation selections, the impact of the di-photon vertex selection, and the estimation of the photon energy scale and resolution. All other photon-related uncertainties are assessed using Run 2 data, with additional uncertainties accounting for changes in conditions between Run 2 and Run 3, as well as changes to the MC simulation.

Trigger efficiency : The efficiency of the di-photon trigger is estimated with a preliminary uncertainty of about 4% for Run 3 data based on the bootstrap method, detailed in [233, 234]. The single photon trigger contributes only to 0.1% of the selected signal events and its uncertainty is therefore neglected.

Vertex selection efficiency : The vertex selection uses pointing information from the diphoton system to select the primary vertex candidate of the event, as described in Section 4.3.1.2. Differences in the efficiency of selecting the primary vertex between data and simulation can impact the correction factors. Consequently, an uncertainty on the correction factor is assigned based on the difference in the vertex selection efficiency between data and simulation using $Z \rightarrow ee$ events. The ratio of the efficiencies is used to increase the weights of events in the simulation with $|z_{\text{reconstructed}} - z_{\text{true}}| > 0.3$ mm. The resulting impact on $\mathcal{C}_{\mathcal{F}}$ from this efficiency uncertainty amounts to below 0.03%.

Photon identification efficiency : The selected photons are required to pass tight identification criteria as outlined in Section 4.3.1.3. The efficiency of this selection, denoted as $\epsilon_{\text{tightID}}$, in simulated events is corrected to match the efficiency observed in data, as outlined in [235]. A per-photon correction factor is subsequently derived to accommodate discrepancies in efficiency between data and simulation. The uncertainties associated with these correction factors are then propagated to the unfolding correction factors by adjusting the photon identification efficiency correction factors within their uncertainties. This variation will cause events to migrate across the boundaries of the fiducial region. The difference between the correction factor under these variations and the nominal one is regarded as the uncertainty, estimated to impact $\mathcal{C}_{\mathcal{F}}$ by about 5%, as summarized in Table 4.9 (PH_EFF_ID_Uncertainty).

Photon isolation efficiency : The uncertainty on the photon isolation efficiency is determined using a methodology similar to that of the photon identification, as detailed in [235]. This uncertainty is estimated to have a 1.6% impact on $\mathcal{C}_{\mathcal{F}}$ as shown in Table 4.9 (PH_EFF_ISO_Uncertainty).

Photon energy scale and resolution : The PES and PER uncertainties not only affect the signal invariant mass distribution, as detailed in Section 4.3.3.1, but also impact the correction factors due to migrations across the boundaries of the fiducial region, with a maximal impact on $\mathcal{C}_{\mathcal{F}}$ below 0.1%. Table 4.9 shows the combined effect of all scale (EG_SCALE_ALL) and resolution (EG_RESOLUTION_ALL) uncertainties on the correction factors.

Pileup uncertainties : A pileup reweighting procedure is performed, wherein the distribution of the average number of interactions per bunch crossing, $\langle \mu \rangle$, in the simulation is reweighted to match that of the data, as outlined in Section 4.2.2.3. The pileup modeling is based on simulations of inelastic pp collisions. The pileup reweighting is varied to account for the uncertainty in the ratio between the predicted and measured inelastic cross-section in the fiducial volume. This uncertainty is evaluated by varying the inelastic cross-section value by $\pm 9\%$ to match the observed pileup distribution in the data with that in the simulation [236]. The impact of these variations on the correction factors is summarized in Table 4.9 (PRW).

Variation	Reco yield n_{reco}	Truth n_{truth}	Ratio	Uncertainty
Nominal	1519.3	2121.3	0.7162	
EG_SCALE_ALL_up	1520.0	2121.3	0.7166	0.0006
EG_SCALE_ALL_down	1518.2	2121.3	0.7157	-0.0007
EG_RESOLUTION_ALL_up	1519.1	2121.3	0.7162	-0.0001
EG_RESOLUTION_ALL_down	1519.3	2121.3	0.7162	0.0001
PH_EFF_ID_Uncertainty_up	1602.4	2121.3	0.7554	0.0547
PH_EFF_ID_Uncertainty_down	1438.4	2121.3	0.6781	-0.0532
PH_EFF_TRIGGER_Uncertainty_up	1532.9	2121.3	0.7226	+0.02
PH_EFF_TRIGGER_Uncertainty_down	1505.7	2121.3	0.7098	-0.02
PH_EFF_ISO_Uncertainty_up	1544.4	2121.3	0.7280	0.0165
PH_EFF_ISO_Uncertainty_down	1494	2121.3	0.7045	-0.0164
PRW_up	1492.1	2121.3	0.7280	-0.0128
PRW_down	1541.2	2121.3	0.7045	0.0103
TheorySig_SigComp_ggH_up	1610.2	2248.7	0.7161	+0.000059
TheorySig_SigComp_ggH_down	1428.0	1993.9	0.7162	-0.000066
TheorySig_SigComp_VBF_up	1531.5	2138.4	0.7162	+0.000094
TheorySig_SigComp_VBF_down	1506.7	2104.2	0.7160	-0.000096
TheorySig_SigComp_ZH_up	1524.0	2128.1	0.7161	+0.000013
TheorySig_SigComp_ZH_down	1514.5	2114.8	0.7161	-0.000013
TheorySig_SigComp_ggZH_up	1520.0	2122.5	0.7161	+0.000016
TheorySig_SigComp_ggZH_down	1518.3	2120.2	0.7161	-0.000015
TheorySig_SigComp_WmH_up	1521.7	2125.0	0.7161	+0.000004
TheorySig_SigComp_WmH_down	1516.6	2117.8	0.7161	-0.000004
TheorySig_SigComp_WpH_up	1522.8	2126.4	0.7161	+0.000005
TheorySig_SigComp_WpH_down	1515.6	2116.4	0.7161	-0.000005
TheorySig_SigComp_ttHtH_up	1522.2	2125.6	0.7161	+0.000005
TheorySig_SigComp_ttHtH_down	1516.3	2117.4	0.7161	-0.000005

Table 4.9: Summary of theoretical and experimental uncertainties on the unfolding correction factors.

4.3.4 Signal Yield Extraction

The Higgs boson signal yield, ν^{sig} (see Equation 4.3.4), within the inclusive fiducial region, is determined by performing an unbinned maximum likelihood fit to the reconstructed di-photon invariant mass spectrum spanning 105–160 GeV. This fit utilizes probability density functions (PDFs) for the signal parametrization and the background model, as described by analytic functions outlined in Sections 4.3.2.1 and 4.3.2.2, respectively. The likelihood function, presented in Equation 4.3.7, is constructed for the inclusive region, and the product of these likelihoods is maximized.

$$\mathcal{L}(m_{\gamma\gamma}; \nu^{\text{sig}}, \nu^{\text{bkg}}) = \frac{e^{-\nu}}{n!} \prod_j \frac{1}{\nu} \left[\nu^{\text{sig}} \mathcal{S}(m_{\gamma\gamma}^j; \theta_k^{\text{sig}}) + \nu^{\text{bkg}} \mathcal{B}(m_{\gamma\gamma}^j; \theta_k^{\text{bkg}}) \right] \quad (4.3.7)$$

Here ν^{sig} and ν^{bkg} represent the fitted number of signal and background events, respectively. $\nu = \nu^{\text{sig}} + \nu^{\text{bkg}}$ is the mean value of the underlying Poisson distribution for the n events, $m_{\gamma\gamma}^j$ is the di-photon invariant mass for event j , $\mathcal{S}(m_{\gamma\gamma}^j; \theta_k^{\text{sig}})$ is the signal PDF, a function of the vector of nuisance parameters θ_k^{sig} describing the signal shape and the different uncertainties affecting it, as detailed in Section 4.3.3.1, and $\mathcal{B}(m_{\gamma\gamma}^j; \theta_k^{\text{bkg}})$ is the background PDF, a function of the vector of nuisance parameters θ_k^{bkg} , describing the different shape and normalization parameters of the background function detailed in Section 4.3.2.2.

Signal shape nuisance parameters In the simultaneous fit of the di-photon mass spectrum, two sources of uncertainty on the signal shape are considered: uncertainties in the resolution due to photon energy resolution (θ_{EnRes}) and uncertainties in the peak position due to photon energy scale (θ_{EnScale}). These uncertainties in the signal shape are incorporated into the likelihood as multiplicative constraints $\prod_k C_k$. The choice of constraint, C_k , depends on the type of uncertainty.

The energy scale uncertainties are implemented using a Gaussian constraint. For each uncertainty in θ_{EnScale} , the pulls are treated asymmetrically. The constraint term $C_{\text{EnScale}}(\theta_{\text{EnScale}}; 0, 1)$ has a mean of $\theta_{\text{EnScale}} = 0$ and a width of 1, ensuring that values of $\theta_{\text{EnScale}} = \pm 1$ correspond to $\pm 1\sigma$ pulls on the nuisance parameters, thereby correctly penalizing the likelihood accordingly.

The energy resolution uncertainties are implemented using a log-normal constraint, as they can

only take on positive values. The log-normal constraint is formulated as follows:

$$\Theta_{EnRes} = \exp\left(\theta_{EnRes} \sqrt{\log(1 + \delta_{EnRes}^2)}\right), \quad (4.3.8)$$

Here, θ_{EnRes} and δ_{EnRes} represent the nuisance parameter and the resolution uncertainty values for a given source of resolution uncertainty.

Higgs mass nuisance parameters The uncertainty associated with the measurement of the Higgs boson mass, $m_H = 125.09 \pm 0.24$ GeV, is incorporated as an extra nuisance parameter enabling shifts to the signal peak position. Within the likelihood, it is represented by a symmetric Gaussian constraint $C_{MassUncert}(\theta_{MassUncert}; 0, 1)$.

The nuisance parameters are allowed to float in the fit to data, and any deviations from the central value of these parameters will result in a decrease in the likelihood. Uncertainties that do not affect the shape of the diphoton mass spectrum are excluded from the fit and are addressed as components of the correction for detector effects (see Section 4.3.3.3). The spurious signal, as outlined in Section 4.3.2.2, is not incorporated into the fit. Instead, it is combined in quadrature with the uncertainty in the signal yield derived from the fit.

The total number of nuisance parameters in the fitting equals to 85+N, where it encompasses 74 (PES uncertainties) + 10 (PER uncertainties) + N (background function parameters) + 1 (Higgs mass uncertainty). Therefore, the free parameters in the fit are $\theta_{EnScale}$, θ_{EnRes} , $\theta_{Background}$, ν_{sig} , and ν_{bkg} .

4.3.5 Results

The invariant mass spectrum, superimposed with the background and signal functions obtained from the fit to the data, is shown in Figure 4.7.

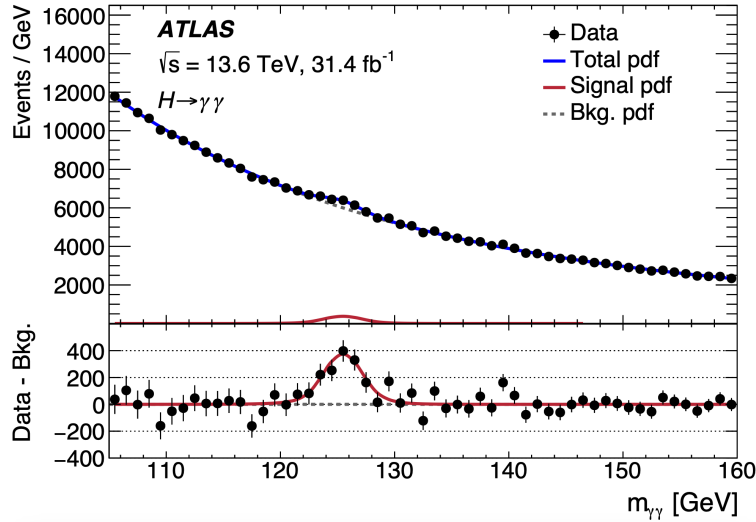


Figure 4.7: The diphoton invariant mass spectrum within the $H \rightarrow \gamma\gamma$ fiducial region, as observed in the data. The signal, background, and total probability density functions (PDFs) derived from the fit to the data in the $m_{\gamma\gamma} = 105 - 160$ GeV range are also displayed.

The fiducial cross-section value, extracted from the fit to this $m_{\gamma\gamma}$ spectrum, is measured to be $\sigma_{fid}(pp \rightarrow H \rightarrow \gamma\gamma) = 76^{+14}_{-13} \text{ fb} = 76 \pm 11(\text{stat})^{+9}_{-7}(\text{syst}) \text{ fb}$. This measurement is consistent with the SM prediction of $67.5 \pm 3.4 \text{ fb}$. The SM prediction is derived using state-of-the-art cross-section calculations [200], corrected for acceptance effects, which are assessed using simulated samples, described in Section 4.2.2.

The fit to the data provides an estimate of the signal yield along with its total uncertainty. Table 4.10 provides a detailed breakdown of the total uncertainty into its individual components, while Figure 4.8 illustrates the ranking of nuisance parameters based on their impact on the fit to the data. The statistical component is obtained by fixing all the nuisance parameters associated with systematic uncertainties to their best-fit values. The grouped systematic uncertainties are determined by subtracting the uncertainties in quadrature between two fits: one with the corresponding nuisance parameters fixed to their best-fit values, and the other with those parameters free-floating during the fit. The largest source of uncertainty arises from the data statistics. Among the systematic uncertainties, the most significant contributors are the spurious signal, followed by photon energy scale and resolution, and photon selection efficiency uncertainties. Tables 4.5, 4.6, 4.7, 4.9 summarizes all nuisance parameters and their respective groups.

Source	Uncertainty [%]
Statistical uncertainty	14.0
Systematic uncertainty	10.9
Photon trigger and selection efficiency	6.7
Background modelling (spurious signal)	6.0
Photon energy scale & resolution	5.5
Luminosity	2.2
Pile-up modelling	1.1
Higgs boson mass	0.1
Theoretical (signal) modelling	<0.1
Total	17.7

Table 4.10: Breakdown of the relative uncertainties in the inclusive di-photon fiducial cross-section measurement.

Additionally, assuming SM values for the acceptance and the di-photon branching fraction, the fiducial measurement is extrapolated to the full phase space. This extrapolation yields a total cross-section value of $\sigma(pp \rightarrow H) = 67_{-12}^{+13}$ pb at 13.6 TeV, which is consistent with the SM prediction of $\sigma(pp \rightarrow H) = 59.8 \pm 2.6$ pb. When performing this extrapolation, additional uncertainties on the acceptance and the branching fraction are considered (see Section 4.3.3).

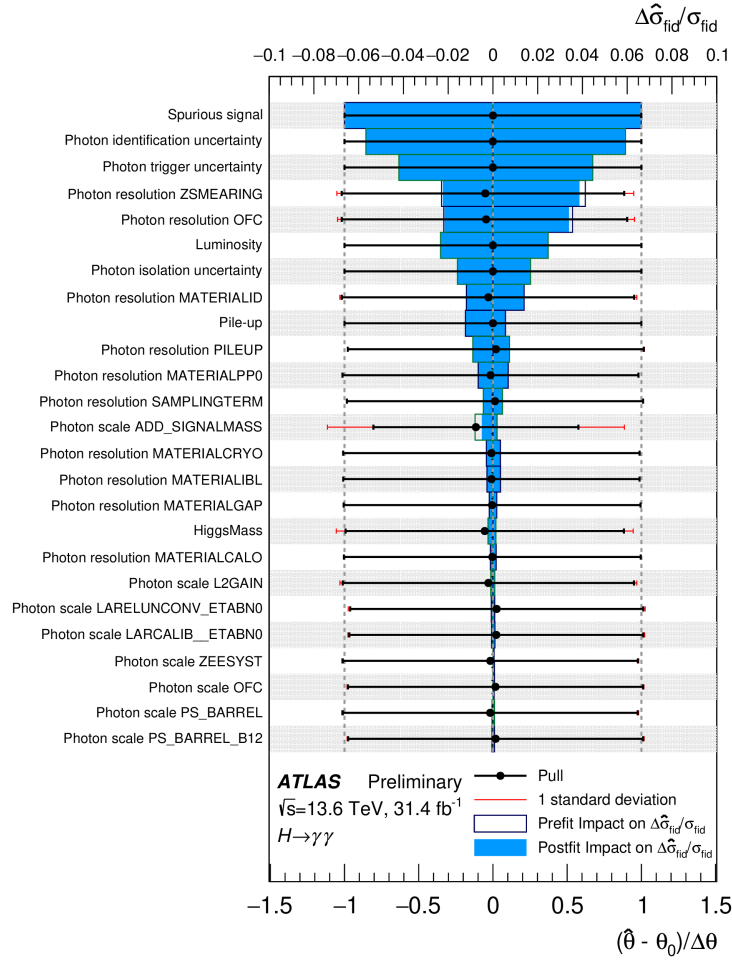


Figure 4.8: Impact of systematic uncertainties on the fitted Higgs boson cross-section. The figure displays the effect of the 25 most significant systematic uncertainties, ranked by their impact on the cross-section. The filled boxes illustrate the relative impact (see top x-axis) of varying each individual nuisance parameter by its fitted uncertainty (both upward and downward), while allowing all other parameters to vary. This method accounts for correlations between uncertainties. The dots (see bottom x-axis) indicate deviations of the fitted nuisance parameters from their nominal values, normalized to their nominal uncertainties, with error bars showing the fitted uncertainties relative to these nominal uncertainties. The nuisance parameter Photon scale ADD_SIGNALMASS represents an additional 0.4% uncertainty in the photon energy scale and is constrained by data due to its sensitivity to the Higgs boson mass.

4.3.5.1 Combination with the $H \rightarrow ZZ^* \rightarrow 4l$ channel

The measurement of the Higgs boson inclusive fiducial cross-section is also performed in the $H \rightarrow ZZ^* \rightarrow 4l$ channel using the early Run 3 2022 dataset. A summary of the fiducial selection in the $H \rightarrow 4l$ channel is presented in Table 4.11. The results of this measurement, shown in Figure 4.9, are in excellent agreement with the Standard Model, similar to the observations in the $H \rightarrow \gamma\gamma$ channel.

The fiducial cross-section value, extracted from the m_{4l} template fit detailed in Ref [173], is measured to be $\sigma_{fid} = 2.80 \pm 0.70(\text{stat.}) \pm 0.21(\text{syst.}) \text{ fb}$. This result is consistent with the Standard Model prediction of $\sigma_{fid,SM} = 3.67 \pm 0.19 \text{ fb}$.

Assuming SM values for the fiducial acceptances and branching fractions of the two channels, the fiducial measurements are extrapolated to the full phase space. The total Higgs boson production cross-section at 13.6 TeV is measured to be $\sigma(pp \rightarrow H) = 67^{+12}_{-11} \text{ pb}$ using the $H \rightarrow \gamma\gamma$ channel and $\sigma(pp \rightarrow H) = 46 \pm 12 \text{ pb}$ using the $H \rightarrow 4l$ channel. The two measurements are compatible with a p-value of 20% [173].

Leptons	
Leptons	$p_T > 5 \text{ GeV}, \eta < 2.7$
Lepton selection and pairing	
Lepton kinematics	$p_T > 20, 15, 10 \text{ GeV}$
Leading pair (m_{12})	SFOC lepton pair with smallest $ m_Z - m_{\ell\ell} $
Subleading pair (m_{34})	remaining SFOC lepton pair with smallest $ m_Z - m_{\ell\ell} $
Event selection (at most one quadruplet per event)	
Mass requirements	$50 \text{ GeV} < m_{12} < 106 \text{ GeV}$ and $12 \text{ GeV} < m_{34} < 115 \text{ GeV}$
Lepton separation	$\Delta R(\ell_i, \ell_j) > 0.1$
J/ψ veto	$m(\ell_i, \ell_j) > 5 \text{ GeV}$ for all SFOC lepton pairs
Mass window	$105 \text{ GeV} < m_{4\ell} < 160 \text{ GeV}$
If extra lepton with $p_T > 12 \text{ GeV}$	quadruplet with largest matrix element value

Table 4.11: Summary of the event selection criteria defining the fiducial phase space for the $H \rightarrow ZZ^* \rightarrow 4l$ cross-section measurement. SFOC lepton pairs refer to same-flavour-opposite-charge lepton pairs [173].

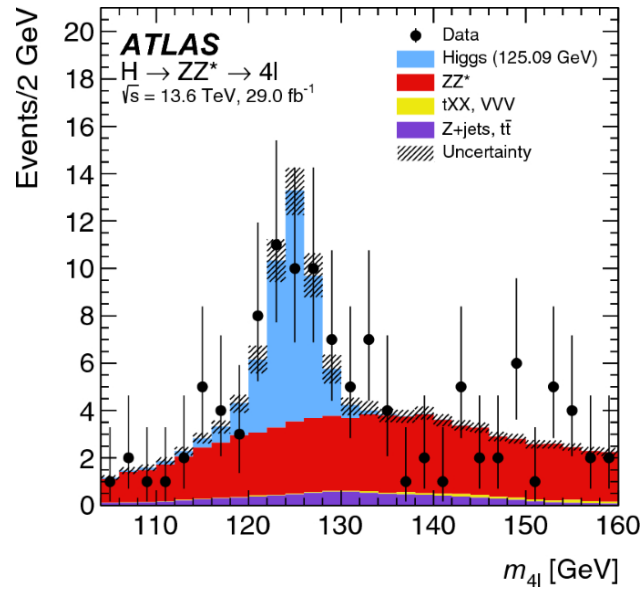


Figure 4.9: The observed and expected inclusive four-lepton invariant mass distribution for the selected Higgs boson candidates, shown for an integrated luminosity of 29.0 fb^{-1} at $\sqrt{s} = 13.6 \text{ TeV}$. The hatched band represents the uncertainty in the prediction, including the theoretical uncertainties in the SM cross-section for the signal and the main background processes. The label tXX indicates the sum of the $t\bar{t}W$ and $t\bar{t}Z$ processes.

Experimental and theoretical uncertainties that affect both channels are correlated through common nuisance parameters. The correlated experimental uncertainties include those related to the integrated luminosity, the description of pile-up in the simulation, the common electron-photon energy scale, the Higgs boson mass value, and the relative contributions of the different Higgs boson production modes. Additionally, the common sources of theoretical uncertainty in the $H \rightarrow ZZ^* \rightarrow 4l$ and $H \rightarrow \gamma\gamma$ branching fractions such as α_s , b - and c -quark masses, and partial decay widths into the main decay channels, like two vector bosons, two gluons, or a $b\bar{b}$ pair are also correlated. Furthermore, the theoretical uncertainties in the acceptance factor, due to missing higher-order QCD effects, PDF variations, variations in the modeling of the parton shower, and signal composition, are also correlated.

The total Higgs boson production cross-section, obtained by combining the $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ^* \rightarrow 4l$ results, is $\sigma(pp \rightarrow H) = 58.2 \pm 7.5(\text{stat.}) \pm 4.5(\text{syst.})$ pb at 13.6 TeV. All three results; $H \rightarrow \gamma\gamma$, $H \rightarrow ZZ^* \rightarrow 4l$, and their combination, are in agreement with the Standard Model prediction of $\sigma(pp \rightarrow H)_{SM} = 59.9 \pm 2.6$ pb. The values of the total cross-section determined from this analysis, along with those from previously published ATLAS studies [171, 172], are shown in Figure 4.10 as a function of the pp center-of-mass energy. The measurements at the new center-of-mass energy of 13.6 TeV are in good agreement with the SM prediction.

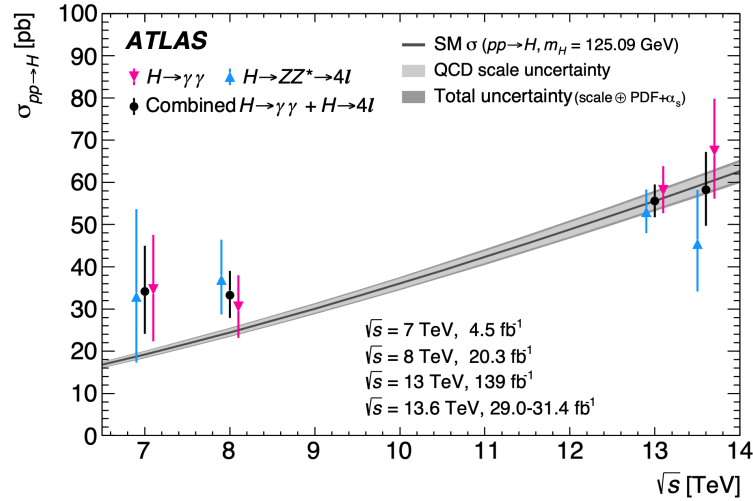


Figure 4.10: Values of the $\sigma(pp \rightarrow H)$ measurements from this study and previous ATLAS publications [171, 172] as a function of the pp center-of-mass energy. The SM predicted values and their uncertainties are depicted by the shaded band. The results for individual channels are offset along the x-axis for clarity [173].

4.3.6 Outlook

The pp collision data recorded by the ATLAS detector in 2022 at $\sqrt{s} = 13.6$ TeV are utilized to obtain the first measurements of the Higgs boson production cross-sections for the $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ^* \rightarrow 4\ell$ channels, with integrated luminosities of 31.4 fb^{-1} and 29.0 fb^{-1} , respectively. These measurements are restricted to kinematic phase spaces of the Higgs boson decay products that closely match the selection criteria applied at the detector level and are corrected for detector effects.

Assuming SM values for the acceptances and branching fractions, the fiducial cross-sections are extrapolated to the full phase space. The total Higgs boson production cross-sections are determined to be $\sigma_{fid,\gamma\gamma} = 76^{+14}_{-13} \text{ fb}$ for the $H \rightarrow \gamma\gamma$ channel and $\sigma_{fid,4\ell} = 2.80 \pm 0.74 \text{ fb}$ for the $H \rightarrow ZZ^* \rightarrow 4\ell$ channel. These results are consistent with the corresponding SM predictions of $67.6 \pm 3.7 \text{ fb}$ and $3.67 \pm 0.19 \text{ fb}$, respectively.

Furthermore, extrapolating the fiducial measurements to the full phase space, the total Higgs boson production cross-sections are $\sigma(pp \rightarrow H \rightarrow \gamma\gamma) = 67^{+12}_{-11} \text{ pb}$ and $\sigma(pp \rightarrow H \rightarrow ZZ^* \rightarrow 4\ell) = 46 \pm 12 \text{ pb}$ at 13.6 TeV. Combining these measurements yields a total cross-section of $\sigma(pp \rightarrow H) = 58.2 \pm 8.7 \text{ pb}$, which is in agreement with the SM prediction of $\sigma(pp \rightarrow H)_{\text{SM}} = 59.9 \pm 2.6 \text{ pb}$.

CHAPTER 5

The High-Luminosity LHC and the ATLAS Inner Tracker

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Section 2.1 presents a comprehensive overview of the LHC and its flagship experiment, ATLAS, emphasizing their pivotal roles in advancing the understanding of fundamental particle physics. Since opening a new frontier in energy exploration in 2010, the LHC has supported a global community of approximately 9,000 scientists dedicated to the study of fundamental particle physics and hadronic matter under extreme conditions of temperature and density [237]. The LHC requires a significant upgrade beyond its Run 3 operations to sustain and extend its discovery potential. The High Luminosity Large Hadron Collider (HL-LHC), an ambitious upgrade project of the LHC, is designed to attain instantaneous luminosities 5 to 7.5 times larger than the nominal LHC design value, thereby enabling the LHC experiments to enlarge their data set by an order of magnitude over the 12 years of HL-LHC operation compared to the LHC baseline program. This novel machine configuration will rely on several innovative technologies, including cutting-edge Nb₃Sn superconducting magnets [238], compact superconducting crab cavities with ultra-precise phase control for beam rotation [239], new technology for beam collimation such as bent crystals [240], and high-power, lossless MgB₂ superconducting links to power the HL-LHC inner triplet magnets,

which play a crucial role in focusing the beam to a diameter of 5 μm just before collisions, among others. To ensure sustained operation over the next decade within this demanding physical environment, the ATLAS detector requires upgrades to its inner trackers, muon systems, calorimeter systems, and trigger and data acquisition system. Similar upgrades will be implemented for the CMS detector, although details are not covered here. This chapter serves as a concise overview of the HL-LHC project (Section 5.1), its profound physics potential (Section 5.2), pioneering work on the new ATLAS Inner Tracker (ITk, Section 5.4), and the module development activities (Section 5.4.4) at Laboratoire de physique nucléaire et de hautes énergies (LPNHE) for quad module preproduction, to which contributions were made.

5.1 The High Luminosity LHC (HL-LHC) Project Overview

Figure 5.1 shows the latest timeline of LHC upgrade program. During Run 1 (2010-2012), the LHC operated at center-of-mass energies of 7 and 8 TeV with an initial bunch spacing of 50 ns, later predominantly using 25 ns, the nominal design value. Following the consolidation of electrical splices between superconducting magnets and various other measures during Long Shutdown 1 (LS1), Run 2 (2015-2018) commenced at a center-of-mass energy of 13 TeV and maintained 25 ns bunch spacing. By 2016, the luminosity reached $1 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$, and a peak luminosity of $2 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$ was achieved in 2018 due to smaller beam emittances from the injectors and a reduced amplitude function at the IP (β^*) of 30 cm compared to the nominal value of 55 cm. Although this luminosity nearly reached the ultimate value outlined in the original LHC design report, it was accomplished with the nominal bunch population of $\approx 1.2 \times 10^{11}$ protons per bunch rather than the ultimate value of 1.7×10^{11} protons per bunch. This high luminosity, coupled with exceptional machine and injector availability, resulted in a record annual integrated luminosity of 65 fb^{-1} in 2018. The Run 3 of the LHC, spanning from 2022 to 2025, aims to increase the total integrated luminosity even further, with the present goal set at 350 fb^{-1} by the end of Run 3 operations, surpassing the initial LHC target of $\approx 300 \text{ fb}^{-1}$. In 2018 it was experimentally confirmed that the peak luminosity is limited at the value of around $2 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$ by the heat deposition from luminosity debris and the lack of sufficient cooling of the inner triplet magnets [237].



Figure 5.1: The LHC roadmap outlines the trajectory for the next decade and beyond, illustrating the progression of collision energy (upper line) and luminosity (lower line). The first long shutdown (LS1) in 2013–2014 achieved the design parameters of beam energy and luminosity. Subsequently, the second-long shutdown (LS2) in 2018–2019 focused on LHC consolidation and HL-LHC underground excavation, along with upgrades to the LHC injectors and Phase 1 enhancements to the LHC detectors. Following the long shutdown (LS3) from 2026 - 2028, the machine will transition into its high-luminosity configuration [237].

To harness the full physics potential of the LHC, CERN launched the HL-LHC project in late 2010 with the goal to deliver an integrated luminosity of at least 250 fb^{-1} per year in each of the two general-purpose detectors, ATLAS and CMS, with the ultimate goal of reaching 3000 fb^{-1} over the span of approximately 12 years following the upgrade. The ATLAS detector will be upgraded to handle an average pile-up of at least 140 (ultimately 200), corresponding to an instantaneous luminosity of $\approx 5 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ (ultimately $7.5 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$) for operation with 25 ns beams consisting of 2760 bunches at 7 TeV [237].

Increasing the instantaneous luminosity results in a higher number of collisions per bunch crossing, which increases the likelihood of observing rare events. However, this also leads to a higher overall interaction rate, including many non-interesting events, necessitating finer detector granularity and larger bandwidth to effectively manage the collision data. The new, all silicon ATLAS Inner Tracker (ITk) replacing the current Inner Detector (Section 2.2.4) is introduced in Section 5.4. The increased integrated luminosity leads to more radiation damage in the detectors, requiring more radiation-tolerant schemes. Section 6.2 provides a detailed discussion of a novel lightweight algorithm for modeling the radiation damage effects in the ITk planar sensors.

5.2 The Physics Potential at HL-LHC

The successful operation of the LHC and the outstanding performance of the ATLAS, CMS, ALICE, and LHCb detectors during the Run 1, 2, and 3 operations of the LHC have enabled diverse physics investigations, confirming the validity of the Standard Model (SM) of particle physics (see Section 1.1) up to unprecedented energy scales with high precision. The HL-LHC upgrade will further enhance our understanding with increased precision and sensitivity to possible anomalies, thanks to tenfold larger datasets, upgraded detectors, and significant advancements in precision calculations and modeling of fundamental interactions at hadron colliders. Higgs boson physics will be a cornerstone of the HL-LHC's physics program with a primary focus on the measurements of Higgs couplings and self-coupling, Higgs differential distributions, rare Higgs decays, and searches for heavy Higgs bosons. Furthermore, significant emphasis is placed on a diverse program covering SM, BSM searches and flavor physics. The subsequent section offers a concise summary of the selected projections, with more comprehensive references available in [241, 242]. The studies summarised below assume an integrated luminosity of 3000 fb^{-1} and an average pile-up of 200.

5.2.1 Measurements of Electroweak Bosons, Higgs Bosons, and Top Quarks

Precision measurements of electroweak bosons and Higgs boson couplings are key in the ATLAS HL-LHC program. Vector boson scattering (WW, WZ, ZZ) can be precisely measured with the full dataset. The main event signature for these processes is $VVjj$, where VV represents the two vector bosons (W or Z) decaying into leptons, and jj denotes two additional jets originating from quarks involved in the scattering as depicted in Figure 5.2. These jets are typically produced in the forward region of the detector. This underscores the necessity for ATLAS detector upgrades to improve forward tracking and jet-finding capabilities, which are essential for enhancing event selection and analysis. ATLAS targets a precision of 6% in the measurement of WW and WZ scattering [243, 244], as depicted in Figure 5.3a, while ZZ scattering is expected to be controlled at the 5% level, primarily limited by theoretical uncertainties [245]. The VV final states also serve as searches for high-mass diboson resonances, with discovery potential up to 4.9 TeV [245]. Despite achieving good precision in measuring inclusive scattering cross-sections, longitudinal W boson scattering measurement remains challenging. ATLAS anticipates a 2σ significance in measuring $W_L^+ W_L^-$ scattering, considering all uncertainties, as depicted in fig 5.3b. More detailed studies of experimental and theory uncertainties will be needed to improve the sensitivity.

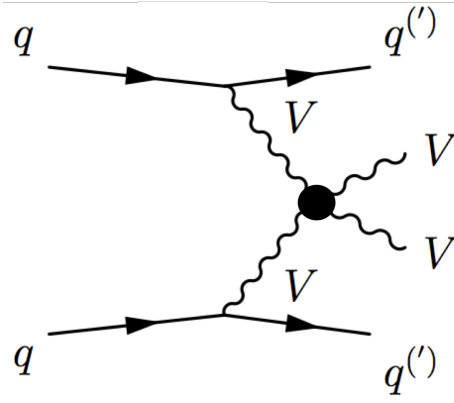


Figure 5.2: Feynman diagram of vector boson scattering (VBS)

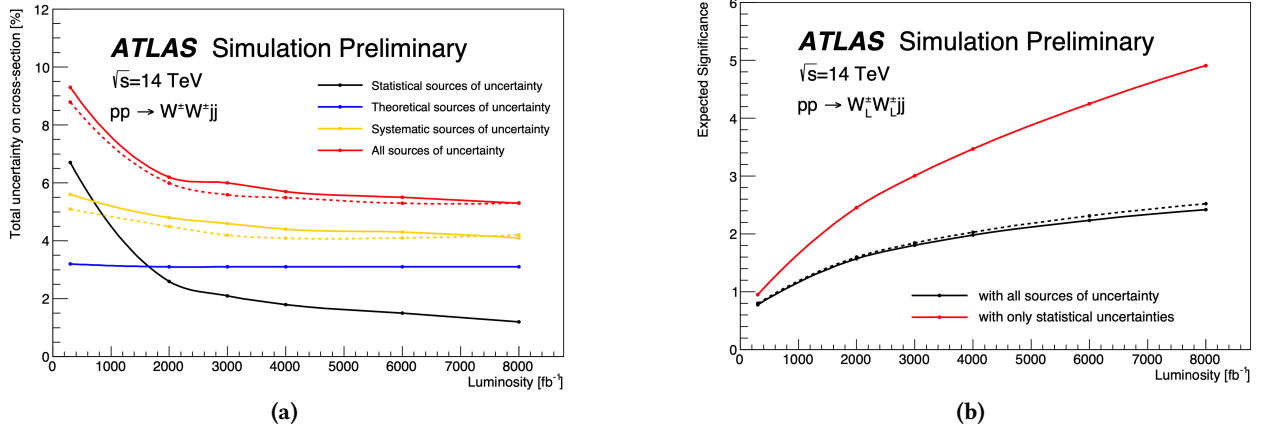


Figure 5.3: (a) Projection of the W^+W^-jj cross-section measurement uncertainties as a function of integrated luminosity. (b) Projection of the expected significance of the $W_L^\pm W_L^\pm jj$ observation as a function of integrated luminosity. The results are presented both with and without systematic uncertainties to emphasize the potential impact of reducing these uncertainties [243].

Measurements of the W boson mass and the electroweak mixing angle $\sin \theta_W$ are anticipated to improve at the HL-LHC. The improvement in the W boson mass measurement stems from enhanced lepton acceptance at high $|\eta|$ rather than from increased luminosity, with studies indicating an achievable precision of 15.9 MeV [246]. Similarly, the $\sin \theta_W$ measurement through the Z boson forward-backward asymmetry benefits from improved lepton acceptance and a large electron data sample, resulting in substantial enhancements compared to current ATLAS measurement [247].

The measurements of Higgs boson couplings are fundamental to the HL-LHC program. With a dataset 20 times larger than that of Run 2, ATLAS aims to achieve a precision of a few percent in Higgs boson production cross-section measurements % [248], as shown in fig 5.4a. The WH associated production cross-section poses the greatest challenge due to larger statistical and systematic uncertainties. By interpreting measurements within the coupling modifier framework, including effective couplings to photons and gluons, the Higgs boson couplings to gauge bosons and fermions of the third generation can be constrained at the 2–4% level, as depicted in fig 5.4b. Systematic uncertainties dominate most measurements, despite the baseline scenario assuming that uncertainties will halve by the end of the HL-LHC program. The largest uncertainties are anticipated for κ_μ (7%) and $\kappa_{Z\gamma}$ (12%), which are associated with the rare decays of $H \rightarrow \mu\mu$ and $H \rightarrow Z\gamma$, respectively, as illustrated in Figure 5.4b.

While the current LHC dataset enables the study of numerous properties of the Higgs boson, determining certain aspects, such as the Higgs self-coupling, remains challenging. The Higgs boson self-coupling (λ_{HHH}) is probed at tree level (see Figure 5.5) in HH production and at loop level

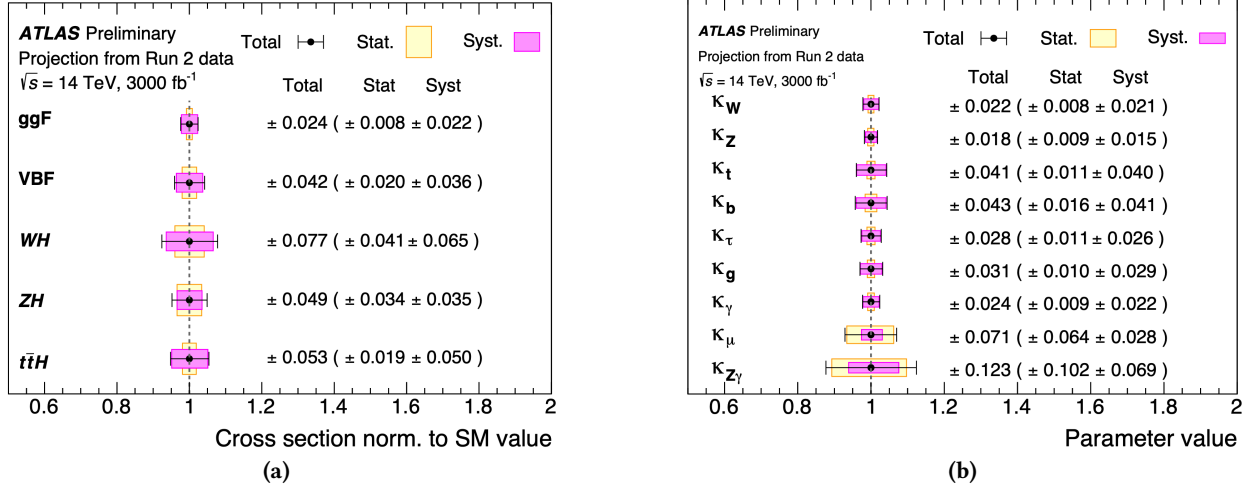


Figure 5.4: (a) Expected results for Higgs boson production cross-section measurements. (b) Higgs boson coupling modifiers for each particle type. The cross-section results are normalized to the Standard Model cross-sections and the coupling modifiers are defined relative to the Standard Model couplings [248].

(see Figure 5.6) in single-H production. The dominant HH production mode at the LHC is the ggF with a cross-section of $\sigma_{ggF}^{HH} = 36.69$ fb at $\sqrt{s} = 14$ TeV at NNLO accuracy in α_S , followed by the VBF production mode with $\sigma_{VBF}^{HH} = 2.055$ fb at $\sqrt{s} = 14$ TeV at N3LO accuracy in α_S [249]. ATLAS has explored the HH production at the HL-LHC via three main event signatures: $b\bar{b}\tau^+\tau^-$, $b\bar{b}\gamma\gamma$, and $b\bar{b}b\bar{b}$, with $b\bar{b}\tau^+\tau^-$ being the most sensitive and $b\bar{b}b\bar{b}$ suffering from significant systematic uncertainties [250]. Combining results from all three final states yields a significance of 3.0σ , accounting for all systematic uncertainties. Furthermore, when combined with similar HH production studies from the CMS Collaboration, an overall significance of 4.0σ can be achieved with the HL-LHC dataset [251].

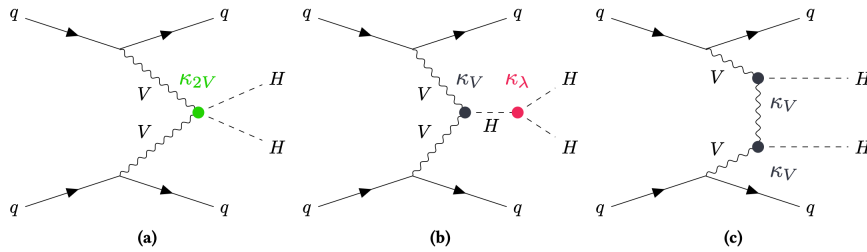


Figure 5.5: Tree-level Feynman diagrams for the vector boson fusion (VBF) production of Higgs boson pairs (HH). The vertices labeled by κ_{VV} , κ_V , and κ_λ represent the couplings for $VV \rightarrow HH$, $VV \rightarrow H$, and HHH , respectively. Figure taken from [252].

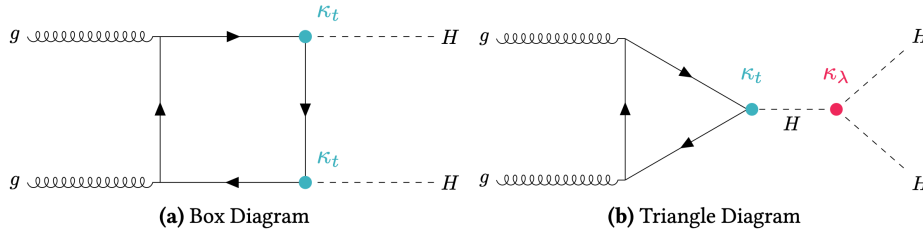


Figure 5.6: Leading-order Feynman diagrams for Higgs boson pair production via gluon fusion (ggF) in the Standard Model. Diagram (a) illustrates the production mediated by the Higgs-top quark Yukawa coupling, with the coupling parameter defined as $\kappa_t \equiv y_t/y_t^{\text{SM}}$. Diagram (b) shows the contribution from the Higgs boson self-coupling, with the coupling parameter defined as $\kappa_\lambda \equiv \lambda_{HHH}/\lambda_{HHH}^{\text{SM}}$. Figure taken from [252].

Another rare process anticipated to be measured with the HL-LHC dataset is the production of four top quarks. ATLAS recently presented evidence for four top quarks in the multi-lepton final state,

utilizing the full Run 2 dataset, with a measured cross-section of 24^{+7}_{-6}fb [253]. The expected $t\bar{t}t\bar{t}$ cross-section at $\sqrt{s} = 14\text{TeV}$ is 16fb , with the extensive HL-LHC dataset enabling a measurement precision of 11% [254]. This production is sensitive to variations in the top quark Yukawa coupling and serves as a search for new particles beyond the Standard Model [255], which may manifest as detectable distortions in the $t\bar{t}$ and $4t$ invariant mass spectra.

5.2.2 Searches for Physics Beyond the Standard Model (BSM)

ATLAS plans diverse searches for new physics at the HL-LHC, spanning from anomalous top quark couplings to supersymmetry and dark matter. Extensive studies have been conducted on the sensitivity to flavor-changing neutral currents (FCNC) in top quark decays. While the Standard Model predicts a branching ratio of 10^{-14} for $t \rightarrow qZ$ ($q = u, c$), this value can significantly increase in certain models, such as the quark singlet model, which predicts FCNC branching ratios as high as 10^{-4} . Utilizing the three-lepton final state and kinematic fits to test the $t\bar{t}$ hypothesis, ATLAS projects a sensitivity of 6.9×10^{-5} for the branching ratio of $t \rightarrow uZ$ and 8.1×10^{-5} for $t \rightarrow cZ$ [256].

The extensive dataset of the HL-LHC serves as an excellent testbench for electroweak supersymmetry searches. Studies demonstrate the potential to probe the TeV mass scale for charginos and neutralinos, despite their low production cross-sections. Fig 5.7a illustrates a significant enhancement in sensitivity to chargino pair production in the dilepton final state compared to current ATLAS exclusions [257]. Additionally, for neutralino-chargino production followed by decay to the lightest Higgs boson (h) and subsequent reconstruction of the $h \rightarrow b\bar{b}$ decay, a search yields sensitivity to $\tilde{\chi}_1^+$ and $\tilde{\chi}_2^0$ masses well above 1TeV , as demonstrated in fig 5.7b [257]. This projection incorporates a comprehensive flavour-tagging simulation and associated uncertainties.

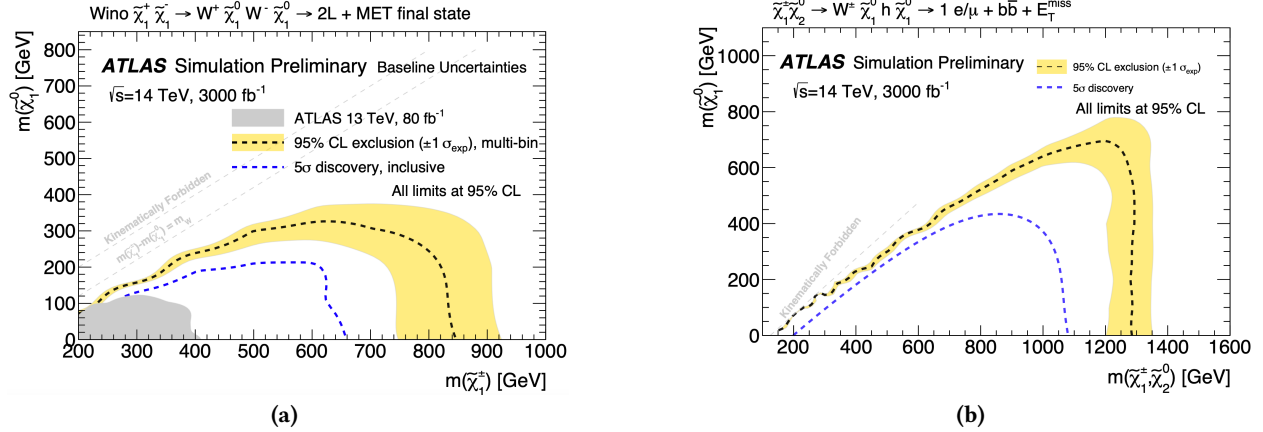


Figure 5.7: Exclusion limits and discovery potential for $\tilde{\chi}_1^+ \tilde{\chi}_1^-$ production, assuming $\tilde{\chi}_1^\pm$ decays to $W^\pm \tilde{\chi}_1^0$ (a) and for $\tilde{\chi}_1^+ \tilde{\chi}_2^0$ production, assuming $\tilde{\chi}_2^0$ decays to $h \tilde{\chi}_1^0$ (b). The baseline uncertainty scenario assumes the systematic uncertainties in the background estimates will be halved relative to the Run 2 uncertainties [257].

If the mass spectrum of supersymmetric particles is compressed, resulting in a small mass splitting between $\tilde{\chi}_1^0$ and $\tilde{\chi}_2^0$, the leptons from $\tilde{\chi}_2^0$ decay will have low transverse momentum. Projections for a search targeting low-momentum leptons (with $p_T \geq 3\text{ GeV}$) demonstrate sensitivity to $\tilde{\chi}_2^0$ masses around 350 GeV with the HL-LHC dataset, surpassing the exclusions of LEP2 and ATLAS. Alternatively, if the mass splitting between $\tilde{\chi}_1^\pm$ and $\tilde{\chi}_1^0$ is small, the $\tilde{\chi}_1^\pm$ lifetime is prolonged and the chargino can produce a visible disappearing track in the inner tracking layers. A search for such disappearing tracks, coupled with significant missing transverse energy, yields a broad mass exclusion at small mass splittings, as depicted in fig 5.8a. The combined result of the soft lepton and disappearing track searches is presented in fig 5.8b [257].

Searches for dark matter using signatures of missing energy, such as jet + missing transverse en-

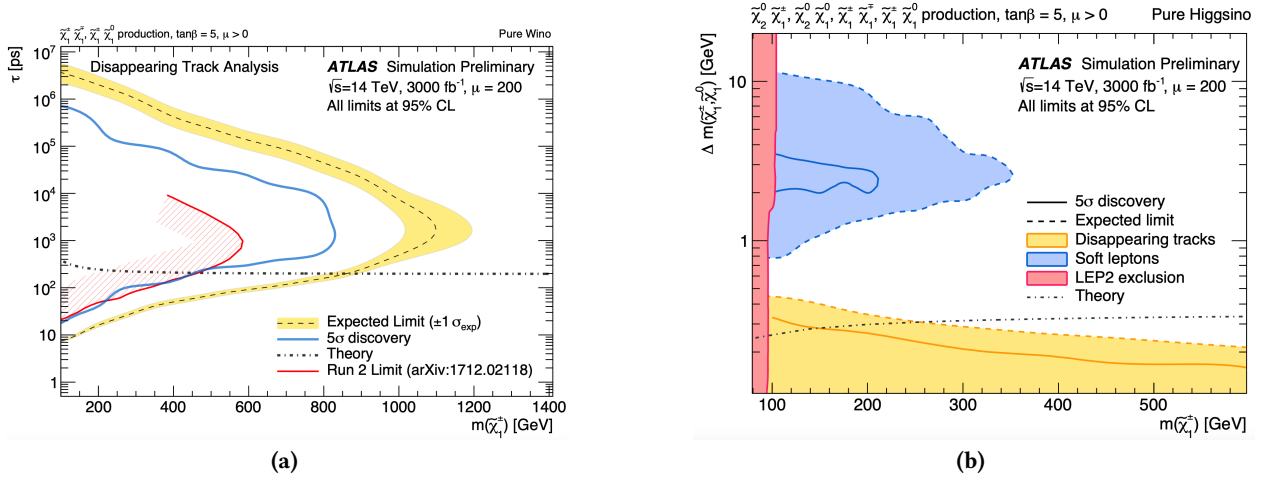


Figure 5.8: (a) Exclusion limits from the disappearing track search as a function of $\tilde{\chi}_1^\pm$ mass and lifetime (b) Combined exclusions and discovery potential from a combination of the disappearing track and soft lepton searches. The chargino and neutralino masses in this scenario are assumed to satisfy the relation

$$m(\tilde{\chi}_1^\pm) = \frac{1}{2}[m(\tilde{\chi}_1^0) + m(\tilde{\chi}_1^\pm)] \text{ [257].}$$

ergy, benefit from the increased center-of-mass energy and integrated luminosity. Projections for these searches with the 3000fb^{-1} dataset indicate sensitivity to dark matter particles coupling to mediators with masses up to 2.7 TeV [258, 259].

5.3 The ATLAS Phase II Upgrade

Under the forthcoming challenging operating conditions of HL-LHC, as outlined in section 5.1, major upgrades are imperative for the ATLAS detector to uphold its current performance capabilities to fully exploit the rich physics potential provided by these large HL-LHC data sets.

The primary detector challenges at the HL-LHC involve maintaining excellent performance in vertex and track reconstruction, lepton identification, and heavy flavor tagging. To tackle these challenges, four fundamental detector upgrades are necessary: a complete replacement of the current tracking system with a new full silicon Inner Tracker (ITk) (Sec 5.3.1), addition of a new High Granularity Timing Detector (HGTD) (Sec 5.3.5) to complement the ITk in the forward region, integration of new radiation-hard readout electronics employing state-of-the-art technologies for the tracking, calorimeter (Sec 5.3.2), and muon detector systems (Sec 5.3.3), and an upgraded Trigger and Data Acquisition (TDAQ) (Sec 5.3.4) architecture to accommodate the increasing particle rates. The aforementioned upgrades, elaborated in [95, 260–264], are essential to mitigate the impacts of aging and the HL-LHC’s rate and radiation environment, and are strategically designed to maximize the LHC’s physics potential.

5.3.1 The Inner Tracker Upgrade

The ATLAS Inner Tracker is vital for reconstructing and identifying leptons, photons, hadronic decays, and for b-jet tagging. The pivotal role of the tracker in the ATLAS physics program becomes even more pronounced in the HL-LHC environment characterized by high luminosity and high pile-up. The current tracker, designed for a ten-year operational lifespan at a peak luminosity of $1 \times 10^{34}\text{cm}^{-2}\text{s}^{-1}$, with an average number of up to 23 pileup events per 25 ns bunch crossing, and a Level-1 trigger rate of 100 kHz, is inadequate for the challenging HL-LHC conditions. At the HL-LHC, the luminosity will increase to $7 \times 10^{34}\text{cm}^{-2}\text{s}^{-1}$, and the expected radiation fluence

in the interaction region will be between 1 and $2 \times 10^{16} n_{eq}/cm^2$, necessitating its replacement. In response to this increase in luminosity, a new all-silicon detector named Inner Tracker (ITk), featuring both pixel and strip technology [95, 260], is currently under construction and slated for installation during LS3. The predictions for particle fluences and ionizing doses for the ITk layout are based on an integrated luminosity of $4000fb^{-1}$ and a center-of-mass energy of 14 TeV for inelastic proton collisions. Figure 5.9 illustrates the fluence distribution for the ITk Pixel Detector during HL-LHC operation, with the 1 MeV neutron equivalent fluences (see Equation 3.5.3) normalized to a total of $4000fb^{-1}$ [95]. As the central focus of this thesis work, this chapter will delve into extensive discussion regarding the baseline design for the ITk.

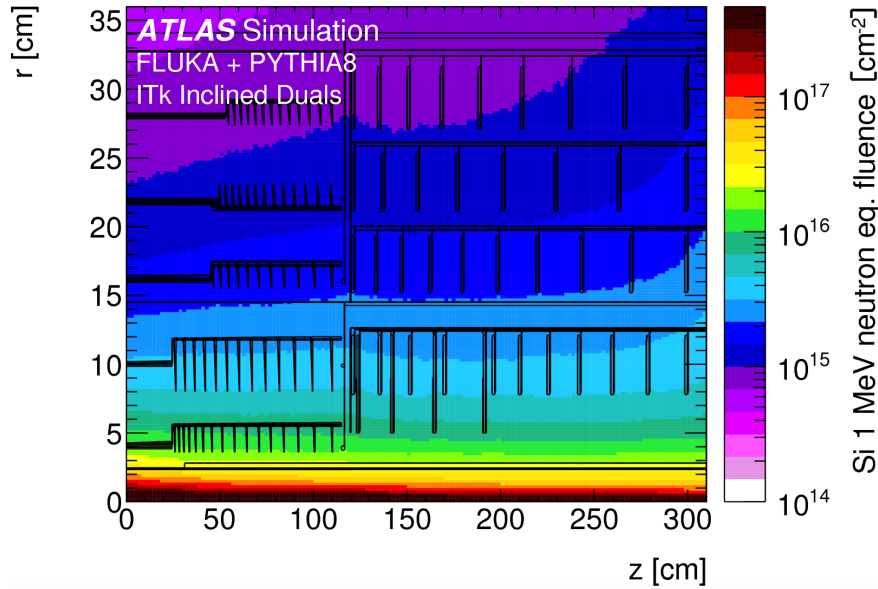


Figure 5.9: Fluence and dose distributions for the Pixel Detector, with fluence set to 1 MeV neutron equivalent and normalised to $4000fb^{-1}$. Radiation background simulations have been performed for the ITk using the PYTHIA8 [265] event generator and the FLUKA [266] particle transport code. Notably, no safety factors are taken into account in this figure [95].

5.3.2 The Calorimeter Upgrade

To withstand the expected high radiation doses and demanding data-taking conditions at HL-LHC, significant upgrades will be made to the front-end (FE) electronics of the ATLAS LAr and Tile calorimeters introduced in Section 2.2.5. These upgrades will capitalize on technological advancements to implement a robust architecture capable of operating effectively in the high-radiation HL-LHC environment [263, 267].

The upgraded LAr readout chain will consist of on-detector electronics comprising FE and calibration boards, and off-detector electronics comprising processing and timing control boards. The FE boards will amplify and digitize the ionization signal with high precision and low noise. The on-detector components share the common requirement of maintaining stable operation under a maximum irradiation of $4.1 \times 10^{13} n_{eq}/cm^2$. Thus, custom-made chips have been developed for signal amplification, shaping, and digitization, demonstrating stability under irradiation tests [268]. Calibration boards equipped with custom Application Specific Integrated Circuits (ASICs) will ensure precise calibration across all channels, also exhibiting stability under irradiation. The off-detector electronics will process the digitized signal from the FE boards for energy estimation and time stamping. As a part of the Phase-II upgrade activities, a dedicated off-detector electronics system known as the LAr Signal Processor (LASP) has been developed. The LASP consists of an Advanced Telecommunications Computing Architecture (ATCA) blade equipped with two Field-

Programmable Gate Arrays (FPGAs) and a Smart Rear Transition Module (SRTM). For further details on the LAr calorimeter upgrades, readers are encouraged to refer to [267–269].

In order to cope with the anticipated high trigger rates and intense radiation environment, the ATLAS Tile Calorimeter will undergo upgrades with redesigned electronic systems, ensuring its optimal performance in future operations. During the LS3, both the on- and off-detector TileCal electronics will be replaced to provide better precision of the calorimeter signals used by the trigger system allowing the development of more complex trigger algorithms. The upgraded front-end system will continuously digitize and read out shaped photomultiplier tube (PMT) signals from every TileCal cell at a rate of 40 MHz, transmitting them over high-speed fiber links to the new back-end electronics to be stored in latency pipelines and digitally summed to produce improved trigger tower data for the Level-1 trigger [270]. The FE electronics features radiation-tolerant commercial off-the-shelf components with extensive redundancy to minimize single point failures [270]. The timing, control and communication interface with the off-detector electronics is implemented with FPGAs and high speed fiber optic links running up to 9.6GBs. The Tile upgrade program has undergone extensive R&D and test beam campaigns. In 2019, a demonstrator module was integrated into ATLAS for testing in the actual detector environment. For further information about the TileCal upgrade program, readers are recommended to consult additional literatures [270–272].

5.3.3 The Muon Spectrometer Upgrade

The muon spectrometer of the ATLAS detector will undergo significant upgrades to meet the demands of the HL-LHC in Run 4 and beyond. This involves replacing a large portion of the FE and on- and off-detector readout and trigger electronics for the RPC [273], TGC [274], and MDT [275] chambers (see Section 2.2.6) to handle higher trigger rates and longer latencies required for the new L0 trigger (see Section 5.3.4). Additionally, MDT chambers, currently excluded from the hardware trigger, will be integrated into the level-0 trigger to sharpen the momentum threshold and enhance system redundancy. New-generation RPC chambers will be installed in the inner barrel layer, alongside the replacement of some MDT chambers with small-diameter MDTs. New TGC triplet chambers will replace TGC doublets in the barrel-endcap transition zone to suppress false triggers. The power system for the RPC, TGC, and MDT chambers and electronics will require replacement due to component obsolescence, ageing, and radiation damage. A high- η tagger is under consideration to extend the angular acceptance for muon identification [264]. The Phase-II upgrade marks the conclusion of adapting the muon spectrometer to the continuously improving performance of the LHC. This process commenced with the Phase-I upgrade NSW project, which will replace the CSC chambers and the MDT chambers of the innermost endcap wheels with Micromegas and small-strip TGCs. For an in-depth discussion on the Phase-II upgrade of the muon spectrometer, readers are encouraged to refer to additional literature [264, 276].

5.3.4 The Trigger and Data Acquisition Upgrade

The Phase-II upgrade of the ATLAS TDAQ system complements upgrades across different ATLAS subdetectors, including the new ITk, which extends tracking system coverage up to $\eta = 4.0$, upgrades to LAr and TileCal calorimeter readout electronics to meet Phase-II requirements, and upgrades to Muon Trigger Chambers and readout electronics to fulfill L0 trigger requirements and extend solid angle coverage. Two architectures are proposed for the Phase-II upgrade: a baseline featuring a hardware-based L0 trigger at 40 MHz and a CPU farm-based Event Filter (EF) with hardware-assisted track reconstruction at 1 MHz; and an advanced version incorporating an intermediate L1 trigger at 2–4 MHz, reducing EF input rates to 800–600 kHz compared to the baseline. Both architectures are designed to provide a 10 kHz output rate. For further details, readers are encouraged to refer to [261, 277, 278].

5.3.5 New HL-LHC Detector: The High Granularity Timing Detector (HGTD)

The detrimental effect of increased pileup interactions at the HL-LHC can be mitigated by using high-precision timing information to distinguish between collisions occurring close in space but well-separated in time. A High-Granularity Timing Detector (HGTD), based on Low gain Avalanche Detector (LGAD) technology [279], is planned for the ATLAS Phase-II upgrade. The HGTD will be installed in the forward region at ± 3.5 m from the interaction point, in a gap region between the end-cap and the barrel calorimeters. Covering the pseudorapidity region from 2.4 to 4.0, HGTD improves the forward object reconstruction with high-precision timing information. Optimized to achieve an average time resolution of 30 ps per track for a MIP at the start of its lifetime, which degrades to 50 ps by the end of the HL-LHC operation, the HGTD mitigates the effects of pileup by resolving the collisions in time within a single bunch crossing and complements the capabilities of the new ITk detector in the forward regions of ATLAS, resulting in improved performance for jet and lepton reconstruction. These enhancements boost sensitivity and extend the reach of the ATLAS physics program. Additionally, the HGTD provides unique capabilities for online and offline luminosity determination, crucial for precision physics measurements. A comprehensive overview of the HGTD project, encompassing its performance, current status, and key highlights of sensitive components, can be found in [262, 280].

5.4 The ATLAS Inner Tracker (ITk)

For the HL-LHC upgrade of the ATLAS detector, the current Inner Detector (ID, Section 2.2.4), consisting of silicon pixel, silicon strip detectors and transition radiation tracker (TRT) is going to be replaced by an all-silicon Inner Tracker (ITk), which has 13 m^2 of pixel detectors with 5 billion readout channels and 160 m^2 of strip detectors with 50 million readout channels. Section 5.4.1 outlines the layout of the ITk detector, while Section 5.4.2 presents an overview of its anticipated performance. Section 5.4.3 offers an in-depth discussion of the ITk pixel detector, which is the primary focus of study in this thesis.

5.4.1 The ITk Layout

The "Inclined Duals" layout, the finalized design of the ITk detector, integrates precise central tracking amidst an average of 200 pile-up events, extending tracking coverage to a pseudorapidity of 4, while maintaining excellent tracking efficiency and performance [95]. The ITk detector comprises a strip subsystem [260] covering $|\eta| < 2.7$ and a pixel subsystem [95] extending to $|\eta| < 4$ as illustrated in Figure 5.10. The strip subsystem consist of four strip module layers in the barrel region and six disks in the endcaps while the pixel detector comprises five flat barrel layers and five layers of inclined or vertical rings providing coverage in the forward region. The Pixel and Strip Detector volumes are separated by a Pixel Support Tube (PST). Additionally, due to the anticipated harsh radiation conditions at the HL-LHC, the inner two layers of the Pixel Detector are replaceable. These inner layers are isolated from the outer three layers by an Inner Support Tube (IST), facilitating their replacement. The combined strip and pixel detectors offer a total of 13 hits for $|\eta| < 2.7$ as illustrated in Figure 5.11a, except at the transition between the barrel and end-cap of the strip detector, where the hit count decreases to 11. The pixel detector is designed to supply a minimum of at least 9 hits for $|\eta| > 2.7$ as shown in Figure 5.11b. Figure 5.10a depicts the planned ITk Inclined Duals layout for the HL-LHC upgrade, while Figure 5.10b illustrates the schematic layout of active detector elements for one quadrant, and Figure 5.10c provides a zoomed-in view of the pixel subsystem.

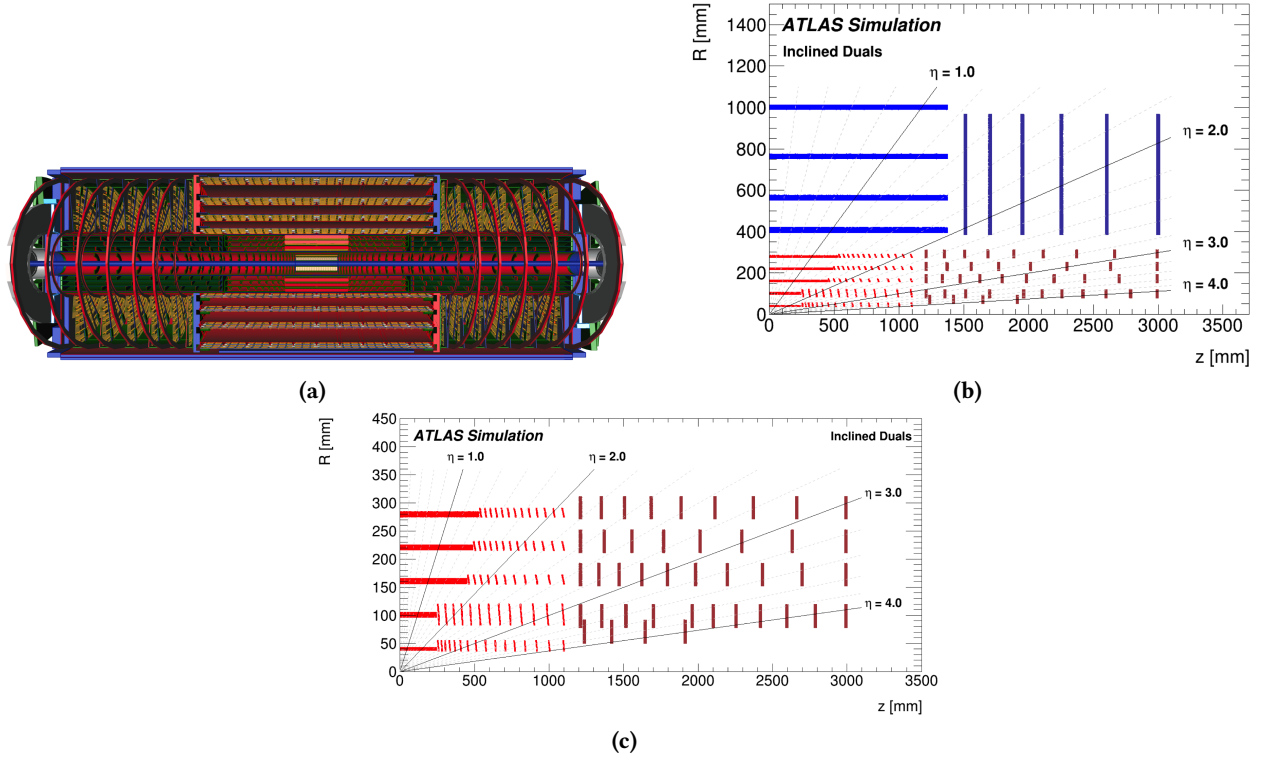


Figure 5.10: (a) Display of the Inner Tracker Inclined Duals layout (b) A schematic layout of the active elements of one quadrant of the ITk detector. The active elements of the barrel and end-cap Strip Detector are shown in blue, for the Pixel Detector the sensors are shown in red for the barrel layers and in dark red for the end-cap rings. The horizontal axis is along the beam line with zero being the interaction point. The vertical axis is the radius measured from the interaction region (c) A zoom into the ITk Pixel Detector. Figures taken from [95, 281]

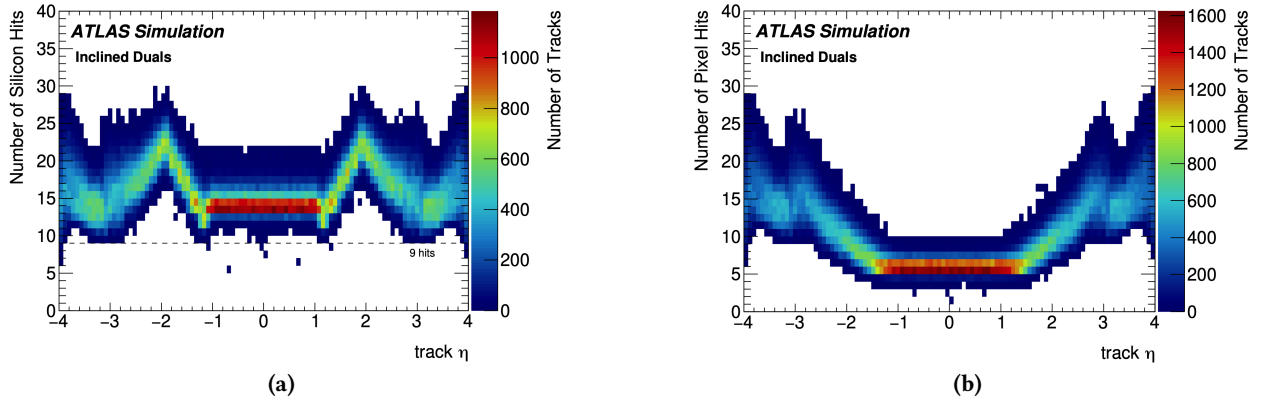


Figure 5.11: (a) The total number of strip plus pixel measurements (hits) on track as a function of η (b) Number of pixel measurements (hits) on track as a function of η . A sample of single muon events with $P_T = 1$ GeV is used. The muons are produced with a flat distribution between -15 to 15 cm in z (beam direction) and between 0 to 2 cm in R (radial direction) [95, 281].

5.4.2 Expected Tracking Performance of the ITk

Under the increased pileup conditions of the HL-LHC, the ITk detector must uphold a tracking efficiency that is either on par with or superior to that of the ID. To assess the tracking efficiency of the ITk, $t\bar{t}$ events were generated at a center-of-mass energy of 14 TeV using POWHEG [194, 195, 282] interfaced with Pythia8 [265], simulating the HL-LHC pileup conditions ($\langle \mu \rangle = 200$). To draw a comparison, these steps are reproduced for the current ID with the pileup equivalent of run 2 ($\langle \mu \rangle = 38$). The detector response is simulated using the GEANT4 toolkit, accurately emulating the particle detector interactions, digitization, and subsequent detector response. The energy depo-

sition in each Geant4 [198] step within the active silicon volume determines free charges and drift time to the readout surface, based sensor parameters such as thickness, carrier mobility, depletion, bias voltages, and Lorentz shift, along with noise and capacitive coupling effects. Collected charge in each channel is determined, and those exceeding a predefined threshold are marked as activated or fired. For channels surpassing the discriminator threshold, a 4-bit Time-over-Threshold (ToT) measurement is emulated using a calibration function, resulting in an average ToT of 7 bunch crossings for a charge of 10000 e. Hits exceeding the threshold are assigned to the bunch crossing corresponding to the particle contributing the most to the charge. The reconstruction chain involves forming clusters from individual channels, converting pixel ToT information into charge measurements, and calibrating analogue clustering for precise position evaluation. Pixel and strip clusters are then transformed into 3D space-points for pattern recognition, utilizing seeds for defining search roads and implementing a combinatorial Kalman filter for track finding. Additional details on track reconstruction and selection studies can be found in [198], while a comprehensive theoretical discussion on the various stages of detecting a charged particle traversing a silicon pixel detector is available in Chapter 3.

5.4.2.1 Efficiencies and Number of Tracks

Figure 5.12 illustrates the tracking efficiency achieved with the Inclined Duals ITk layout for 2, 10, and 100 GeV muons without pileup, demonstrating good compatibility with the results obtained with the Run 2 detector for $|\eta| < 2.4$. A performance reduction of 0.5% is observed in the barrel layers for 2 GeV muons. However, future optimizations of the tracking reconstruction configurations, particularly material corrections tuning, are expected to recover this loss [281].

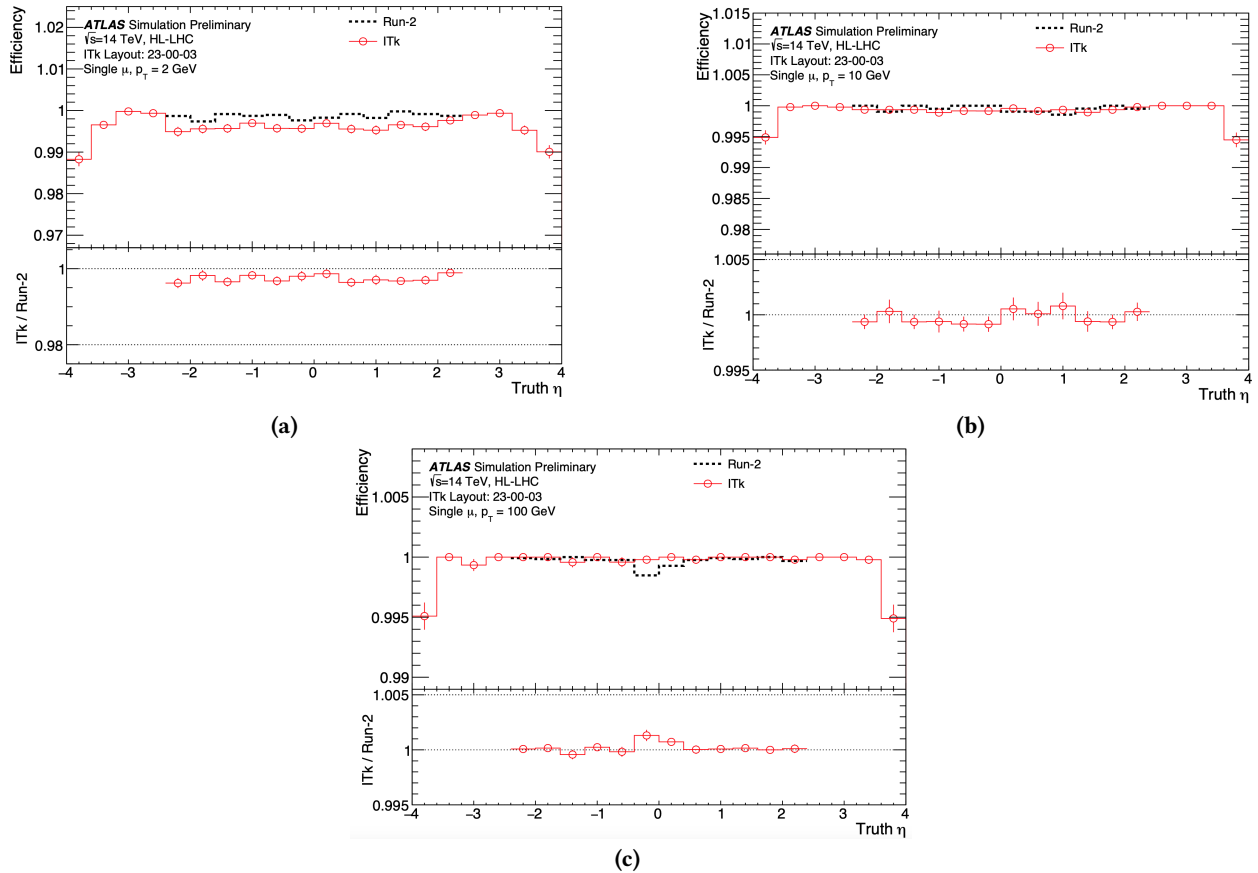


Figure 5.12: The tracking efficiency for single muons with $p_T = 2, 10$, and 100 GeV without pileup is compared between the Run 2 detector and the updated ITk layout. Figures sourced from [281].

Figure 5.13 highlights the expected tracking performance at $\langle \mu \rangle = 200$, illustrating the efficiency

in $t\bar{t}$ events for particles with $p_T > 1$ GeV and within the detector acceptance, considering both hard-scatter and pileup interactions. The efficiency is compared with that obtained with the Run 2 detector at $\langle \mu \rangle = 38$. The tracking efficiency in the central region of the ITk detector is within 5% of that of the current ID, while additionally extending coverage further into the forward directions as depicted in Figure 5.13a. Across the transverse momentum spectrum, the tracking efficiency of the ITk closely matches that of the current ID, with a deviation of only a few percent, as illustrated in Figure 5.13b.

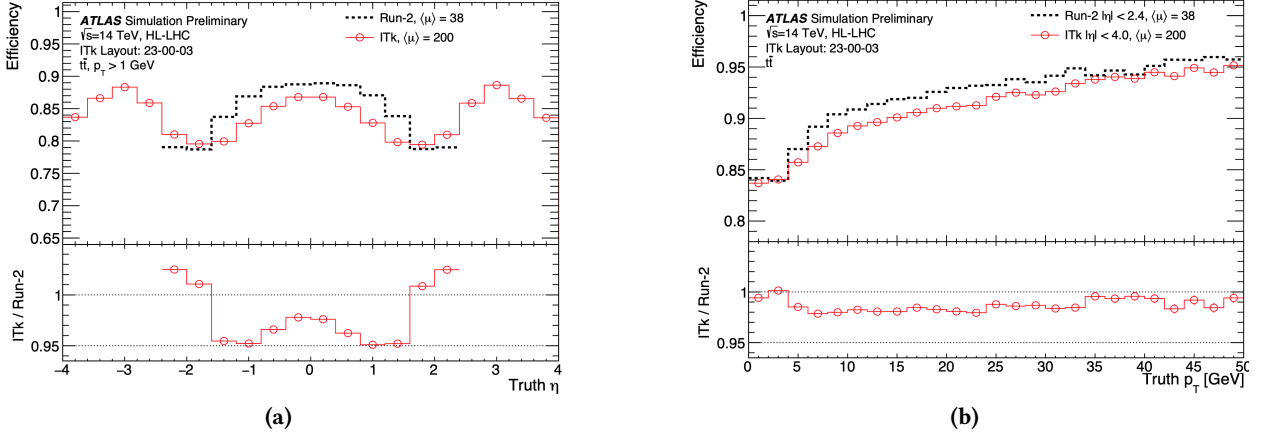


Figure 5.13: Simulated tracking efficiency distributions with respect to pseudorapidity (a) and transverse momentum (b) of $t\bar{t}$ events for the ID in run 2 with $\langle \mu \rangle = 38$ and ITk with $\langle \mu \rangle = 200$. Figures sourced from [281].

Additional metrics, including impact parameters resolution, expected performance of high-level objects such as vertex reconstruction and identification, jet flavor tagging, and tracking-related performance for electron and photon reconstruction and identification can be found in [281].

5.4.2.2 Track Parameter Resolution

Figures 5.14, 5.15, and 5.16 compare the expected resolutions for the transverse and longitudinal impact parameter (d_0 and z_0 , respectively; see Section 5.4.2.2) and transverse momentum, p_T of simulated muons with p_T values of 2 and 100 GeV, between the ITk layout and the Run 2 ATLAS detector.

The d_0 resolution for 2 GeV muons is similar between the ITk and Run 2 detector, as shown in Figure 5.14, due to the similar radius of the innermost pixel layers. However, the z_0 resolution improves by up to a factor of 2 in the ITk detector, thanks to its smaller pixel pitch ($25 \times 100 \mu\text{m}^2$ or $50 \times 50 \mu\text{m}^2$, more details in Section 5.4.3) compared to the IBL's pixel pitch ($50 \times 250 \mu\text{m}^2$), as detailed in Section 2.2.4.1. For 100 GeV muons, which experience minimal material effects, the smaller pixel pitch of the ITk detector leads to significant improvements, enhancing the d_0 and z_0 resolutions by factors of 2 and 4, respectively, as illustrated in Figures 5.14 and 5.15.

The transverse momentum resolution is only marginally affected by changes in the ITk layout and is expected to exceed the Run 2 performance as illustrated in Figure 5.16, thanks to the enhanced resolution in the bending direction provided by the silicon strip sensors in ITk, in contrast to the straw tubes used in the Run 2 ID.

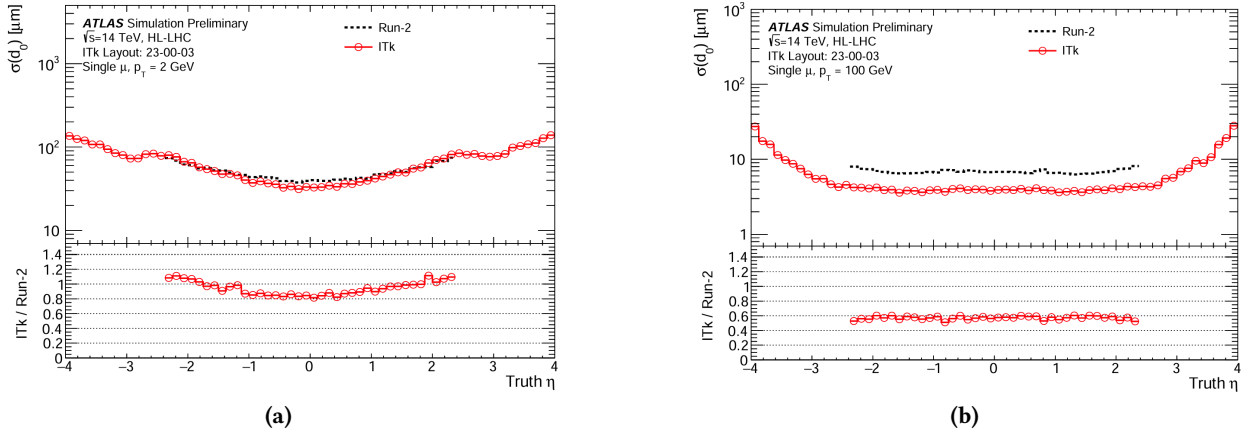


Figure 5.14: Transverse impact parameter (d_0) resolution as a function of pseudorapidity (η) for (a) 2 GeV muons and (b) 100 GeV muons, without pileup, comparing the Run 2 detector with the ITk layout. Figures sourced from [281].

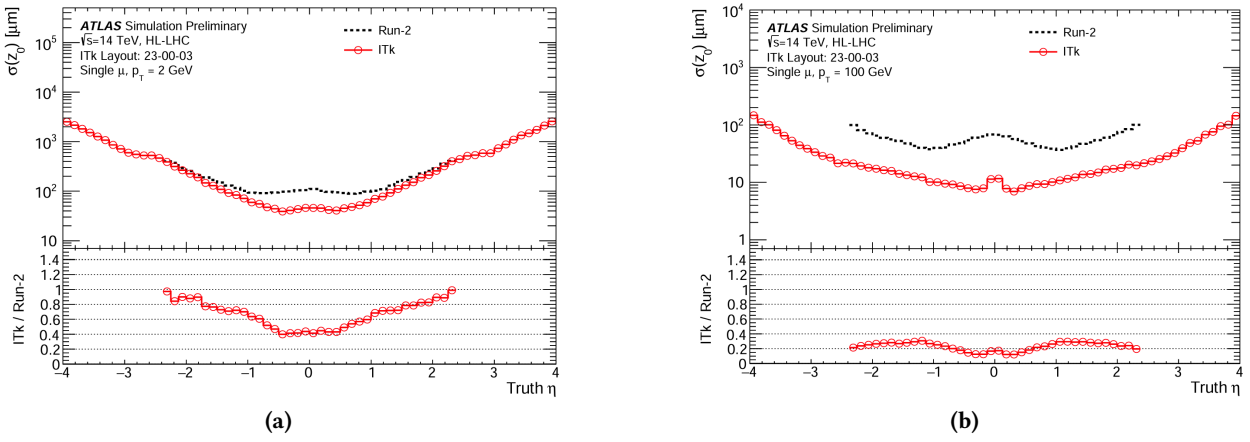


Figure 5.15: Longitudinal impact parameter (z_0) resolution as a function of pseudorapidity (η) for (a) 2 GeV muons and (b) 100 GeV muons, without pileup, comparing the Run 2 detector with the ITk layout. Figures sourced from [281].

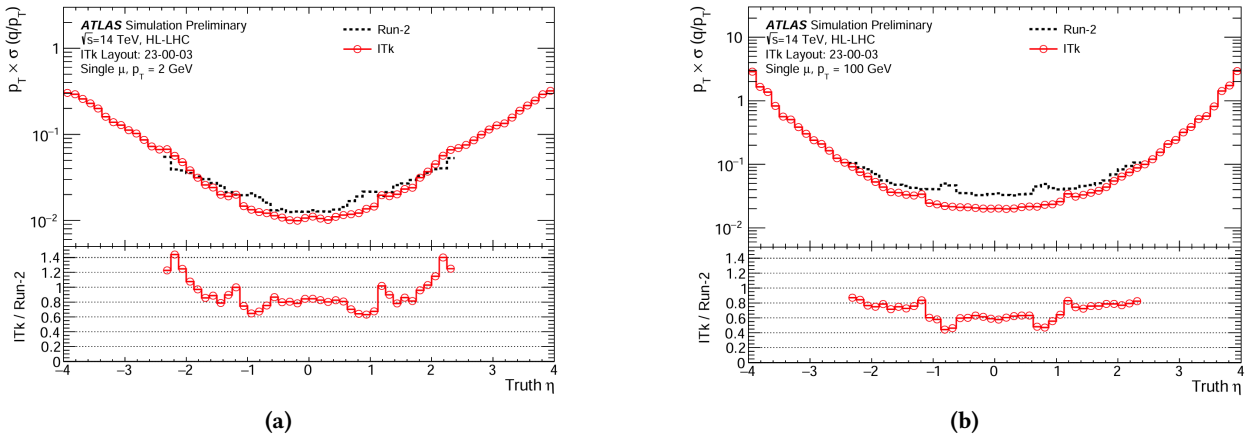


Figure 5.16: Transverse momentum resolution as a function of pseudorapidity (η) for (a) 2 GeV muons and (b) 100 GeV muons, without pileup, comparing the Run 2 detector with the ITk layout. Figures sourced from [281].

5.4.3 The ITk Pixel Detector

This section presents a comprehensive overview of the ITk pixel detector. Sections 5.4.3.1, 5.4.3.2, and 5.4.3.3 introduce the sensors, readout chips, and pixel modules, respectively, which serve as building blocks of the pixel detector, with larger structures built and described in section 5.4.3.4.

The ITk detector will occupy the space currently filled by the ID, with a radius of 1 m and a length of 6 m. Within the innermost part, the pixel system consists of five layers subdivided into three regions: the Inner System (IS), Outer Barrel (OB), and Outer End-caps (OEC). These regions are outlined by different colors, as illustrated in Figure 5.17.

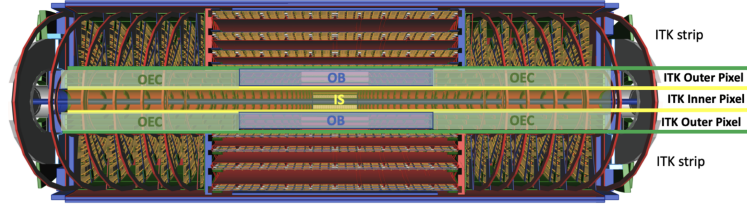


Figure 5.17: The full ATLAS ITk layout, showcasing the distinct sub-detectors comprising the pixel sub-system: the Inner System (IS) highlighted in yellow, the Outer Barrel (OB) in blue, and two Outer End-caps (OECs) in green.

Figure taken from [283].

Each layer of the ITk pixel detector consists of repeated elements, with staves used in the barrel region and rings used in the forward regions (see Section 5.4.3.4). These elements consist of support structures that hold the basic detector units, known as hybrid modules that comprise a sensor and multiple readout chips (see Section 5.4.3.2), which are bonded together using flip-chip technology, as detailed in Section 5.4.3.1. A detailed overview of these components are provided in the subsequent sections.

5.4.3.1 Pixel Sensor Technologies

The choice of the sensors for ITk pixel detector is dictated by the radiation hardness requirement for the different layers of the detector as detailed in Table 5.1. In the baseline scenario, at a maximum integrated luminosity of 2000fb^{-1} , the highest fluence in layer 0 (L0) is $1.31 \times 10^{16} n_{eq}/\text{cm}^2$, corresponding to a dose of 7.2 MGy. For layer 1 (L1), the highest fluence is $3.8 \times 10^{15} n_{eq}/\text{cm}^2$ with a dose of 3.2 MGy. In the outer pixel layers, for a total integrated luminosity of 4000fb^{-1} , the highest fluence is $3.0 \times 10^{15} n_{eq}/\text{cm}^2$ in the barrel and $3.8 \times 10^{15} n_{eq}/\text{cm}^2$ in the end-caps, with a dose of 3.2 MGy. The pixel sensors must maintain a hit efficiency exceeding 98.5% prior to irradiation and remain above 97% post-irradiation as specified by a corresponding end-of-life fluence [95]. Another crucial performance parameter to consider for the sensor technology is power dissipation. Although the total power dissipation of a module is primarily determined by the FE chip, maintaining high reconstruction efficiency after irradiation often necessitates sensor technologies to operate at high operational voltages with moderate leakage currents. Consequently, the resulting power dissipation values set constraints on the necessary thermal performance of the pixel local support structures, as detailed in Chapter 13 of the Technical Design Report (TDR) for the ATLAS ITk Pixel Detector [95]. The ITk pixel detector comprises two baseline sensor technologies: hybrid planar (Section 5.4.3.1) and 3D silicon sensors (Section 5.4.3.1), which are bump-bonded onto the ITkPixV2.0 FE ASIC (Section 5.4.3.2) developed with the RD53 collaboration [284]. The 3D sensors in the innermost L0 layer are organized in triplet modules with three single FE-sensor assemblies on a triplet flex, chosen for their radiation hardness and planar sensors in quad modules in all other layers (L1–L4), feature four frontend chips on a quad sensor tile on a quad flex, selected for their high fabrication yield and lower costs as depicted in Figure 5.18b and Figure 5.18c, respectively. Both technologies utilize n-implant in p-substrate, with a generally thinner active thickness compared to the current pixel detector. Consequently, charge and hit efficiencies saturate at lower bias voltages, resulting in reduced dissipated power. At the moment, a market survey is finished for both technologies and pre-production is ongoing.

Luminosity	Layer	Location	R (cm)	z (cm)	Fluence ($10^{14} n_e q / \text{cm}^2$)	Dose (MGy)
2000 fb^{-1}	0	Flat barrel	3.9	0.0	131	-
			4.0	24.3	-	7.2
		Inclined barrel	3.7	25.9	123	-
			3.7	110.0	-	9.9
		End-cap	5.1	123.8	68	6.3
2000 fb^{-1}	1	Flat barrel	9.9	24.3	27	1.5
		Inclined barrel	8.1	110.0	35	2.9
		End-cap	7.9	299.2	38	3.2
4000 fb^{-1}	2- 4	Flat barrel	16.0	44.6	28	1.6
		Inclined barrel	15.6	110.0	30	2.0
		End-cap	15.3	299.2	38	3.5

Table 5.1: Maximal 1 MeV Neutron equivalent fluences and Total Ionising Dose for various components of the ITk Pixel Detector, under the baseline replacement scenario, all values scaled by a safety factor of 1.5 [95].

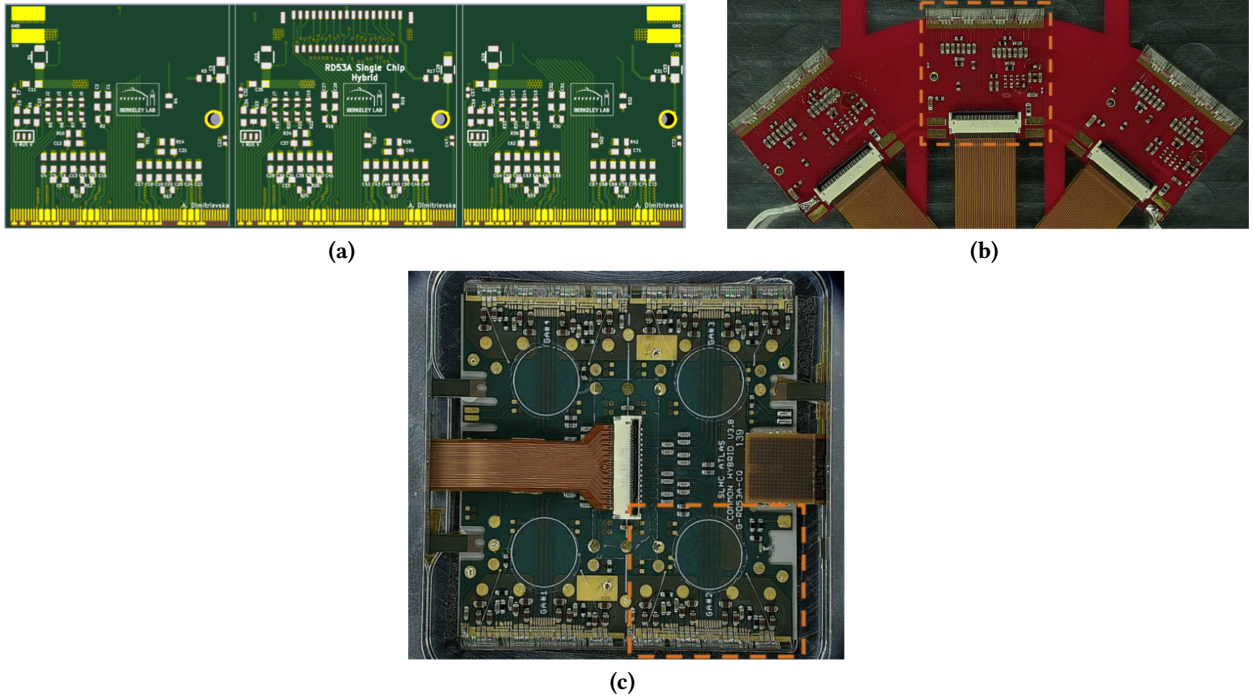


Figure 5.18: (a) Barrel linear triplet module housing three sensors each paired with an individual FE chip. (b) Ring triplet module integrated with flexible PCB, housing three sensors each paired with an individual FE chip. The highlighted orange lines enclose one sensor chip and its corresponding FE chip (c) A quad module with four FE chips bump-bonded onto a single large sensor chip. The highlighted orange region indicates the attachment point of one FE chip to the larger sensor chip. Pictures taken from [285].

Planar Sensors

Planar pixel sensors serve as the baseline for layers L1 to L4 of the ITk Pixel Detector. The potentially cost-effective n-in-p technology has been selected over the n-in-n technology currently employed in the ATLAS Pixel Detector and the IBL due to its single-sided process, requiring processing of only one side of the wafer. Additionally, the n-in-p technology is more radiation hard as it will not undergo space charge sign inversion in the bulk as discussed in Section 3.5.3. The active sensor thickness is 100 μm in Layer 1 and Ring 1, and 150 μm elsewhere. The thickness is cho-

sen based on the radiation hardness requirements and the material budget minimization weighted against the cost implications of using thinner sensors [95]. A reduced sensor thickness improves radiation tolerance by reducing charge carrier trapping during collection. Thinner sensors require lower operational voltage, decreasing power dissipation. Additionally, they decrease readout bandwidth requirements due to fewer pixels traversing inclined tracks. Thin sensors also reduce the material budget and, consequently, multiple scattering within tracking devices, improving the energy resolution of the calorimeters.

The planar n-in-p sensors of the ITk Pixel Detector comprise a boron-doped p-type silicon substrate with concentrations typically around $\approx 10^{12}\text{cm}^{-3}$, and n-type implants with phosphorus at higher doping concentrations exceeding 10^{18}cm^{-3} , DC coupled to an aluminum read-out pad forming one pixel. Inter-pixel isolation is achieved via p-stop and/or p-spray doped to ensure a minimum specified inter-resistance value of $2\text{M}\Omega$. The back-side of the sensor is uniformly metallized to establish a good ohmic contact with the bulk using a p^+ implant with doping concentration typically exceeding 10^{18}cm^{-3} . Additionally, a passivation oxide layer is applied on the front-side to protect the sensor from scratches.

Once the individual sensors are fabricated, they are bump bonded to the readout chip using the flip-chip process described in Section 5.4.3.3, resulting in what are known as hybrid pixel sensors, as illustrated in Figure 5.19.

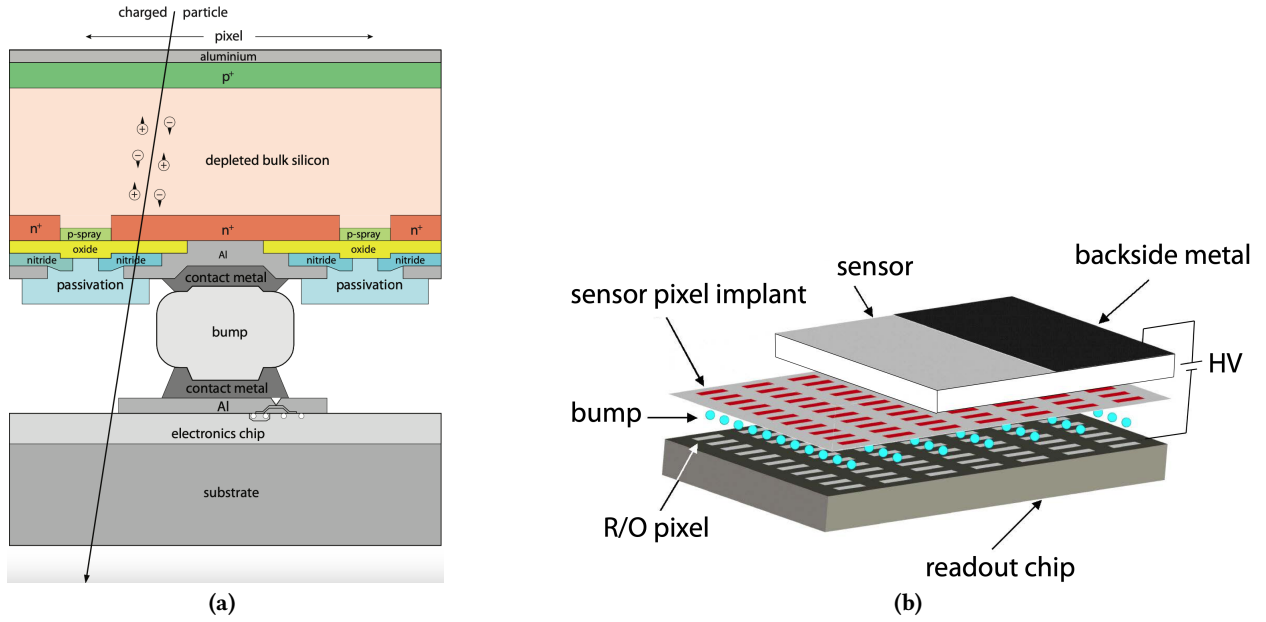


Figure 5.19: (a) The layout of an individual pixel cell with a sensor and an electronics cell arranged in one-to-one correspondence (b) Hybrid pixel matrix where both the sensor and electronics chip feature pixels of identical size, bonded together via bump bond. Figures taken from [286].

Typical auxiliary sensor structures

Several additional structures are implemented in the planar pixel sensor design to improve the sensor performance and broaden testing capabilities. The layout of the sensor surface, including pixel implants and their biasing structure, is illustrated in Figure 5.20. During production, sensors are cut from silicon wafers using a diamond saw, leaving defects that make the edges conductive, linking the front and back at high potential. To prevent breakdown, concentric ring implants called Guard Rings (GR) are placed between the pixel matrix and the sensor border to ensure a smooth potential gradient from the pixel area to the high voltage region. More GRs result in smaller potential steps between the rings, leading to a smoother and lower electric field, thereby improving the breakdown behavior of the sensor. However, adding more guard rings extends the inactive area of

the sensor. The typical width of the inactive surface under the guard rings ranges from about $50\text{ }\mu\text{m}$ to about 1 mm . The guard ring structure is implemented on the p-n junction side; therefore, in the n-in-p sensors, it is on the pixel side.

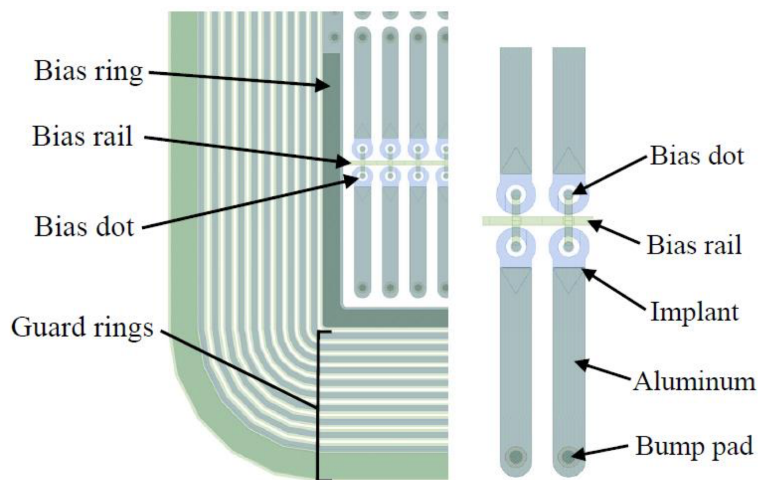


Figure 5.20: Standard layout of a silicon pixel sensor: **Left:** illustrates the sensor's edge, while **Right:** provides a detailed view of the pixel cell structure. Guard rings, biasing structures, and other key components of the pixel cell are indicated. Figure taken from [287].

The inner guard ring, when grounded, can serve as the bias ring, biasing the entire sensor. It provides potential around the pixel matrix and is connected to aluminum bias rails that run between the pixel columns, distributing potential to the pixel implants. The implants receive their potential from the bias rail via a circular implant called the bias dot, which can be implemented in two ways: the "standard" bias dot located within the opening of the pixel implant, or the "common" bias dot situated externally at the corner of four neighboring pixel cells. Pixel connectivity to the bias dot is achieved through bias resistors [145], typically polysilicon or the "punch-through" mechanism [288].

In the standard manufacturing process, sensors cannot be tested before they are interconnected to a readout chip. However, it is crucial to assess the sensors at this stage, as hybridization, the process where readout chips are bump-bonded to the sensor, is the most costly step in module production. The bias structure described above enables the measurement of the electrical properties of sensors before bump-bonding to the readout chip. Conversely, it has been observed that the biasing structure induces efficiency losses near the punch-through bias dots after irradiation to high fluences, as detailed in [95].

3D Sensors

The 3D sensors feature columnar electrode implants of both doping types, penetrating the silicon bulk substrate perpendicular to the sensor surface, unlike planar sensors where the implants are parallel. This process involves etching narrow deep holes in the wafer followed by doping implantation on the hole surfaces, creating p-type and n-type columns as depicted in Figure 5.21a. Subsequently, the hollows are filled with a conductive material to form the anodes and cathodes. The bias voltage is applied between the n and p-type columns to generate an electric field, directing the electrons and holes generated by the ionizing particle towards the respective collection electrodes parallel to the wafer surface.

The 3D silicon detectors offer superior radiation tolerance compared to other sensor technologies. The distance between the columnar electrodes, penetrating the sensor bulk perpendicularly (refer to Figure 5.21), is decoupled from the sensor thickness and can be spaced significantly closer together than the thickness of the standard planar sensors, where electrodes are implanted on the

surface of the sensor Figure 5.19. This reduced electrode spacing minimizes charge trapping from radiation-induced defects and lowers operational voltages, thereby reducing power dissipation post-irradiation.

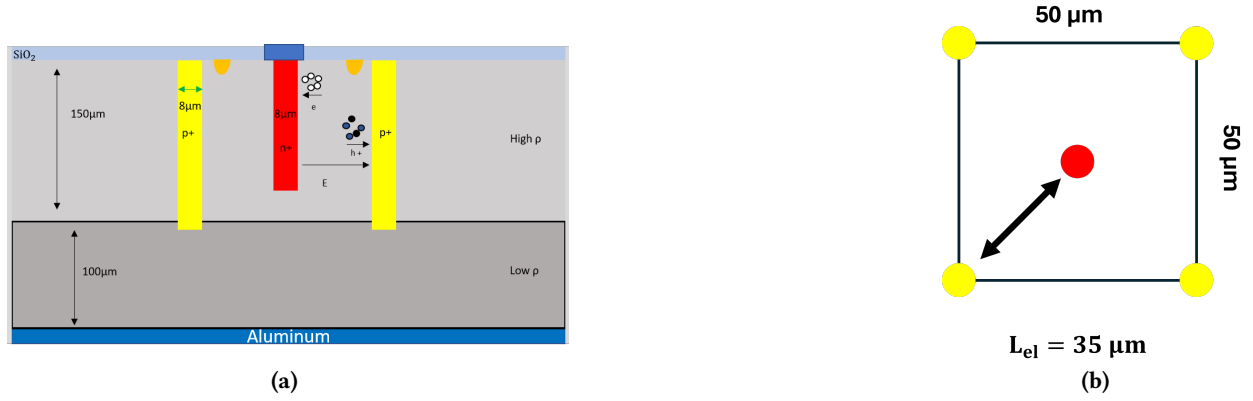


Figure 5.21: (a) Layout of the 3D sensors in the innermost L0 layer of the ITk Pixel Detector. The readout columns (n+) are highlighted in red, while the ohmic columns (p+), depicted in yellow, are connected to the bulk region, which is biased from the backside (b) The top view of the $50 \times 50 \mu\text{m}^2$ pixel with the inter-electrode distance of $35 \mu\text{m}$.

Over the past two decades, 3D sensor technology has evolved into a commercially mature product, meeting high radiation tolerance requirements. Within the ATLAS experiment, both the IBL (see Section 2.2.4.1) and the ATLAS Forward Proton detector (AFP) [289] utilize 3D sensors with inter-electrode distances of $67 \mu\text{m}$ and a sensor thickness of $230 \mu\text{m}$, demonstrating a radiation tolerance of at least $5 \times 10^{15} n_{eq}/\text{cm}^2$, meeting the requirements for both IBL and AFP [94]. The high radiation tolerance and low power dissipation make the 3D sensor technology the baseline option for the innermost layer of the ITk Pixel Detector (Layer 0 and Ring 0).

The ITk Pixel Detector requires specific developments in 3D sensor technology, including smaller pixel sizes, thinner active areas, and exceptional radiation tolerance. The ITk 3D sensors are designed with a $150 \mu\text{m}$ active thickness, complemented by a $100 \mu\text{m}$ passive support wafer added to facilitate handling and bump-bonding. The 3D sensors in the barrel and endcap regions of the L0 are characterized by pixel sizes of $50 \times 50 \mu\text{m}^2$ and $25 \times 100 \mu\text{m}^2$, respectively. Hit reconstruction efficiencies greater than 97% with an associated power dissipation of about $10 \text{mW}/\text{cm}^2$ have been demonstrated for 3D devices with $50 \times 50 \mu\text{m}^2$ pixel geometries irradiated with 24 GeV protons up to $1.4 \times 10^{16} n_{eq}/\text{cm}^2$ as depicted in Figure 5.22 [290]. Additionally, dedicated productions of 3D sensors compatible with the ITk prototype FE chip (RD53A) have been completed or are underway at various foundries such as CNM (Barcelona), FBK (Italy), and Sintef (Norway).

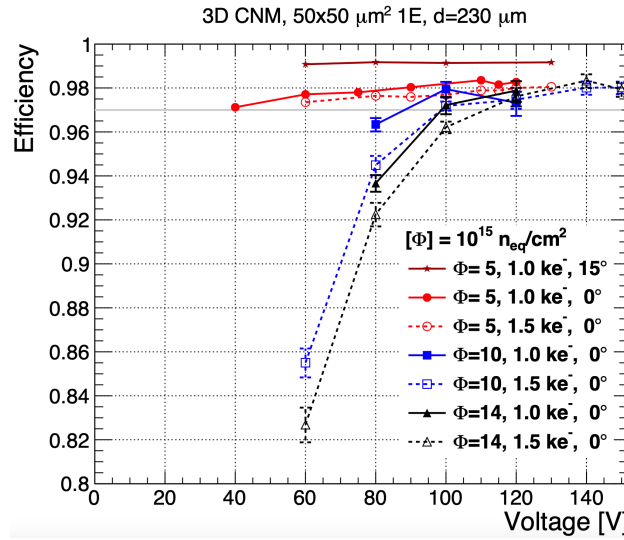


Figure 5.22: Efficiency of a $50 \times 50 \mu\text{m}^2$ CNM 3D sensor plotted against voltage for various fluences, thresholds, and tilts. Uncertainties depicted are statistical in nature [290].

5.4.3.2 ITk Pixel Readout Chips

The stringent requirements on the ATLAS ITk Pixel Detector, including radiation hardness, data handling capacity, and trigger rates, as discussed in Sections 1 and 2, respectively, surpass the capabilities of the current FE-I4 chip (see Section 2.2.4.1). This necessitates R&D efforts for new read-out chip designs tailored to meet the specific requirements of detectors operating within the harsh radiation environment of the HL-LHC. The RD53 collaboration, comprising 24 institutes from Europe and the United States, was established to collectively design the next generation of hybrid pixel read-out chips for the phase-II upgrade of both the ATLAS and CMS detectors. The specific requirements of the read-out chip are determined by the detector's performance and its interface with a range of system components. These connections include electrical interfaces with sensors, module flex, DAQ systems, and test setups, as well as mechanical interfaces with flip chip bump bonding, module assembly, mechanical supports, detector layout, and wafer processing and testing [95]. Table 5.2 summarizes the main requirements of an FE-chip for HL-LHC operations. The planned increase in the trigger rate from ≈ 100 kHz to about 1 MHz at HL-LHC results in the increase of the detector throughput. In order to meet the bandwidth requirements and fulfill all the specifications mandated by the Phase-II ATLAS Experiment, RD53 utilizes 65 nm CMOS technology, which is smaller in scale compared to the 250 nm and 130 nm technologies used in FE-I3 and FE-I4 chips, respectively. The chip dimensions are estimated to be $\approx 20\text{cm} \times 21\text{cm}$, housing 153,600 pixels arranged in 400 rows and 384 columns. The use of 65 nm technology is crucial due to its enhanced radiation hardness and increased integrability, essential for accommodating ≈ 500 million transistors present in the RD53 FE chips. The RD53 read-out chip features programmable internal settings, allowing optimization tailored to each layer of the ITk detector. This capability effectively reduces power consumption, especially considering that the same FE chip is intended for use in both the innermost layer, which encounters the most critical conditions, and all outer layers, which generally experience a more relaxed environment by comparison.

Requirements	Value	Source
Matrix size columns $\times$ rows	400×384	Layout, IC design constraints
Input pitch	$50 \mu\text{m} \times 50 \mu\text{m}$	Tracking performance, occupancy
Final thickness	$150 \mu\text{m}$	Material, bump bonding, local supports
Power dissipation	$< 0.7 \text{ W/cm}^2$	Cooling, local supports, sensor
Current consumption	$< 1.5 \text{ A/chip}$	Services
Temperature range	-40^{deg}C to 40^{deg}C	Cooling, operation, integration
Total ionizing dose tolerance	$\geq 500 \text{ Mrad}$	Inner layer lifetime before replacement
Full chip SEU upset probability	5% per hour	Inner layer operation
Pixel loss due to SEU	$< 1\%$ per run	Hit efficiency, inner layer operation
Trigger rate	1 MHz (4 MHz)	Trigger and DAQ
Trigger latency	$< 35 \mu\text{s}$	Trigger and DAQ
Trigger Protocol	Tagged trigger	DAQ, operation
Single Pixel Noise (ENC)	$100e^-$	Threshold, resolution
Threshold dispersion after tuning	$40e^-$	Uniformity, efficiency
Threshold variation	$< 10\%/K$	Operation
Noise occupancy per pixel	$< 10^{-6}$	Tracking performance
Hit loss at 75 kHz hit rate	$\leq 1\%$	Efficiency for inner layer
Recovery from saturation	$< 1 \mu\text{s}$	Efficiency, pileup
Charge measurement resolution	$< 600e^-$	Tracking performance

Table 5.2: Physical, power, environmental and performance requirements for the ITk Pixel Detector Front-End chip [95].

RD53A Readout Chip

The RD53A read-out chip is the first prototype ASIC developed by the RD53 collaboration to showcase the chosen technology's suitability for the HL-LHC upgrade. The chip was not intended as a final design but rather incorporates design variations specifically for testing purposes [291]. The functional floorplan of the RD53A is illustrated in 5.23a. At the bottom of the chip lies the analog and digital circuitry responsible for biasing, configuration, and readout functions. A row of pads for wirebonding, facilitating all electrical connections, is located along the chip's lower edge. RD53A incorporates three distinct pixel frontend types: synchronous, linear, and differential frontends, arranged on the chip as depicted in 5.23b. This arrangement enables the evaluation of different design performances on the same chip. The differential frontend utilizes a differential gain stage preceding the discriminator and implements threshold adjustment by unbalancing the two branches. The linear frontend features linear pulse amplification preceding the discriminator, which compares the pulse to a threshold voltage. Meanwhile, the synchronous frontend employs a baseline "auto-zeroing" scheme, requiring periodic acquisition of a baseline instead of pixel-by-pixel threshold trimming [292]. More details on the various flavours of FE can be found in [291, 292]. Similar to the FE-I4, the pulse width, also known as ToT, is measured using the discriminator and is proportional to the charge deposited in the sensor.

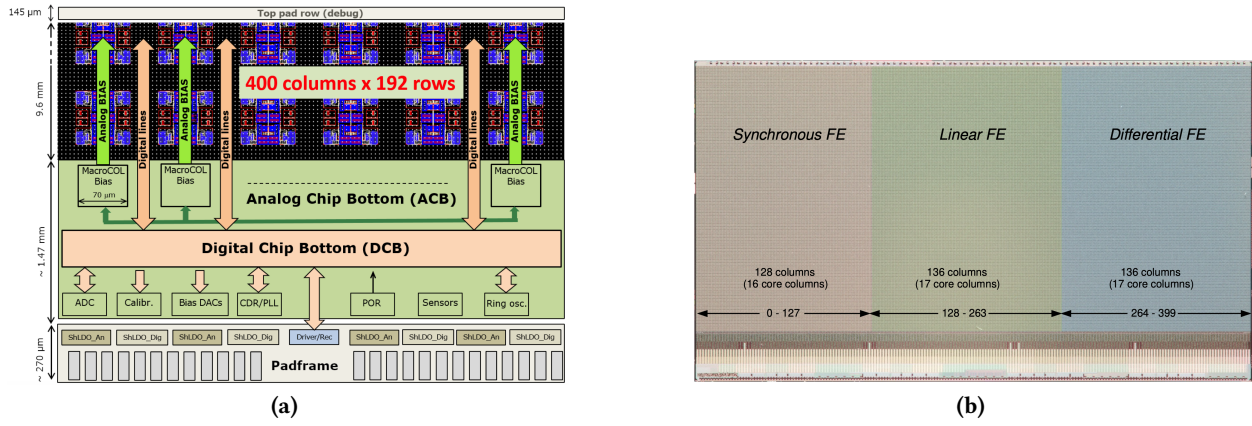


Figure 5.23: (a) RD53A floorplan, functional view (b) Arrangement of front end flavours in RD53A. The pixel column number range of each flavour is shown along the bottom. Figures taken from [291].

ITkPix Readout Chip

The pixel matrix is divided into 8×8 pixels, forming a pixel core, synthesized as a single digital circuit. Four analog pixel FEs are grouped together, surrounded by the digital logic of the pixel cores. The cores provide the digital configuration to the analog FEs and receive the digital outputs from the FEs for processing. The RD53A chip is controlled via a single 160 MB/s link, which also serves as the source for on-chip clocks. Data output is available on up to four links, each operating at up to 1.28 GB/s. The chip is configured for serial powering with integrated regulators, enabling multiple frontends to be linked in a chain supplied with constant current, minimizing power losses in cables and the material budget.

Following the successful development of the RD53A prototype chip, the collaboration expanded its scope to create a unified design adaptable to ATLAS and CMS requirements. This led to the RD53B prototype, serving as the foundation for two distinct chips tailored to each experiment: the ITkPix for ATLAS, featuring a 400×384 pixel array and utilizing a differential frontend, and the CROC for CMS, featuring a 432×336 pixel array and employing a linear frontend. The variation in pixel matrix size between the two chips was implemented to accommodate distinct detector layout constraints, with each chip incorporating experiment-specific features accordingly [293].

The RD53B chip prototype introduces several enhancements over the RD53A, such as improvements to serial powering regulators, clocking mechanisms, a revamped triggering and readout scheme, and a new data encoding method that boosts encoding efficiency by over 20%. Additionally, it enables data merging from other chips, allowing up to four RD53B-based chips to be connected together. The data from up to three slave chips connected to the input lanes is merged into the output of the master chip [293].

The pre-production chip for the ITk Pixel Detector is referred to as the ITkPixV1. Table 5.3 compares its basic design parameters with those of the previous FE chips in ATLAS. The initial version, ITkPixV1.0, encountered a Time over Threshold (ToT) issue upon its submission in March 2020, resulting in a significant current increase and rendering it unusable for data collection. In 2021, an updated version, ITkPixV1.1, was released, addressing the ToT problem by disabling ToT reading through modification of the topmost layer of the silicon wafer during chip production, limiting functionality to binary hit readout. As a result, ITkPixV1.1 remains a prototype, with the final iteration, ITkPixV2, submitted by the end of 2022 and currently undergoing rigorous testing at various institutes.

	FE-I3	FE-I4	RD53A	ITkPixV1
Feature size [nm]	250	130	65	65
Chip Size [mm ²]	7.6 × 10.8	20.2 × 18.8	20 × 11.6	≈ 20 × 20
Pixel Size [μm ²]	50 × 400	50 × 250	50 × 50	50 × 50
Pixel matrix	18 × 160	80 × 336	400 × 192	400 × 384
Data bandwidth	40 MB/s	160 MB/s	4 × 1.28 GB/s	4 × 1.28 GB/s
Data encoding		8b10b	64b66b	64b66b

Table 5.3: Comparison of Design Parameters for Frontend Chips in the Current and Future ATLAS Pixel Detectors [96, 292–294]

5.4.3.3 Pixel Modules

The hybrid pixel module comprises two primary components: a passive high-resistivity silicon sensor and a FE read-out chip manufactured using CMOS technology, referred to as the bare module and a flexible PCB, called a module flex. The silicon sensor and the FE read-out chip are interconnected using a high-density connection technique called flip-chip bump-bonding [295]. All connections to the bare modules are routed to the active elements via the module flex, which is affixed to the backside of the sensor [95]. Figure 5.24 illustrates a schematic representation of the constituent elements of a bare pixel module.

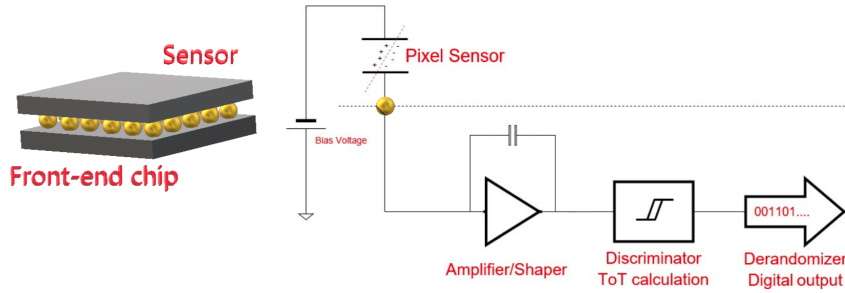


Figure 5.24: Schematic view of a bare pixel module [95].

Three types of hybrid pixel modules are envisioned for the ITk Pixel detector: quad modules with four FE chips bump-bonded to a single sensor ($4 \times 4\text{cm}^2$), designated for outer barrel layers and end-cap rings; dual modules with two FE chips per sensor ($4 \times 2\text{cm}^2$), intended for innermost barrel layers and outer barrel inclines to optimize radial tiling while minimizing material; and single-chip modules with one front-end chip bump-bonded to a sensor ($2 \times 2\text{cm}^2$), tailored for the inclined part of the innermost barrel layer.

Over the next three years, approximately 10,000 modules will be manually assembled for the ITk Pixel detector. This assembly process involves bonding bare, hybridized sensor-frontend assemblies onto module flexes using custom-built tools, where the glue distribution is performed through a laser-cut stencil, and the thickness of the glue layer is meticulously controlled via a calibration procedure described in detail in Section 5.4.4.3. An overview of the module development activities conducted at one of the assembly sites of the outer barrel pixel modules, LPNHE-Paris, is presented in Section 5.4.4.

5.4.3.4 Mechanical Support

In the ITk detector (see Figure 5.10b), the modules are placed on the local supports, with the backside of the FE chips in contact with the support. These local support structures provide mechanical support, alignment, service routing, and thermal management for the pixel modules. These

supports are typically crafted from lightweight, high-rigidity materials with excellent thermal conductivity, such as carbon fiber laminates, pyrolytic graphite, and other carbon-based composites featuring a titanium pipe for heat extraction through a CO₂ cooling system.

The Inner System (IS) consists of two layers of barrel staves (L0 and L1) and three endcap ring designs (R0, R0.5, and R1), as depicted in Figure 5.25a. The integration of IS occurs in quarters, as shown in Figure 5.25b, with services such as power, data transmission, and cooling running along the outer shell. The carbon foam local support structure for an endcap ring is illustrated in Figure 5.25c. A circular connection board that supplies power and transmits data, referred to as a Type-0 service ring, acts as an intermediate layer between pixel modules and patch panels, connecting to the patch panels via pigtail connectors on the integrating structure's shell [285].

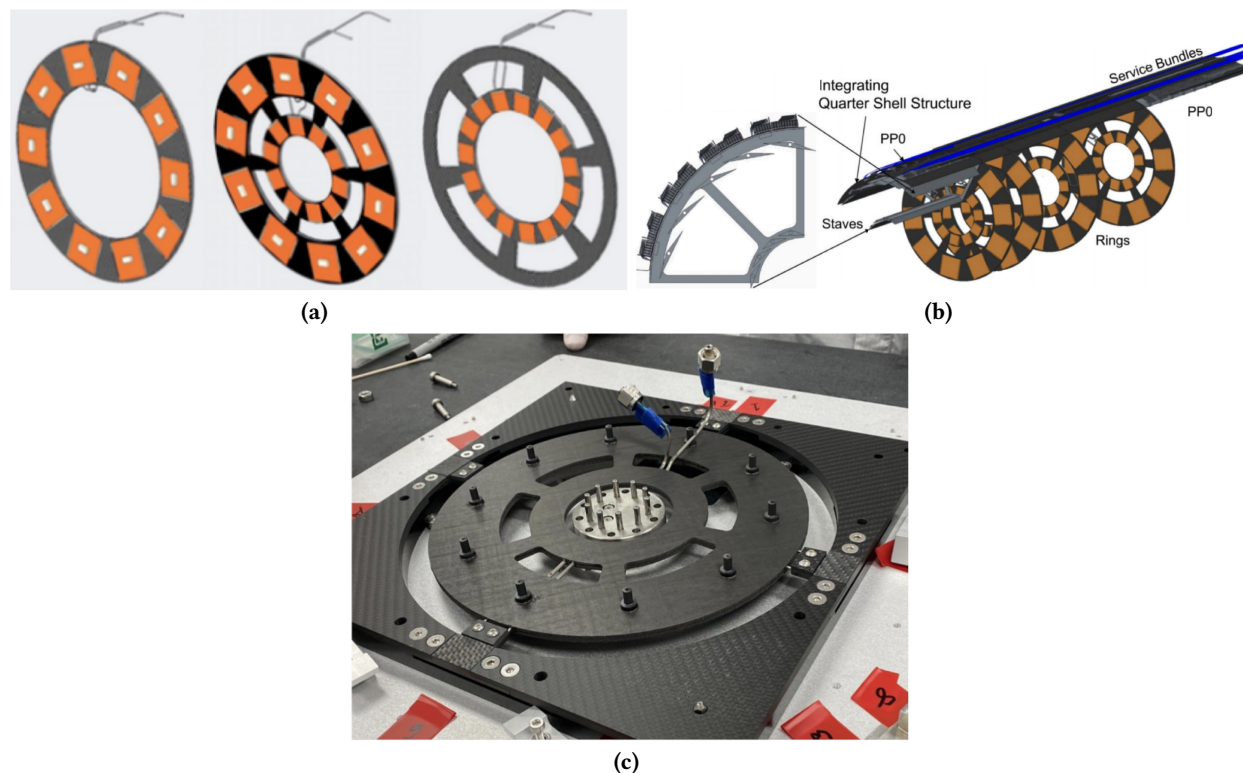


Figure 5.25: (a) Three distinct ring designs for the Inner System. From left to right: R1 featuring only quad modules, R0.5 with quads and triplets, and R0 with only triplets (b) An integrating quarter with rings and the two layers of barrel staves. Service bundles and patchpanels are located along the Quarter Shell structure (c) A carbon local support for a R0.5 prototype. Figures taken from [285].

The Outer Barrel (OB) layout consists of two distinct sections: flat and inclined. Within the flat section, the local supports are referred to as longerons, while in the inclined section, they are known as inclined rings. In the OB, modules are loaded onto module cells, which are then fastened to base blocks on the local supports during a subsequent integration stage. A flowchart of the integration scheme is illustrated in Figure 5.26.

The loading procedure for local supports in the Outer Endcaps (OE) involves half-rings, as depicted in Figure 5.27b, available in three different sizes accommodating 8, 11, and 13 modules. The pixel modules will be loaded on both sides of half-rings where a flex PCB bus tape will also be attached to route power and monitoring signals to each module. These half-rings are subsequently assembled into a half-barrel, shown in Figure 5.27a, for the integration into the ITk pixel system.

A comprehensive overview of local supports, including design qualification and prototyping programs, as well as quality assurance and control during production, is detailed in Chapter 13 of [95].

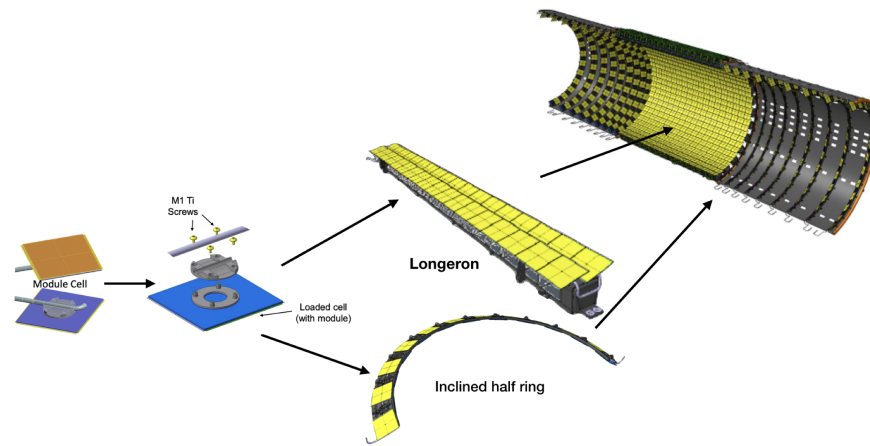


Figure 5.26: Outer barrel assembly scheme: module cells are loaded onto baseblocks for cooling which are then screwed onto the local support structure of the OB, either longerons or inclined rings. The local support structures are then assembled into a half barrel as shown to the right [285].

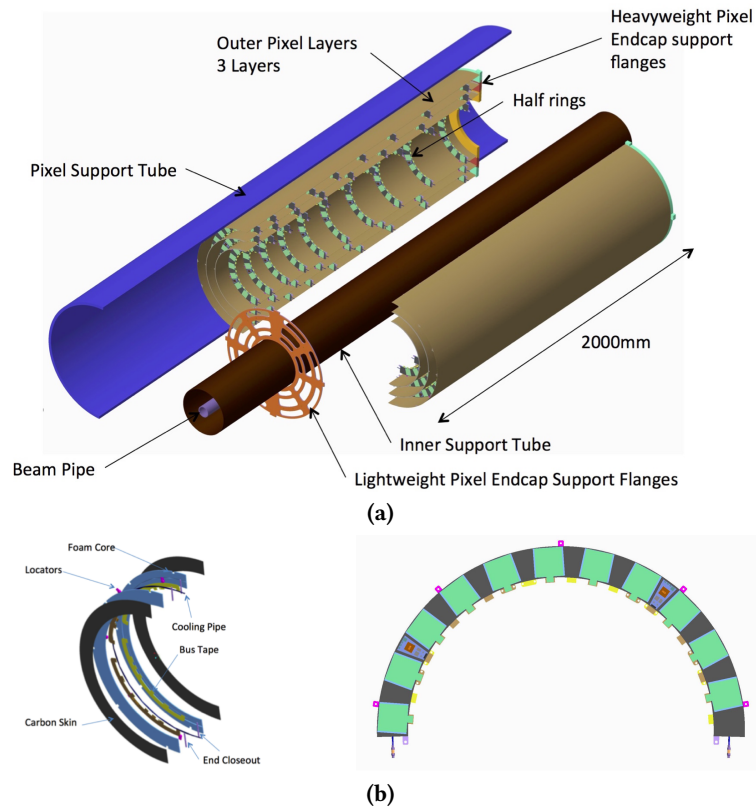


Figure 5.27: (a) Schematic 3D illustration of one Outer End-cap. (b) Left: an exploded view of a half-ring depicting the internal components. Right: a view of the surface of a half-ring showing 11 pixel modules (green). Figures taken from [95].

5.4.4 Module Development

Pixel quad modules are designated for all layers of the ITk pixel detector except the innermost layer (L0), as outlined in Section 5.4.3.3. The final production modules will consist of the ITkPixV2.0 FE read-out chip paired with either planar or 3D sensors, along with the finalized flex design. In the ATLAS experiment, several qualification stages must be completed before commencing the production of the actual ITk modules. Delays in the design and delivery of the final read-out chip and flex prompted the decision to conduct design qualification using the prototype RD53A chip. Following this, the RD53A module campaign was initiated to evaluate the module construction process and subsequent testing procedures. Following the successful conclusion of the RD53A program, which validated numerous production, assembly, integration tests, and the broader infrastructure necessary for commissioning the ITk, the pre-production phase of the modules has begun, with some sites already having successfully completed this stage. With the maturation of these tools and procedures, the focus has turned towards optimizing module production to manage the target throughput across multiple global sites effectively. Currently, tests are underway with the production ITkPixV2 FE [296]. This section offers an overview of the stages involved in the quad module assembly process for the ITk Pixel Detector, emphasizing the work carried out at LPNHE, Paris, as part of site qualification for actual ITk quad module production.

5.4.4.1 Module Assembly Tooling

The University of Göttingen, Germany, developed a standardized tooling for quad module assembly, serving as the default equipment for the entire ITk Pixel Collaboration. A module (Section 5.4.3.3), as depicted in Figure 5.28, comprises a silicon sensor bump-bonded to a FE chip, forming a bare module. The bare module is subsequently glued to a flexible PCB, which facilitates data and power connections via dedicated pigtail cables. Module assembly involves attaching the flex to the bare module using adhesive applied by a stencil, followed by wire bonding after curing. The tooling for quad module assembly, as shown in Figure 5.29, comprises two jigs that support the flex and the bare module, allowing them to be precisely aligned on top of each other with 50 μm [297] precision using rods and ball bearings. Additionally, a stencil tooling and a spatula facilitate the application of a predetermined amount of adhesive onto the flex before closing the tooling for attachment and curing. The module assembly process entails several key stages such as Visual Inspection, Metrology, Flex Attachment, Parylene Coating, and Mechanical Wire-bond Protection Assembly. The subsequent sections offer an overview of each of these stages.

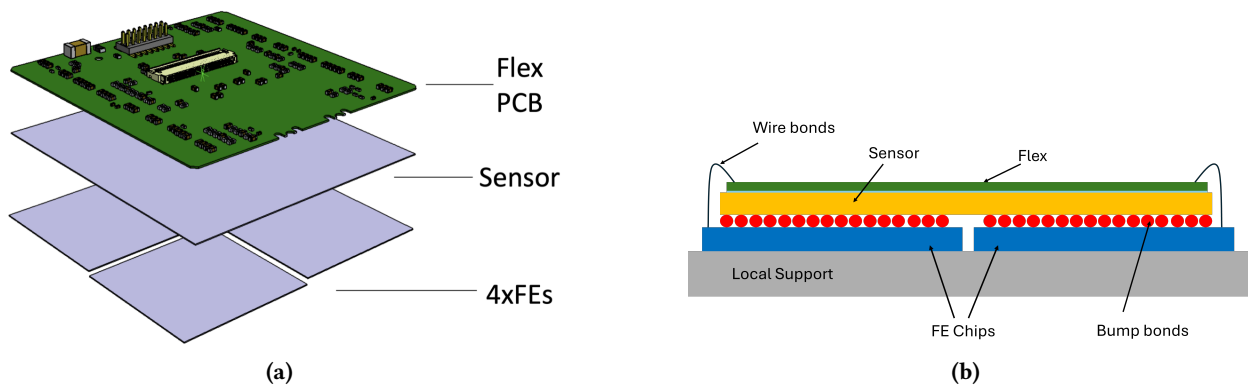


Figure 5.28: (a) Exploded view of a quad module and its constituent components. Figure taken from [296] (b) Schematic of an assembled module.

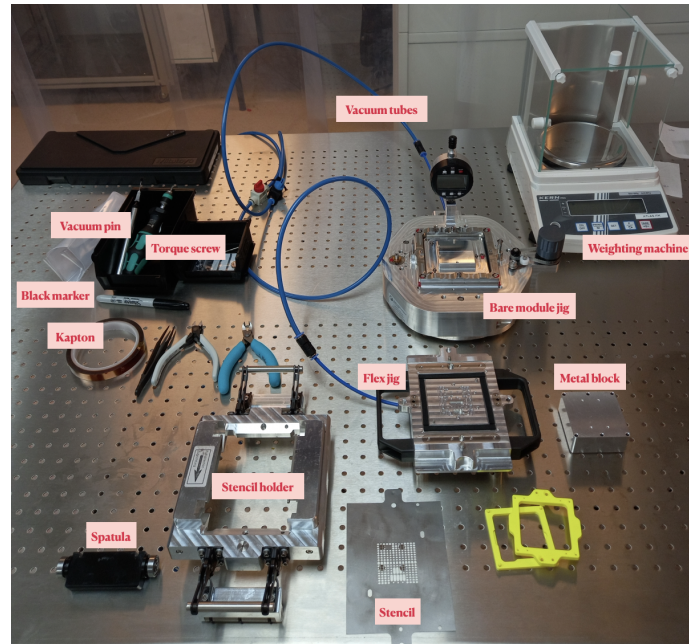


Figure 5.29: LPNHE quad module assembly setup in the lab with two jigs, stencil, stencil holder, spatula, metal block and vacuum supply.

5.4.4.2 Assembly Specifications

Before assembling the pre-production quad modules, the module assembly sites must be qualified to demonstrate their capability of building modules that meet the general requirements. In order to fulfill this purpose, glass and silicon dummies were used instead of bare modules along with the preliminary version (v3.2) of the common quad flex at LPNHE. The assembly of actual ITk quad modules will be carried out using fully functioning ITkPixV2 bare modules and v3.8 of the common module flex. This section briefly outlines the various requirements and specifications that must be met for the module assembly process.

The precise dimensions of the bare components must be known in order to validate the functionality of the module assembly tooling. The overall flatness of both the bare module and the Si-dummy should be within $\pm 25\mu\text{m}$, with coplanarity within $\pm 50\mu\text{m}$ [298]. Additionally, the bump bond layer between the FE chip and sensor should range between 10 - 25 μm . The specifications for OB modules, as outlined in [95] is utilized for the design of the tooling. In the case of assembled modules, in terms of mechanical requirements, a module should be attached with a precision of $\pm 50\mu\text{m}$ in both the x and y directions to ensure proper wire bonding angles and suitable connector positions. The glue coverage under the flex must be at least 80%, without spreading beyond the edge of the flex, to facilitate wire bonding and ensure module stability. This necessitates an adhesive thickness of $(40 \pm 15)\mu\text{m}$ and a defined adhesive weight [297].

The module assembly procedure was developed to meet all the aforementioned requirements and is presented in the following section.

5.4.4.3 Assembly Procedure

The module assembly process begins with a visual inspection, which involves assessing all the components upon reception and at every assembly and testing stage to identify any damage to the module, like scratches, dirt, or broken chips. Digital microscopes are used to perform visual inspections of the components, and any surface defects identified are documented with pictures and stored in the production database (PDB).

Metrology measurements are performed to ensure that bare components and assemblies conform to their specified parameters. These measurement procedures are iterated after each significant modification stage in the assembly chain to consistently evaluate the integrity and compliance of the module [296]. Figure 5.30 shows the MMT machine at LPNHE used for conducting metrology measurements of the bare module, flex, and assembled modules.

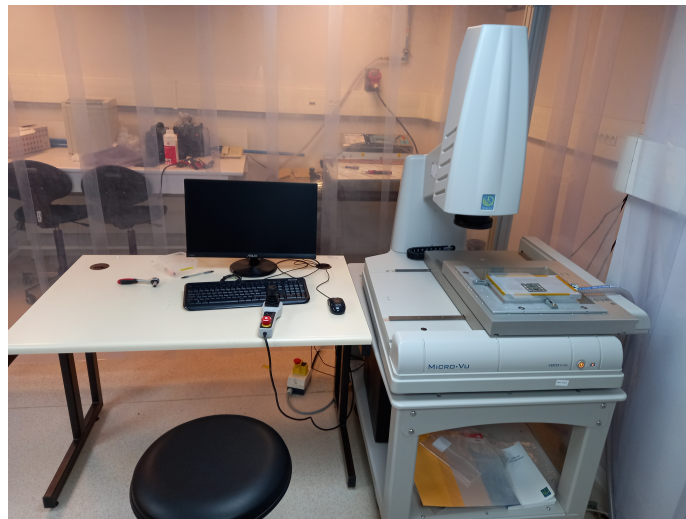


Figure 5.30: The MMT machine in the clean room at LPNHE for metrology measurements.

In addition to metrology measurements before and after flex attachment, the assembly procedure also includes a meticulous calibration of the tooling. The following measurements are carried out for all the modules:

- Measurement of the dimensions of the raw components prior to assembly.
- Weighing the bare components and the module after assembly.
- Height measurements of the module and thickness of the adhesive.
- Pull tests on the wire bonds.
- Visual inspection at various processing stages.

Calibration of the Tooling

The calibration of the tooling is essential in order to ensure that the glue height is within the required specifications, enabling the building of modules with a uniform adhesive layer. This step should be performed before any module assembly to customize the tooling according to the specific module parts. The alignment of the surfaces on the jigs where the bare module and flex make contact should be parallel. This alignment is ensured through the mating principle involving guide rods and bushings rather than relying on their angle with the back-plane of the respective tooling jigs. The process of the calibration of the tooling encompasses the following steps:

1. Alignment of the flex onto its respective jig.
 - Place the flex in the flex jig.
 - Use a metal block to flatten the flex.
 - Make sure that the flex does not move relative to the inlay and turn on the vacuum.
2. Position and align the bare module onto the bare module jig. Figure 5.29 illustrates the tools required for this task, including the bare module jig, bare module, and vacuum pen.

- Gently put the bare module on the bare module jig with the help of the vacuum pin.
- Ensure that the bare module is positioned on the jig so that it makes contact with all three alignment pins, as depicted in Figure 5.31.
- Turn on vacuum on the bare module jig.
- Gently lower the right knob of the bare module jig to the lowest position without applying force.

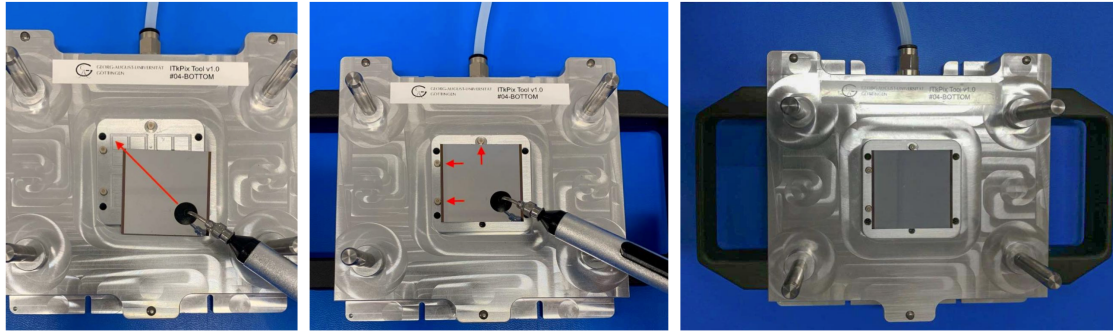


Figure 5.31: **Left:** Placing a bare module on the bare module jig with vacuum pen **Middle:** Aligning the bare module to the alignment pins. **Right:** Dummy bare module aligned with alignment pins on bare module jig. Figures taken from [297].

3. Set the glue height.

- Place the flex jig very carefully onto the bare module jig by mating the guide rods and the guide bushings.
- Insert the two mating long screws using the torque driver already set to the correct force. Simply screw them until they click.
- Turn on the micrometer gauge of the gluing tool.
- Use the right knob to raise the bare module jig plate to its maximum height. Do not force it; at a certain point, the knob will become very light, and the micrometer gauge will stop increasing in value.
- Gently unscrew the height calibration screw until the micrometer gauge stops increasing. Exercise caution and apply minimal vertical pressure during this step.
- Now that the flex and bare module are in contact, reset the micrometer gauge to 0.
- Screw the height calibration screw down to $-40\text{ }\mu\text{m}$.
- Gradually unscrew the height calibration screw until it reaches $-35\text{ }\mu\text{m}$. Ensure to approach $-35\text{ }\mu\text{m}$ from below. If needed, repeat the operation.

4. Check the calibration.

- Lower the bare module jig to a distant value using the right knob and raise it back until the micrometer gauge stops.
- Ensure that the reading is approximately near $-35\text{ }\mu\text{m}$, possibly slightly higher. It should be within $35\text{ }\mu\text{m}$ from the set value.

Flex Attach Procedure

Assuming the flex and the bare module remain in their contact position following the calibration stage (Section 5.4.4.3), the following set of steps must be followed for flex attachment:

1. Remove the flex from the flex jig.

- Lower the bare module jig to its lowest position and then unscrew the mating screws.
 - Cut off the vacuum supply to the flex jig.
 - Use tweezers to gently remove the flex off the jig.
2. Cover the HV hole with a Kapton tape.
- Utilize a combination of cutters, scissors, and ESD plastic tools to cut a small rectangle of Kapton tape. Ensure it is larger than the HV hole but small enough not to extend over the soldering pad or other features.
 - Position the Kapton tape to cover the HV hole and then place the flex in the MMT to inspect the HV hole. Ensure complete coverage of the hole and check for any visible air bubbles trapped under the Kapton tape where it meets the flex.
3. Perform post-Kapton attachment checks on the flex jig.
- Place the flex back in the flex jig.
 - Press the flex firmly using the metallic cube.
 - Turn on the vacuum supply and mate the flex jig with the bare module jig.
 - Raise the bare module jig to maximum position to ensure the same gap as before, $\approx 35\mu\text{m}$. If the gap is significantly larger, inspect for contact with the metal pad, traces, or other components with Kapton tape. Verify the use of the correct (thin) Kapton tape.
 - Lower the silicon jig to the minimum position and un-mate the flex jig from the bare module jig. Ensure to maintain the vacuum supply!
4. Preparation of the adhesive: Araldite (shown in Figure 5.32), a two-part epoxy mixed at glue time, used for attaching the bare module to the flex.
- Dispense between 1/2 to 3/4 pump from the Araldite glue gun into the mixing cup.
 - Mix the glue thoroughly using the mixer. The mixer should start with the correct program; if not, set it to 2 minutes at 2000 rpm for mixing without de-foaming option switched on. Figure 5.32 illustrates the mixer used at LPNHE for preparing the adhesive.
5. Deposition of glue on the flex.
- Position the stencil over the flex jig, ensuring that all alignment pins are correctly aligned.
 - Position the stencil holder/spatula guide over the flex jig and secure it in place by closing it.
 - Place the spatula in the stencil holder, see Figure 5.33a.
 - Use the black marker to indicate on the stencil the position of the glue zone of the spatula.
 - Remove the spatula and apply the glue between the black marks as shown in Figure 5.33b.
 - Insert the spatula back into the guide and carefully pull it down (see Figure 5.34a) to spread the glue into the stencil holes in a controlled motion. Afterward, the stencil should resemble the depiction in Figure 5.34b on the right. Figure 5.34c illustrates a flex with adhesive distributed using the stencil method.
 - Carefully retract the spatula and remove it gently to prevent spreading the glue filaments.
 - Open and remove the stencil holder / spatula guide block from the flex jig, then inspect the glue deposition on the flex.

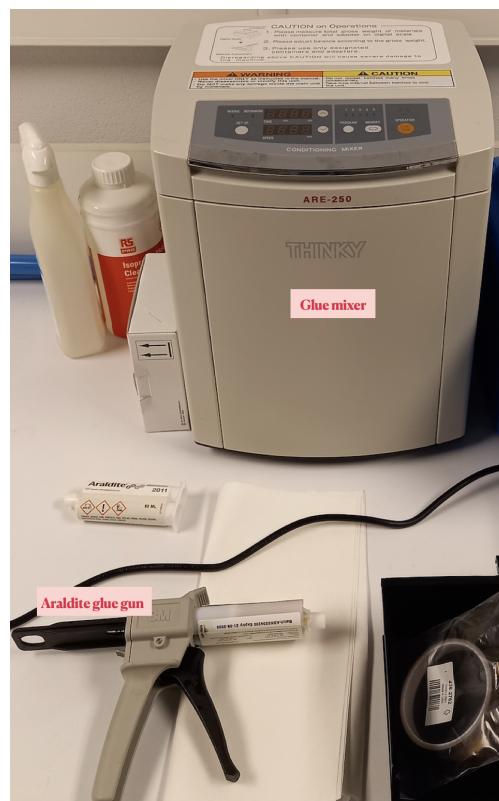
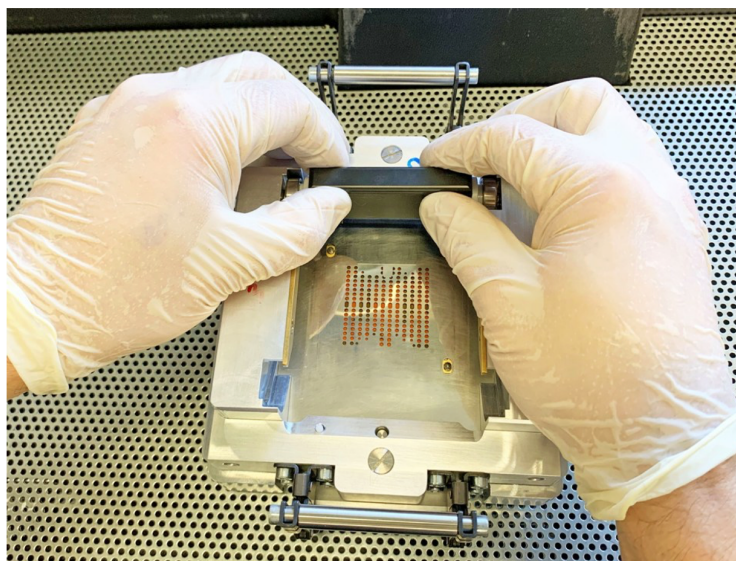
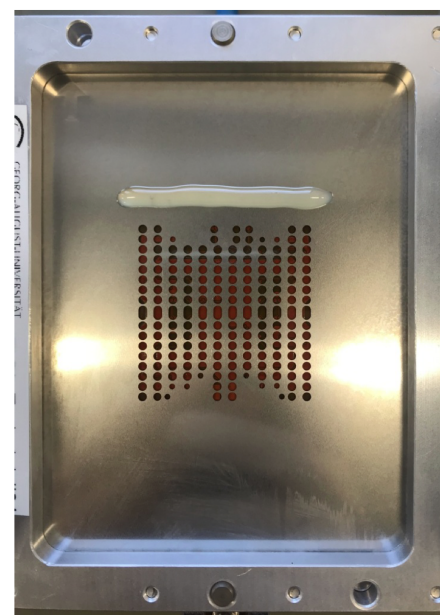


Figure 5.32: Araldite used with a glue gun and mixer for preparing the adhesive.

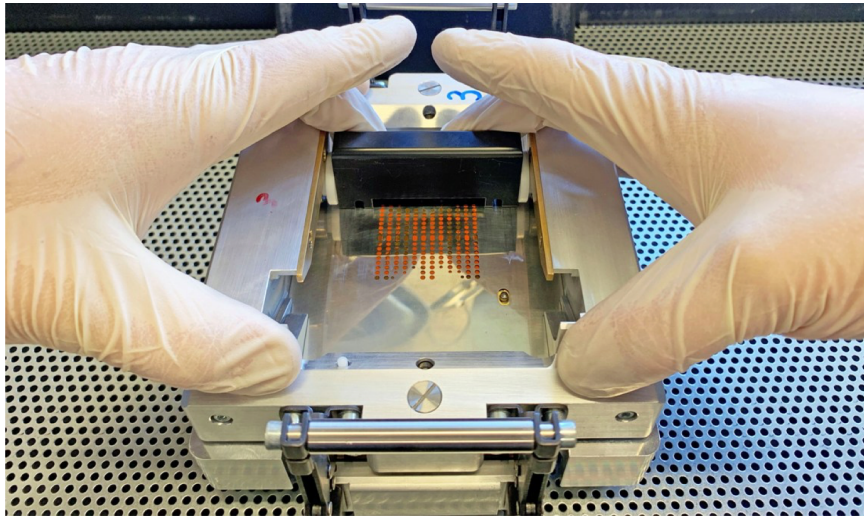


(a)

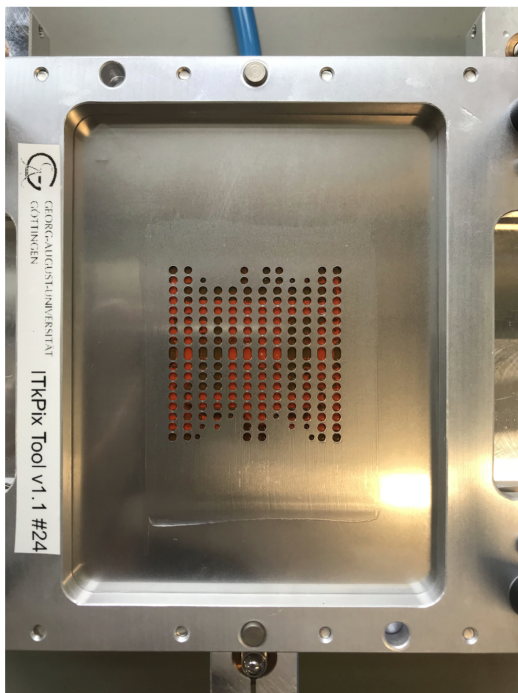


(b)

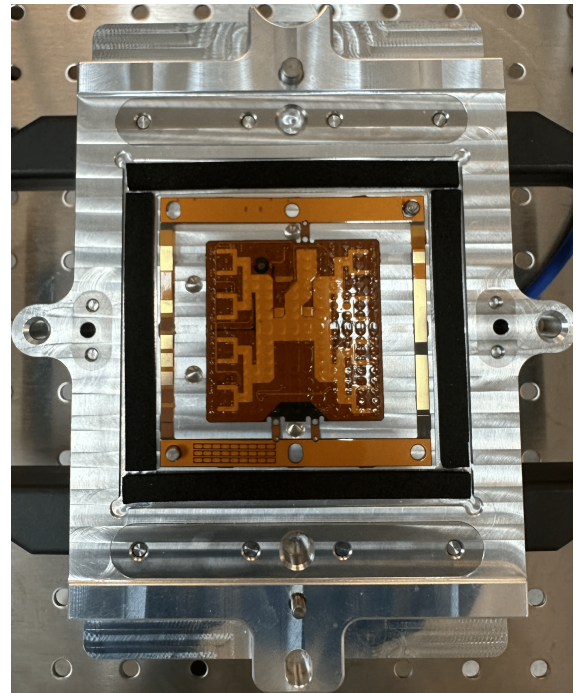
Figure 5.33: (a) Insert spatula (b) Put the glue on the stencil.



(a)



(b)



(c)

Figure 5.34: (a) Pull spatula (b) Adhesive spread on the stencil (c) The adhesive pattern on a flex distributed with the stencil method.

6. Flex attach

- Gently place the flex jig onto the bare module jig while keeping the vacuum active
- Using the torque driver, insert the mating screws and raise the bare module jig to the maximum position (until the right knob feels light). The micrometer gauge may not immediately reach the target value but will approach it at around 10-15 μm before gradually reducing the gap; this indicates the glue is making contact and spreading
- Leave the flex jig on the bare module jig for at least 8 hours to allow the adhesive to cure completely

After ensuring complete curing of the glue by leaving the flex jig on top of the bare module for at least 8 hours, the mating screws are removed and the vacuum supply to the bare module jig is cut off. The bare module jig is then lowered to its lowest position using the right knob of the tooling, and then the jigs are un-mated. If there were no major incidents, the bare module will remain attached to the flex jig. Next, the flex vacuum is switched off and the module is gently detached from the flex jig using tools to release the flex frame from the alignment pins.

Following the gluing application, the module undergoes quality control (QC) procedure to verify the flex attachment process. The visual inspection of the module should indicate no glue seepage on wire bonding pads and HV connection hole. Once the module passes the visual inspection, non-contact metrology with MMT measures module height and alignment in x-y directions, with and without vacuum to assess flatness of the glued module. Glue thickness is determined by the weight difference between bare components and the assembled module. Module alignment is determined by measuring the distance between the bare module and flex edges on all sides and the maximum dimensions must adhere to module envelope specifications outlined in [299]. The recorded data, including glue mass, should be uploaded in the PDB.

In the subsequent stage of the module assembly process, aluminum wedge wire-bonds are used for wire-bonding followed by parylene coating. Wire bonding creates a link between the readout chips and the flex for electrical connectivity, facilitating module readout. The parylene coating enhances mechanical robustness of the delicate wire-bonds, shields against potential high-voltage sparks near sensor edges, and ensures protection from atmospheric corrosion. Wire bonding QC involves visual inspection with a microscope to ensure absence of mis-bonded wires, straight alignment between bond pads, uniform wire loops without kinks, and the absence of wire interconnection. Furthermore, bond pull-strength tests are conducted to evaluate wire-bond quality by measuring the force required to break the bonds. Specifically, 8 wires per chip are pulled, with a minimum breaking force requirement of 5 g for each wire and an average breaking force of 8 g or higher [300].

Once assembled, the modules undergo comprehensive testing, including electrical scans and front-end tuning, monitoring parameters such as high-voltage, low-voltage, currents, environmental temperature, humidity, and dew point with software interlocks, as well as source scans to assess pixel functionality. The results of module testings are available in additional literature beyond the scope of this thesis for interested readers to explore [296–298, 300].

The pre-production phase of the ATLAS Pixel Inner Tracker (ITk) is expected to conclude by mid-2024, marking the transition to full production. The insights and expertise gained during the pre-production phase will facilitate the integration of optimizations into the module production workflow, including the streamlining of assembly procedures and the simplification of electrical quality checks for the modules [296].

ITk Pixel Digitization

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The following chapter explores two critical aspects of ITk pixel detector development in the ATLAS MC software Athena for HL-LHC experiments. Section 6.1 focuses on modeling ITk pixel digitization in Athena, ensuring accurate simulation of the behavior of the readout chip. Section 6.2 introduces a novel, lightweight fast algorithm designed to model radiation damage effects in MC events for high-luminosity experiments.

6.1 Implementation of Pixel Digitization in Athena

This section presents the results of studies on the implementation of digitization for the ITk pixel modules within the ATLAS software framework, Athena. The digitization of the ITk pixel detector in Athena is primarily based on the FEI4 readout chip used in the current ATLAS pixel detector, despite significant differences between it and the RD53-type readout chip planned for the ITk pixel detector. The studies presented in the subsequent sections focus on developing ITk pixel digitization in Release 22 to achieve a more realistic modeling of the RD53-type chip in Athena. Section 6.1.1 elaborates on the digitization step in the charged particle detection chain introduced in Section 3.4. Following a brief introduction to the Athena software framework in Section 6.1.2, a comparison of pixel digitization between Release 21.9 and Release 22 of Athena is presented in

Section 6.1.3. Section 6.1.4 discusses the modelling of Time-Walk effects, a salient feature of the RD53-type detector readout chip and Section 6.1.5 presents a realistic model for the charge-to-ToT response of the chip. The studies presented herein contribute to my ATLAS qualification task.

6.1.1 Digitization and Beyond

Particle detection in silicon pixel detectors consist of four main stages as illustrated in Figure 6.1. The interaction of charged particles with the silicon atoms causes ionization generating about 80 electron-hole pairs per micrometer along the particle's path, as discussed in Section 3.1. In a reverse-biased n-in-p silicon pixel detector, electrons migrate towards the n^+ implant, while holes move towards the high-voltage p-type backside. This movement induces a current on the pixel electrodes, which is modeled using the Shockley-Ramo theorem discussed in Section 3.3.3. The induced current is typically small; thus, it is amplified by a preamplifier integrated into the readout electronics of each pixel. Subsequently, the signal undergoes shaping to filter out noise and optimize the signal-to-noise ratio, tailoring it to a suitable form for digitization. During the digitization stage, analog signals are converted into a digital format, representing the magnitude of collected charge as a digital value.

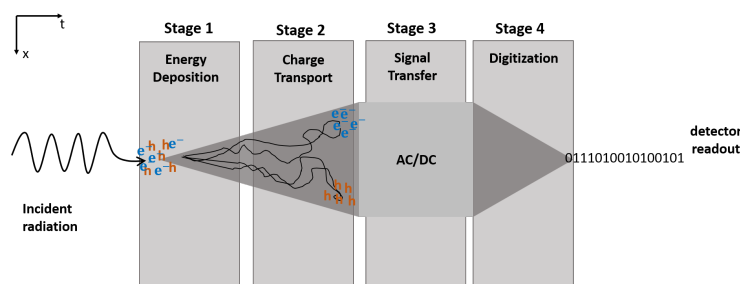


Figure 6.1: The four main stages of charged particle detection in silicon detectors. Adapted from [301].

The readout chip's electronics have a predefined threshold to detect charged particles passing through the detector. When the signal surpasses this threshold, a timer starts to measure the Time-Over-Threshold (ToT), proportional to the deposited charge. A longer ToT indicates a larger charge as depicted in Figure 6.2. Calibration procedures, outlined in Section 6.1.5, convert the ToT measurements into precise charge estimates.

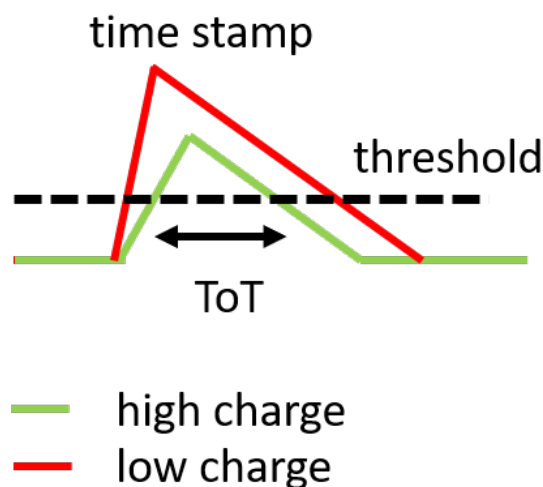


Figure 6.2: Illustration of the Time-over-Threshold (ToT) response of a readout chip to charge depositions from a charged particle, showing both large and small energy deposits.

Pixels detecting charge above the threshold are identified as hits, and adjacent hits are grouped into clusters. The cluster centroid provides an accurate determination of the particle's position. Clusters are formed independently in each detector layer, and clusters from different layers likely caused by the same particle are matched based on their positions and expected trajectory.

Track seeds, initial guesses of the particle's trajectory, are formed by connecting clusters from different layers. Typically, three or more clusters are required to form a seed, and a linear extrapolation provides a preliminary trajectory estimate. Once track seeds are generated, a more sophisticated algorithm, such as the Kalman Filter [302], refines this estimate by considering multiple measurements and uncertainties. Tracks are subsequently evaluated for quality using the Chi-Square test, which measures the agreement between the fitted track and the measured clusters, and hit residuals, which quantify differences between measured and predicted positions. Tracks with poor quality or large residuals are discarded or flagged for further investigation. The final output is the reconstructed particle trajectory, used for momentum calculation, vertex determination, and particle identification [303, 304].

6.1.2 Overview of Athena Software Framework

The Athena framework [305, 306] is the main software infrastructure used by the ATLAS collaboration. It uses Python as a scripting and interpreter language to configure and load C++ algorithms and objects. Instead of creating an entirely new data processing infrastructure for high-energy physics, Athena is built on the Gaudi framework [307], originally developed for the LHCb collaboration. This framework supports various applications through base classes and common functionalities, providing communication tools between different components. Athena also depends on the CLHEP [308] common libraries, which consist of utility classes specifically created for use in high-energy physics software, such as vectors and rotations.

The Athena framework is used to run the complete software stack, primarily involving simulation, digitization, reconstruction, and, to some extent, physics analysis [309]. It works by iterating over an input dataset associated with single particle collisions, referred to as events. This iteration over each event is known as the *Event Loop*, and Athena manages the sequencing of different algorithms within the Event Loop through the *Athena AlgSequence*. The full software chain can be summarized with the following steps:

- Step 1 - Event Generation : Simulates outgoing particles from LHC collisions with specific energies and directions and stores the results in EVNT files, which serve as the input for subsequent steps in the data processing chain.
- Step 2 - Simulation : The generated particles are transported through the detector, simulating their interactions with its components. This process produces HITS files, which represent the energy deposits of particles on the sensitive detector cells.
- Step 3 - Digitization : The ATLAS detector's response is calculated and converted into a digital format from the HITS file generated in the previous step, producing the Raw Data Object (RDO) files, which mimic the signals that would be produced by the actual detector electronics and serve as the input for the reconstruction step.
- Step 4 - Reconstruction: The digitized signals are processed and analyzed to reconstruct physics objects such as tracks, vertices, and energy deposits. These analysis objects are stored in Analysis Object Data (AOD) and Event Summary Data (ESD) files.
- Step 5 - Derivation and Physics Analysis: The vast amount of data stored in AOD and ESD files is filtered and refined to retain only the relevant information for specific physics analysis. The refined data is stored in Derived Analysis Object Data (DAOD) files, which contain a compact representation of the relevant physics objects and event information needed for the specific analysis.

Athena-based programs are tailored to the specific requirements of data processing tasks by configuring the data flow of algorithms, such as event generation, simulation, digitization, reconstruction, and data analysis, in sequence, using *jobOptions*, generated by Python job transform wrapper scripts. An overview of the ATLAS simulation data flow is depicted in Figure 6.3.

Algorithms and applications to be run are represented in blue ovals, while persistent data objects are shown in red boxes. Optional steps required for pile-up or event overlay are indicated with a dashed outline. Generators produce outgoing particles from LHC collisions in HepMC formats, and Monte Carlo truth is saved alongside the hits that represent energy deposition in the detector.

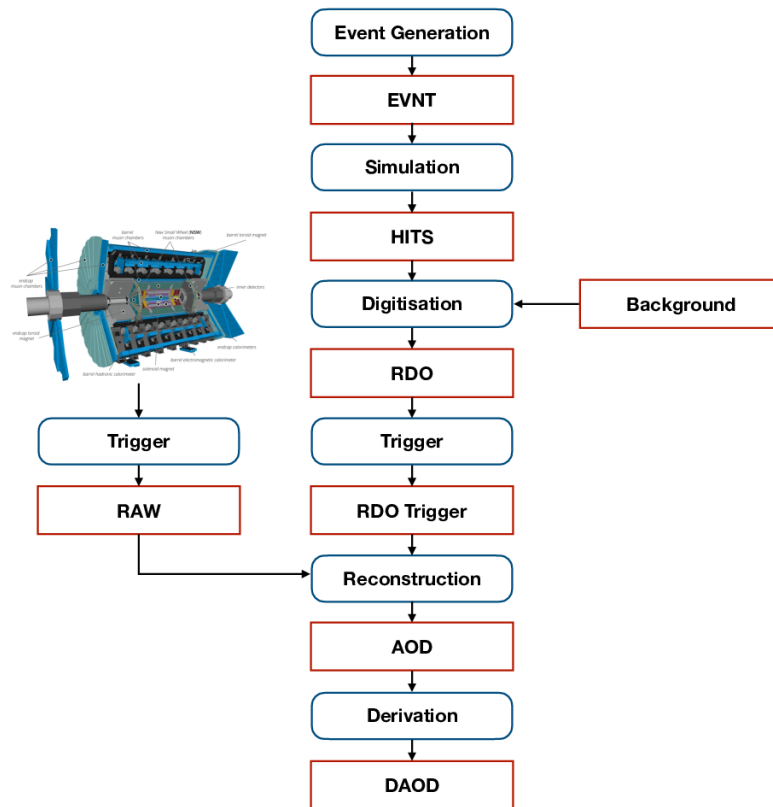


Figure 6.3: The standard software workflow of the ATLAS experiment. Processing steps are represented by blue ovals, with output formats represented as red boxes. The various steps and data formats are described in the text. The background entering digitisation may be additional simulated HITS files, pre-digitised RDO files, or specially processed RAW detector data. Figure taken from [310].

The ATLAS simulation software chain efficiently utilizes computational resources and simplifies software validation by breaking the simulation process into multiple steps, each handling a specific part of data processing, as described above and illustrated in Figure 6.3. Event generation jobs, typically fast, produce relatively small output (EVNT) files and can handle several thousand events at a time. By storing the generated events rather than regenerating them each time, the same set of events can be reused across different versions of the simulation software or various detector configurations. The simulation step is particularly slow and computationally intensive, often taking several minutes per event. The simulation jobs are therefore divided into smaller groups, typically handling 50 or fewer events per job. Digitization jobs, discussed in detail in Section 6.1.1, are generally configured to run approximately 1000 events, easing file handling by producing a smaller number of RDO files. The detector geometry used for a digitization job is selected based on the input hit file from the simulation step, ensuring consistency between the simulated hits and the detector configuration used in digitization. The detector description is built from the GeoModel [311] toolkit, which provides a complete set of mechanisms for describing large and complex detector ge-

ometries with minimal memory consumption. The toolkit includes tagged variants on the ATLAS detector, such as extra material and subdetector element misalignments. The detector description is regularly updated to incorporate improvements based on comparisons between data and MC simulations. This ensures that the simulations remain accurate and reflect the actual detector performance. Furthermore, the reconstruction step converts the raw detector signals stored in RDO files into higher-level physics objects such as tracks, vertices, and energy deposits. The reconstruction process is identical for both simulated and real data, ensuring consistency in processing the detector signals and allowing for direct comparisons between data and MC simulations. During data acquisition, the ATLAS high-level trigger (HLT, see Section 2.2.7) processes data directly from the bytestream files generated by the detector electronics. Bytestream files contain raw detector data in a format optimized for real-time processing. While the HLT mainly works with bytestream files during data acquisition, it is possible to evaluate hypotheses and run additional tests by converting the RDO files (used in offline reconstruction) into bytestream format. This adaptability allows for exploring alternative hypotheses or conducting specialized analyses after the initial event selection by the HLT [312].

6.1.3 Comparison of ITk Pixel Digitization in Athena Releases 21.9 and 22

This section presents the results of comparing pixel digitization for the ITk pixel detector between Athena Releases 21.9 and 22.0. The goal of this comparison is to quantify any differences in observable distributions, such as ToT and charge, across the various layers of the ITk pixel detector in the two releases. Additionally, this comparison study aims to identify and address necessary corrections correct in the simulation of the ITk pixel detector geometry, which has been rebuilt from scratch using the new GeoModelXML framework in Athena Release 22. The input HITS file comprises single muon events with a p_T of 100 GeV and no pileup ($\mu = 0$). The digitization job is run with 1000 events, applying a threshold of 600 e. Figure 6.4 presents a comparison of the charge distribution across the five barrel layers of the ITk pixel detector between Athena Release 21.9 (blue) and Release 22 (red). The mean charge of the histograms for each barrel layer is very similar, except for layer 0, where a significant relative charge difference of $\approx 16\%$ is observed between the mean values of charge distributions in Athena Releases 21.9 and 22.

To understand the observed differences in charge distributions in layer 0 between Athena Releases 21.9 and 22.0, the energy loss distribution at each pixel radius was investigated in both releases and is depicted in Figure 6.5.

The innermost layer in Athena Release 22.0 (Figure 6.5b) exhibits roughly 50% higher energy loss compared to Release 21.9 (Figure 6.5a), while the other layers show reasonable agreement between the two releases. This difference was determined to stem from incorrect simulation of the dead area in the 3D sensors (layer 0) in R22. In the correct design, as implemented in R21.9, the dead region is 0.1 mm and the active silicon is 0.15 mm, resulting in a combined dead and active area of 0.25 mm. In R22, the active silicon area was modeled to be 0.25 mm, leading to more active silicon and consequently larger deposited charge. A merge request (MR) incorporating the correct separation of the dead and active silicon as in Athena R21.9 was implemented. The energy loss as a function of pixel radius with the corrected dead area and active silicon separation in Athena R22 is shown in Figure 6.6a, illustrating better agreement with the energy loss observed in Athena R21.9 (Figure 6.5a). The comparison of barrel charge distributions in layer 0 between R21.9 and R22, after correctly simulating the 3D sensors, is depicted in Figure 6.6b. The mean charge of the histograms is now very similar, and the previously observed difference of 280e, as shown in Figure 6.4, is no longer present.

Figure 6.7 illustrates the ToT distributions in layer 0 for R21.9 and R22, both before (Figure 6.7a) and after (Figure 6.7b) properly simulating the 3D sensors with the correct dead and active area separation. In Figure 6.7a, the mean ToT and the shape of the ToT distributions (indicated by the

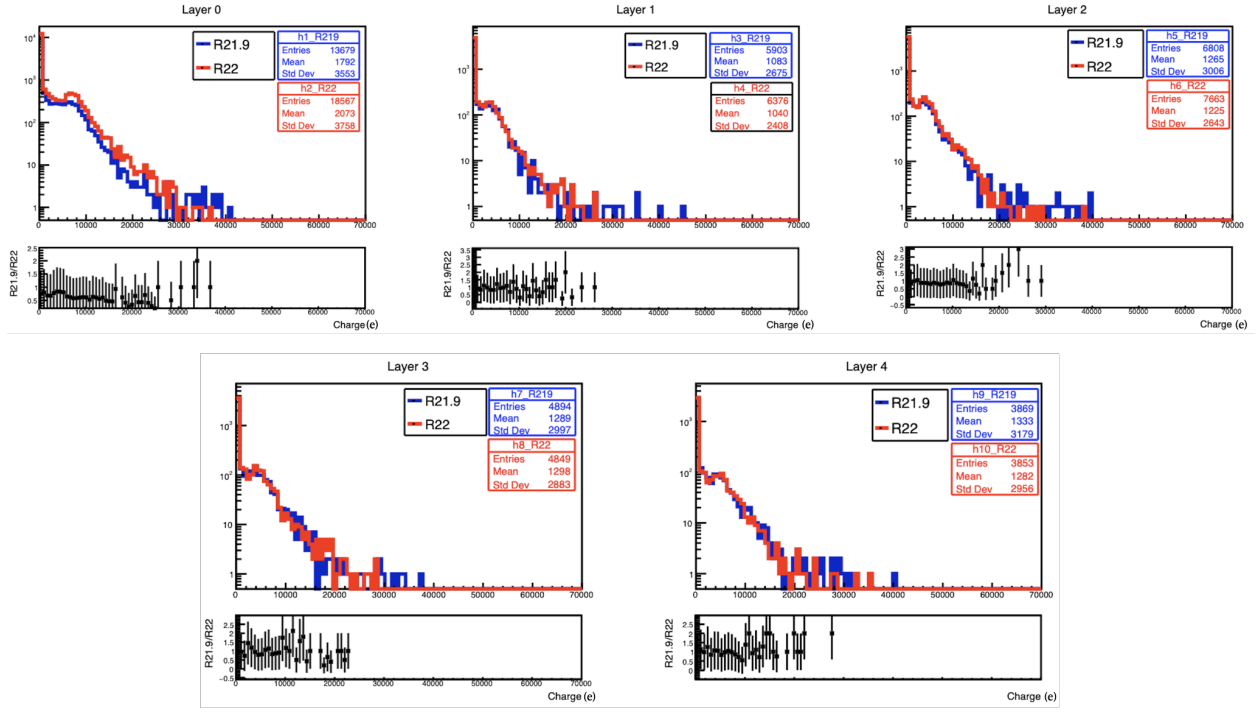


Figure 6.4: Comparison of charge distributions in Athena Releases 21.9 (blue) and 22.0 (red) for each barrel layer of the ITk pixel detector. A significant difference in the mean charge is observed for layer 0, while the other layers exhibit similar mean charges in both releases.

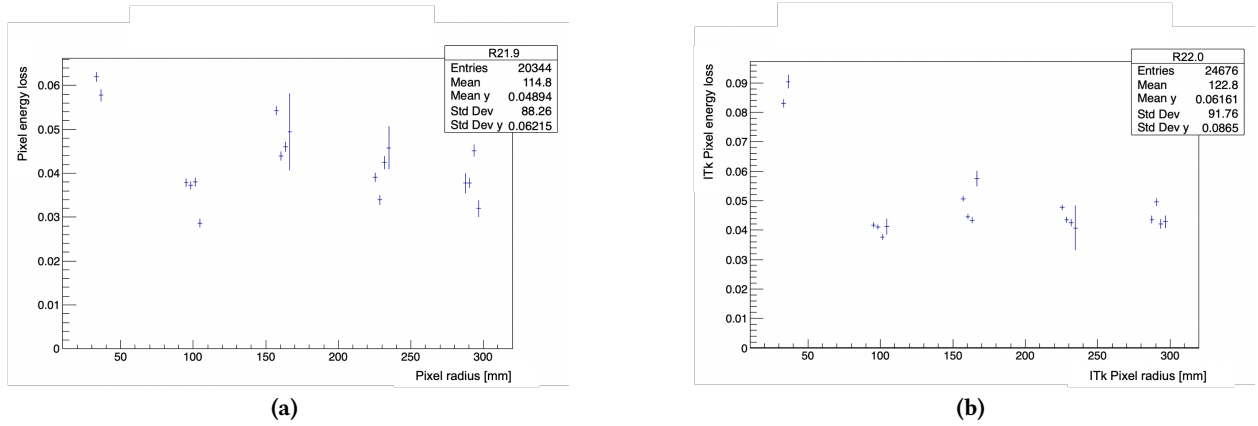


Figure 6.5: Energy loss as a function of pixel radius in (a) Athena Release 21.9 and (b) Athena Release 22.0. The innermost layer exhibits approximately 50% higher energy loss in Athena Release 22.0.

standard deviation) in R21.9 and R22 are quite similar, although a scaling effect can be observed in each ToT bin. The number of entries in each ToT bin of the histogram corresponding to Athena R22 (red) is approximately twice that of R21.9 (blue). However, after correctly simulating the 3D sensors, this difference in the number of entries between R21.9 and R22 is no longer observed, as illustrated in Figure 6.7b.

The preliminary comparison studies of various observables between Athena Releases 21.9 and 22 is presented in this section. The studies identified inaccuracies in the simulation of the separation between passive material and active silicon in the 3D pixel sensors, prompting necessary corrections to the geometry.

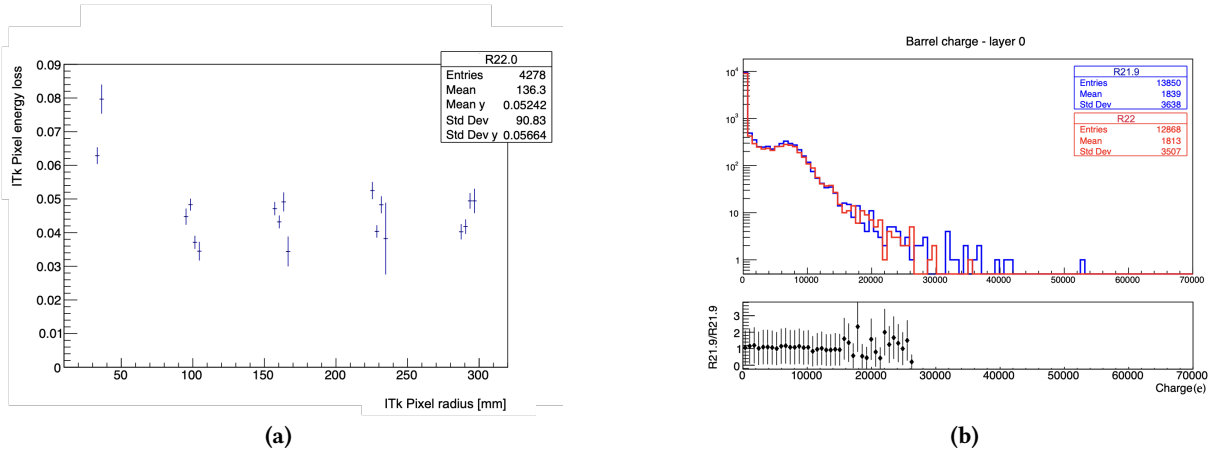


Figure 6.6: (a) Energy loss as a function of pixel radius with corrected dead area and active silicon separation in the 3D sensors (layer 0) simulated in Athena Release 22. (b) Barrel charge distributions in R21.9 and R22 after correctly simulating the 3D sensors in R22.

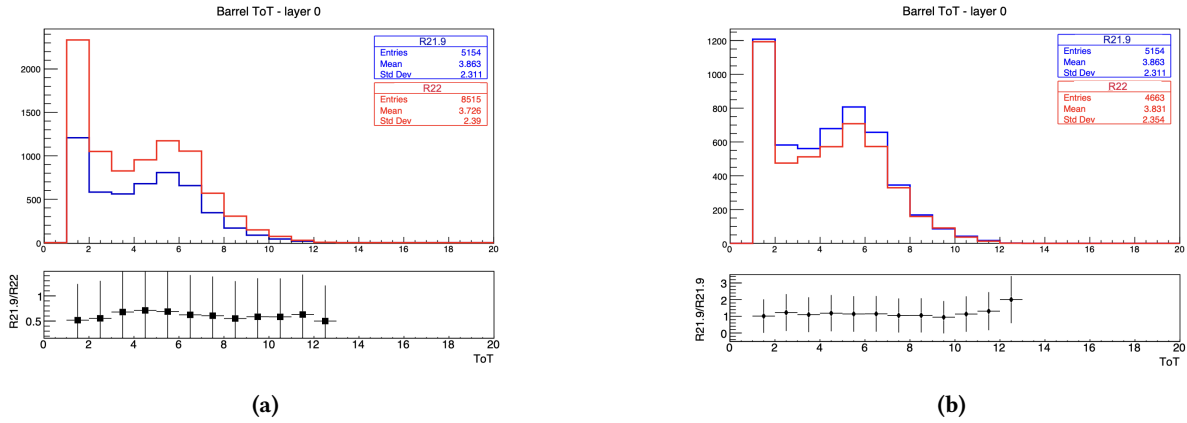


Figure 6.7: Comparison of ToT distributions in barrel layer 0 in Athena R21.9 (blue) and R22 (red): (a) before and (b) after implementing the correct dead and active silicon separation in Athena Release 22.

6.1.4 Modelling Time-Walk effects in Athena

The following section presents the results of modeling the Time-Walk effects for the RD53A-type readout chip, such as the ITkPix V2.0, in Athena. As discussed in Section 3.4, Time-Walk is a phenomenon affecting small amplitude signals, where the time for preamplifier signals to cross a fixed threshold varies with pulse height. A lower pulse height results in a delayed signal crossing, leading to delayed hit detection by the pixel. Time-Walk is one of the limiting factors for the time resolution of the pixel chip. Therefore, it is crucial to correct for this effect during digitisation and to accurately model it in Monte Carlo simulations.

Implementing Time-Walk corrections in Athena adjusts the timing of detected signals based on the charge collected by each pixel diode. If the charge exceeds a predefined threshold and is track-associated, the initial bunch crossing time is calculated using the Geant4 simulation time, which is the time at which the particle interaction is simulated to occur, along with a time offset accounting for systematic delays in the detector. The corresponding pixel hits are then assigned to the nominal bunch crossing with a BCID of 0. If the charge is below the sum of the threshold and the chip overdrive, a parameter that measures the difference between the in-time and absolute thresholds (see Section 3.4), a correction of up to 25ns (one bunch crossing) is applied, assigning the pixel hits to the next bunch crossing with a BCID of +1. For non-track-associated charges, a random bunch crossing number is assigned. This correction ensures accurate timing adjustments, enhancing the precision of particle tracking.

A single muon HITS (see Section 6.1.2) file with a p_T of 100 GeV and no pile-up is used as the input for the studies presented here, with a threshold of $600e$ configured via the condition tag in the digitization *jobOption*. The measured overdrive for the ITKPix V2.0 readout chip is $\approx 150e$. The initial modeling of the charge-to-ToT conversion in Athena for the RD53-type readout chip is based on a simplified parametric formula, as shown in Equation 6.1.1.

$$\text{ToT} = \frac{A*(E+Q)}{(C+Q)}, \quad (6.1.1)$$

Here, Q represents the collected charge, while A , E , and C are the charge calibration constants with values of 14, -1000 , and 8000 , respectively, stored and retrieved from the Athena database (db). For a threshold of $600e$ and an overdrive of $150e$, the Time-Walk effects are significantly pronounced for Q in the range $[600, 750]$. Plugging a charge value within this range into Equation 6.1.1 yields a ToT value less than 1, and in Athena, such low charges are explicitly assigned a minimum ToT value of 1. In contrast, a ToT greater than 2 in Equation 6.1.1 corresponds to a charge greater than $1690e$ (above $750e$), a charge regime where Time-Walk effects are not significant. Thus, with the implementation of Time-Walk effects in Athena, it is anticipated that all ToT bins larger than 2 will be unaffected by Time-Walk, as illustrated in Figure 6.8.

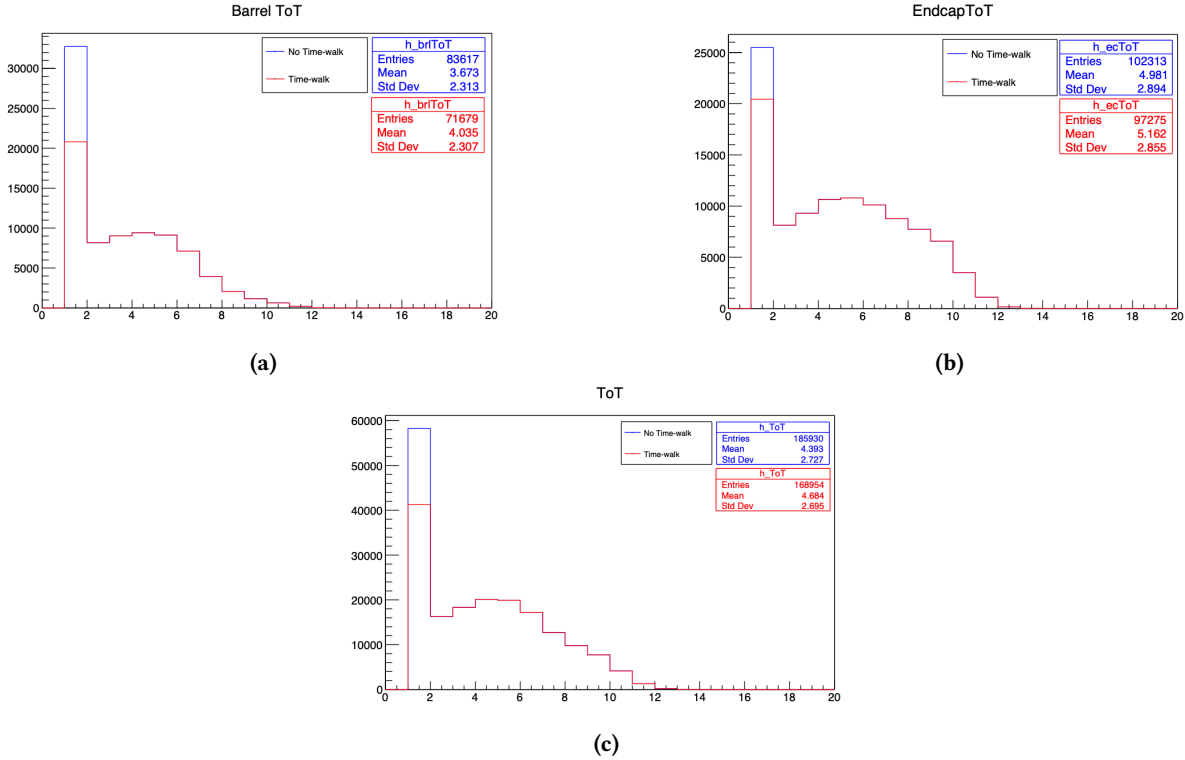


Figure 6.8: ToT distribution with (red) and without (blue) the implementation of Time-Walk effects in Athena: (a) barrel, (b) endcap, and (c) full detector.

The ToT distribution in the barrel, endcap layers, and the full detector with (red) and without (blue) the modelling of Time-Walk effects in Athena is depicted in Figure 6.8a, Figure 6.8b, and Figure 6.8c, respectively. The two distributions are exactly similar in higher ToT bins, as anticipated, indicating that these bins are unaffected by the Time-Walk effects. The effect of including Time-Walk effects can be observed in the lowest ToT bin as a reduction in the number of entries, as illustrated in Figure 6.8. This observed reduction occurs because only hits assigned to the nominal BCID of 0 are taken into account for further processing, while hits with a charge larger than $750e$ assigned to BCID 1 are not used, resulting in a lower number of entries with the inclusion of Time-Walk effects.

The results of digitization studies presented in this section assumes a simplistic parametric formula, as shown in Equation 6.1.1, to model the charge-to-ToT response of the RD53-type readout chips. A more realistic modeling of the charge-to-ToT conversion is discussed in Section 6.1.5.

6.1.5 Modelling of Realistic Charge Calibration in Athena

The initial modeling of the charge-to-ToT conversion for the RD53-type readout chip in Athena was based on the simplified parameterization used for the FEI3 readout chip, as given by Equation 6.1.1. While the parametric formula provides charge calibration curves similar to those of the RD53-type readout chip, it does not accurately represent the exact response of the chip. A lookup-table (LUT) based method for modeling charge calibration for the RD53-type readout chip in Athena has been devised, involving the creation of a local database that stores the charge calibration constants for ToT values in the range of 0 to 15, which is then picked with the digitization *jobOption* for charge-to-ToT conversion.

The studies on single-LUT based charge calibration implementation in Athena are discussed in Section 6.1.5.1. A first look at the ITkPix V1.0 readout chip data for charge-to-ToT conversion studies is presented in Section 6.1.5.2, followed by studies on the implementation of multi-LUT based charge calibration in Athena, discussed in Section 6.1.5.4. The section concludes with an outlook and the future scope of this project detailed in Section 6.1.6.

6.1.5.1 Implementation of Single-LUT Based Charge Calibration in Athena

The single-LUT based method of charge calibration for the RD53-type readout chip involves creating and storing the LUT in a local database, with the structure depicted in Figure 6.9, and picking up the LUT in the digitization *jobOption* instead of using the default FEI4 parameterization indicated in Equation 6.1.1 for charge calibration.

The structure of the single-LUT comprises the charge calibration constants for quad modules with a pixel pitch of $50 \times 50 \mu\text{m}^2$, as well as for single chip modules with pixel pitches of $50 \times 50 \mu\text{m}^2$ and $25 \times 100 \mu\text{m}^2$. In addition to the analog threshold and noise, the calibration constants used in the single-LUT, shown in Figure 6.9, are derived from the FEI4 parameterization in Equation 6.1.1 for ToT values ranging from 0 to 15. This approach serves as an initial test to verify the implementation of single-LUT based charge-to-ToT conversion in Athena, allowing for a comparison of the resulting ToT distributions with those obtained using the default FEI4 parameterization.

```
## Format:
#KN
# analog threshold value,noise for normal,long/ganged pixels
# Q0-Q16 charge calibration constants for normal and long/ganged pixels
else:
    calibQuad = [
        [600, 75, 600, 75, 1000, 1692.31, 2500, 3454.55, 4600, 6000, 7750, 10000, 13000, 17200, 23500, 34000, 55000, 118000, 999999999., 999999999.],
        [600, 75, 600, 75, 1000, 1692.31, 2500, 3454.55, 4600, 6000, 7750, 10000, 13000, 17200, 23500, 34000, 55000, 118000, 999999999., 999999999.],
        [600, 75, 600, 75, 1000, 1692.31, 2500, 3454.55, 4600, 6000, 7750, 10000, 13000, 17200, 23500, 34000, 55000, 118000, 999999999., 999999999.],
        [600, 75, 600, 75, 1000, 1692.31, 2500, 3454.55, 4600, 6000, 7750, 10000, 13000, 17200, 23500, 34000, 55000, 118000, 999999999., 999999999.],
    ]
    # single chip 50x50
    calibSingle = [
        [600, 75, 600, 75, 1000, 1692.31, 2500, 3454.55, 4600, 6000, 7750, 10000, 13000, 17200, 23500, 34000, 55000, 118000, 999999999., 999999999.],
    ]
    # single chip 25x150 (L0)
    calibSingleL0 = [
        [900, 110, 900, 110, 1000, 1692.31, 2500, 3454.55, 4600, 6000, 7750, 10000, 13000, 17200, 23500, 34000, 55000, 118000, 999999999., 999999999.],
    ]
```

Figure 6.9: The structure of single LUT

Figure 6.10 shows the resulting ToT distributions obtained using the default FEI4 parameterization (black) and the single-LUT based charge calibration (red). The calibration constants for the single LUT are derived from the FEI4 parameterization given in Equation 6.1.1 for ToT values ranging from 0 to 15. Although the two ToT distributions are expected to be identical, observed differences arise from a rounding issue. The charge-to-ToT conversion with the default FEI4 parameterization

truncates the obtained ToT, while the conversion using the single LUT returns the ToT bin with the charge closest to the deposited charge in the sensor.

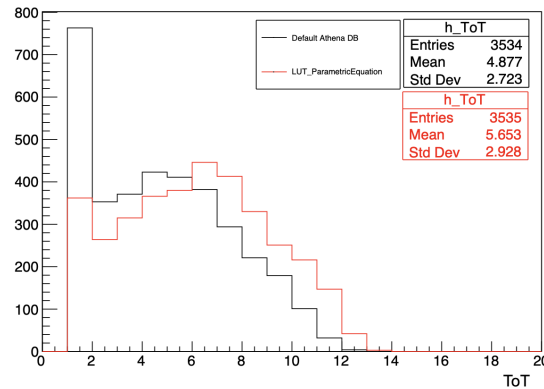


Figure 6.10: The ToT distributions obtained using the default FEI4 parameterization (black) and the single LUT-based charge calibration (red), with the LUT created using charges derived from the FEI4 parametric formula indicated in Equation 6.1.1.

A standalone C++ script outside Athena is used to determine the optimal charges for creating a LUT that emulates the ToT response of the default FEI4 parameterization. Figure 6.11a illustrates the ToT vs. charge distribution obtained with the default FEI4 parameterization (blue) and the single LUT (magenta), using calibration constants shown in Figure 6.9 to create the LUT. The differences between the two curves stem from rounding variations inherent in the respective methods described above. Figures 6.11b, 6.11c, and 6.11d depict the ToT versus charge distributions with the FEI4 parameterization (blue) and the single LUT (magenta) with calibration constants calculated from the FEI4 parametric formula in Equation 6.1.1, each with a ToT offset of 0.5, 1, and finely-tuned (trial and error) calibration constants, respectively. A good agreement between the two distributions is observed with the LUT created using charge calibration constants calculated from the FEI4 parameterization with a ToT offset of 1 as depicted in Figure 6.11c. Further fine-tuning is performed manually to achieve the ToT vs. charge distribution illustrated in Figure 6.11d.

Comparisons of ToT distributions using the default FEI4 parameterization (black) and four single-LUTs with calibration constants calculated using the FEI4 parametric formula (red), parametric formula with a ToT offset of 0.5 (green), 1 (blue), and manually optimized calibration constants (red) are depicted in Figures 6.10, 6.12a, 6.12b, and 6.12c, respectively. The excellent agreement in the ToT versus charge distributions shown in Figures 6.11c and 6.11d indicates a good agreement between the ToT distributions obtained using the default FEI4 parameterization and the LUTs created using charge calibration constants calculated from the FEI4 parametric formula with a ToT offset of 1, as depicted in Figure 6.12b, and the optimized charge calibration constants, as illustrated in Figure 6.12c.

The aim of the studies presented herein is not to exactly reproduce the ToT response of the FEI4 parameterization but rather to achieve a more realistic charge calibration of RD53-type readout chip using LUTs. Currently, the single-LUTs are populated with charge calibration constants from the FEI4 parametric formula due to the unavailability of real calibration data from the ITkPix V2.0 readout chip. This study demonstrates the feasibility of performing charge calibration using the single-LUT method in Athena.

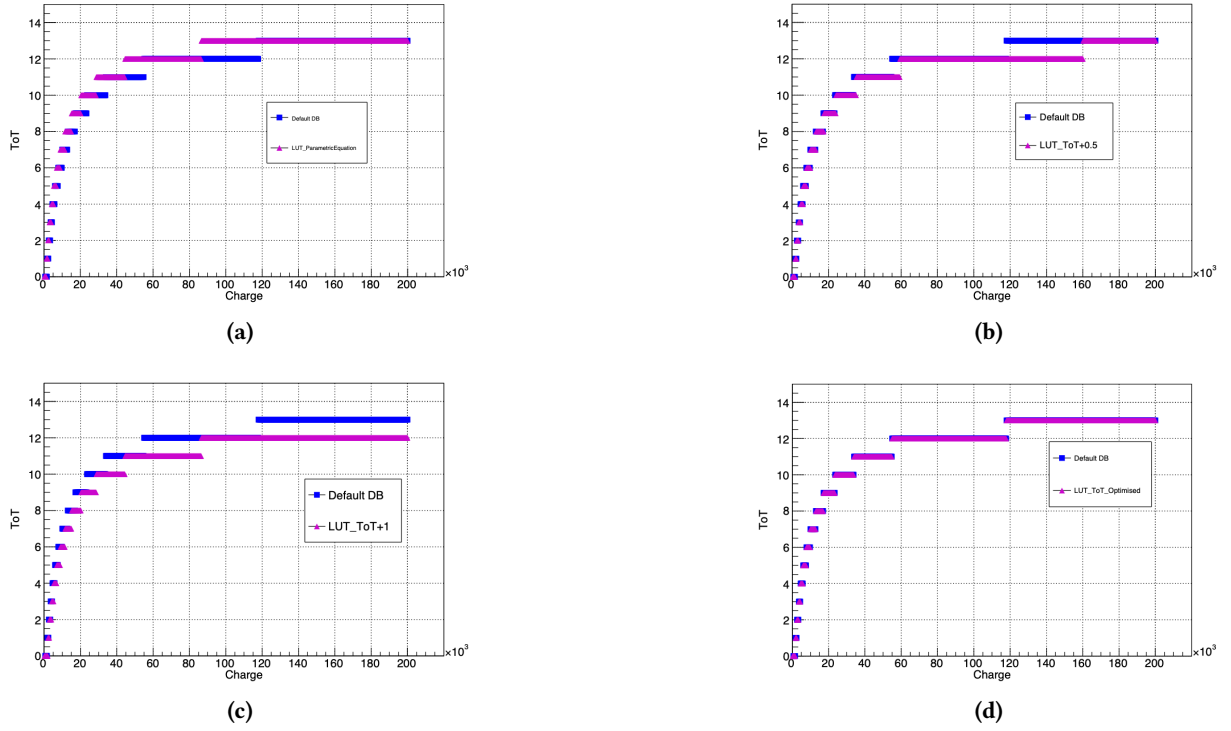


Figure 6.11: The ToT vs. charge distributions comparing the default FEI4 parameterization (blue) and the single LUT (magenta), with calibration constants calculated from (a) the FEI4 parametric formula, (b) the FEI4 parametric formula with a ToT offset of 0.5, (c) a ToT offset of 1, and (d) finely-tuned calibration constants.

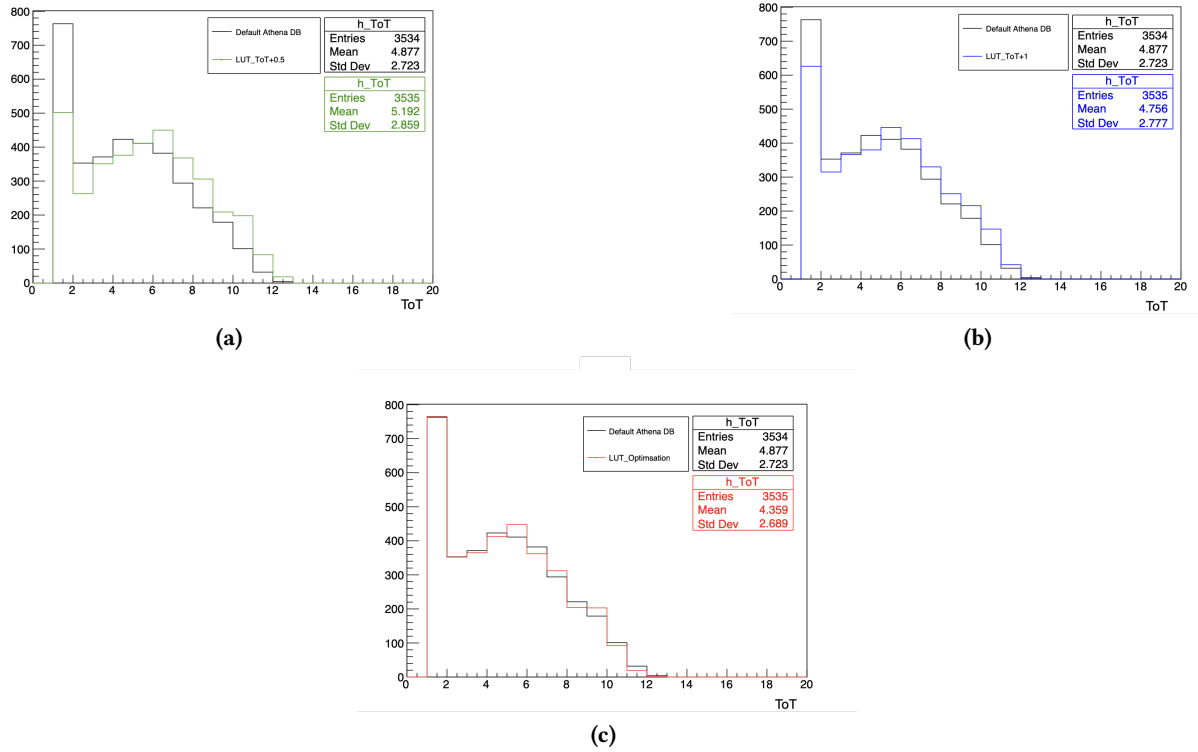


Figure 6.12: The comparison of ToT distribution obtained using the default FEI4 parameterization (black) and the single LUT, with calibration constants calculated from (a) the FEI4 parametric formula with a ToT offset of 0.5 (green), (b) a ToT offset of 1 (blue), and (c) finely-tuned calibration constants (red).

6.1.5.2 A First Look at ITkPix V1.0 Data for Multi-LUT Based Charge Calibration

A single-LUT based charge calibration method has been implemented in Athena for the RD53-type readout chip, as discussed in Section 6.1.5.1, in addition to the default FEI3 parameterization. Due to the unavailability of real chip data, the method has been validated by creating the LUT with charges emulating the FEI3 parameterization. The resulting comparison of ToT distributions with those obtained from the default FEI3 parameterization is illustrated in Figure 6.12c. However, the current single-LUT based charge calibration implementation does not incorporate the spread in individual pixel calibration curves. Initially, the plan was to apply a random Gaussian smearing with a width significantly larger than that of the FEI4 readout chip (greater than $3\times$). However, this approach would not realistically model the charge-to-ToT conversion of the RD53-type readout chip as a single LUT with random Gaussian smearing would fail to account for the return to baseline experienced by each pixel. Thus, an ideal scenario would involve storing one LUT per pixel. However, the ITkPix V1.0 readout chip comprises a pixel matrix of 384×400 pixels, and storing one LUT per pixel in the Athena database would significantly increase the digitization memory footprint. A possible realistic approach to model pixel charge calibration in Athena would involve storing a fixed small number of LUTs in the Athena database and randomly selecting a LUT for the digitization charge. However, this multi-LUT based charge calibration method requires further investigation using chip data. The subsequent sections present the data analysis using the first set of chip data kindly provided by the ATLAS colleagues at Lawrence Berkeley National Laboratory (LBNL).

Insights from ITkPix V1.0 Readout Chip

The following section presents a first look at the ITkPix V1.0 (RD53-type) readout chip data. The dataset corresponds to a bare chip card tuned to a threshold of $1000e$. Charges are injected into the ITkPix V1.0 pixel matrix from $1000e$ to $35000e$ at $500e$ intervals. Figure 6.13 illustrates the mean ToT maps for various charge injections.

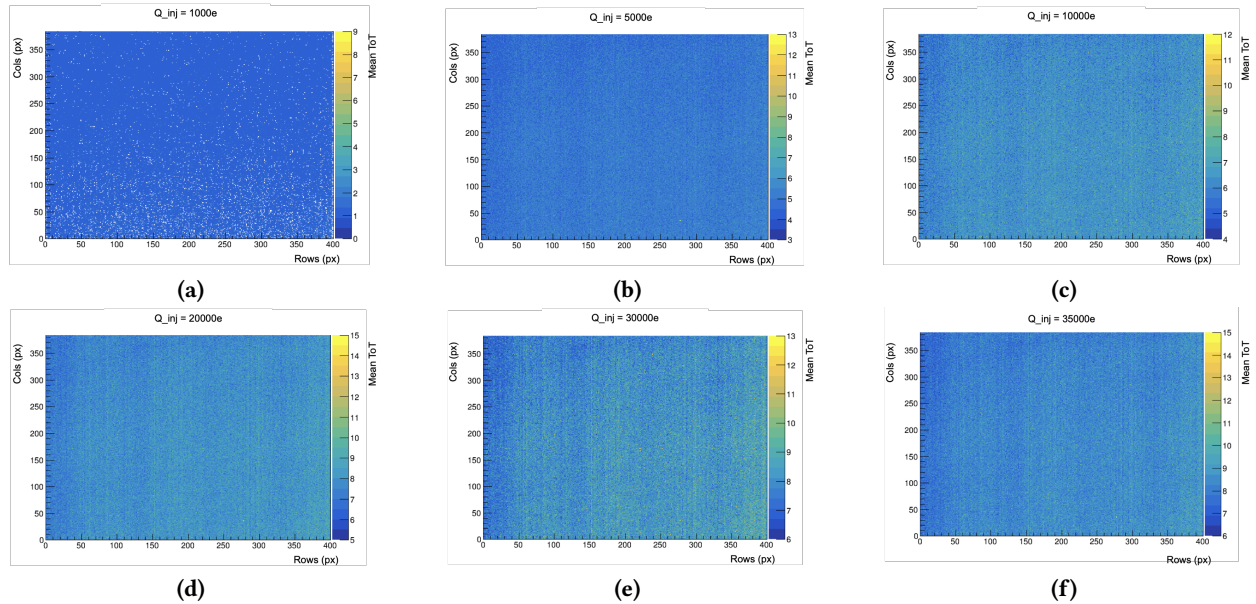


Figure 6.13: Mean ToT maps for a digital single-chip ITkPix V1.0 card with injected charges of (a) 1000 e (b) 5000 e (c) 10,000 e (d) 20,000 e (e) 30,000 e (f) 35,000 e [313].

The novel ITkPix readout chip is characterized by low module-to-module variation in the ToT, in contrast to the significant per-pixel variations observed within a small region of the pixel matrix. This inherent feature of the chip provides a unique advantage for realistic modeling of charge-to-

ToT conversion using multi-LUTs in Athena. Thus, for a realistic modeling of charge calibration, instead of storing 153,600 LUTs - one for each pixel in the Athena database - a small representative group of pixel submatrices can be selected from the ITkPix pixel matrix. This approach allows for a small number of LUTs to be efficiently stored in the database without significantly increasing the digitization memory footprint.

The ITkPix V1.0 pixel matrix, consisting of 400 rows and 384 columns, is divided into groups of 8×8 pixel submatrices. A preliminary study is conducted to determine if an 8×8 pixel submatrix accurately represents the ToT dispersion observed across the entire pixel matrix. The 8×8 pixel submatrix is chosen initially because 64 pixels exceed any usual cluster size and analog clustering is a process significantly affected by realistic modeling of charge-to-ToT conversion. The study on optimal pixel dimensions for realistic charge calibration are discussed in Section 6.1.5.3. Figure 6.14 and Figure 6.15 illustrate the mean ToT and the RMS of the mean ToT distributions for various charge injections across the 2400 8×8 pixel submatrices. The mean ToT distributions across the 2400 pixel submatrices for various charge injections are very narrow, as illustrated in Figure 6.14. This is further corroborated by the minimal variations in the RMS of the mean ToT distributions, as shown in Figure 6.15.

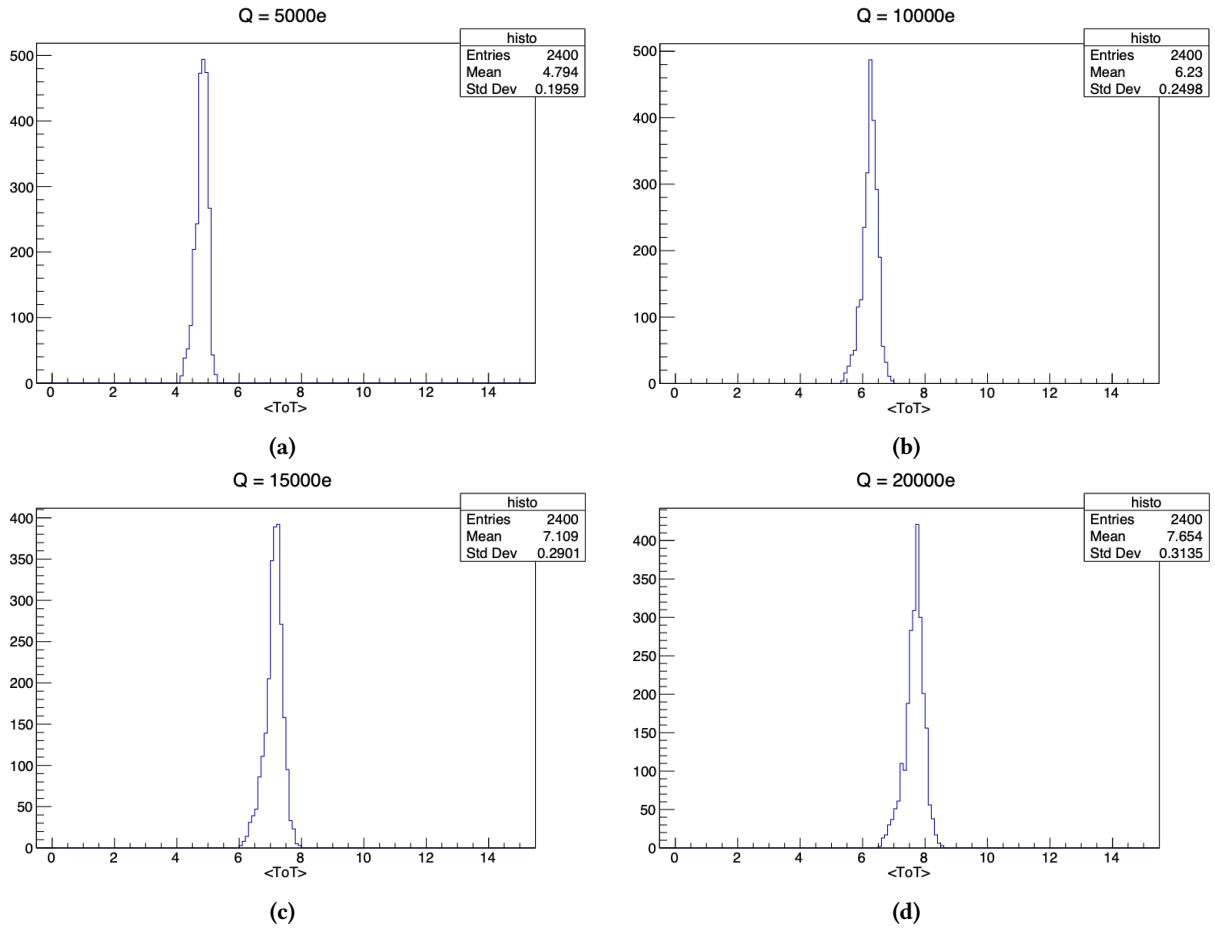


Figure 6.14: The distribution of mean ToT across 2400 8×8 pixel submatrices for injected charges of (a) 5000 e (b) 10,000 e (c) 15,000 e (d) 20,000 e.

Figure 6.16 compares the ToT distributions between a single 8×8 pixel submatrix, located at the bottom-left corner of the ITkPix V1.0 pixel matrix, and the entire matrix for injected charges of 5000e and 10000e. Table 6.1 further compares mean ToT values for the same submatrix and the entire matrix, covering injected charges of 5000e, 10000e, 15000e, and 20000e. The mean ToT from the single 8×8 pixel submatrix does not closely match the values from the entire pixel matrix. The largest relative difference observed is 8% for an injected charge of 20000e.

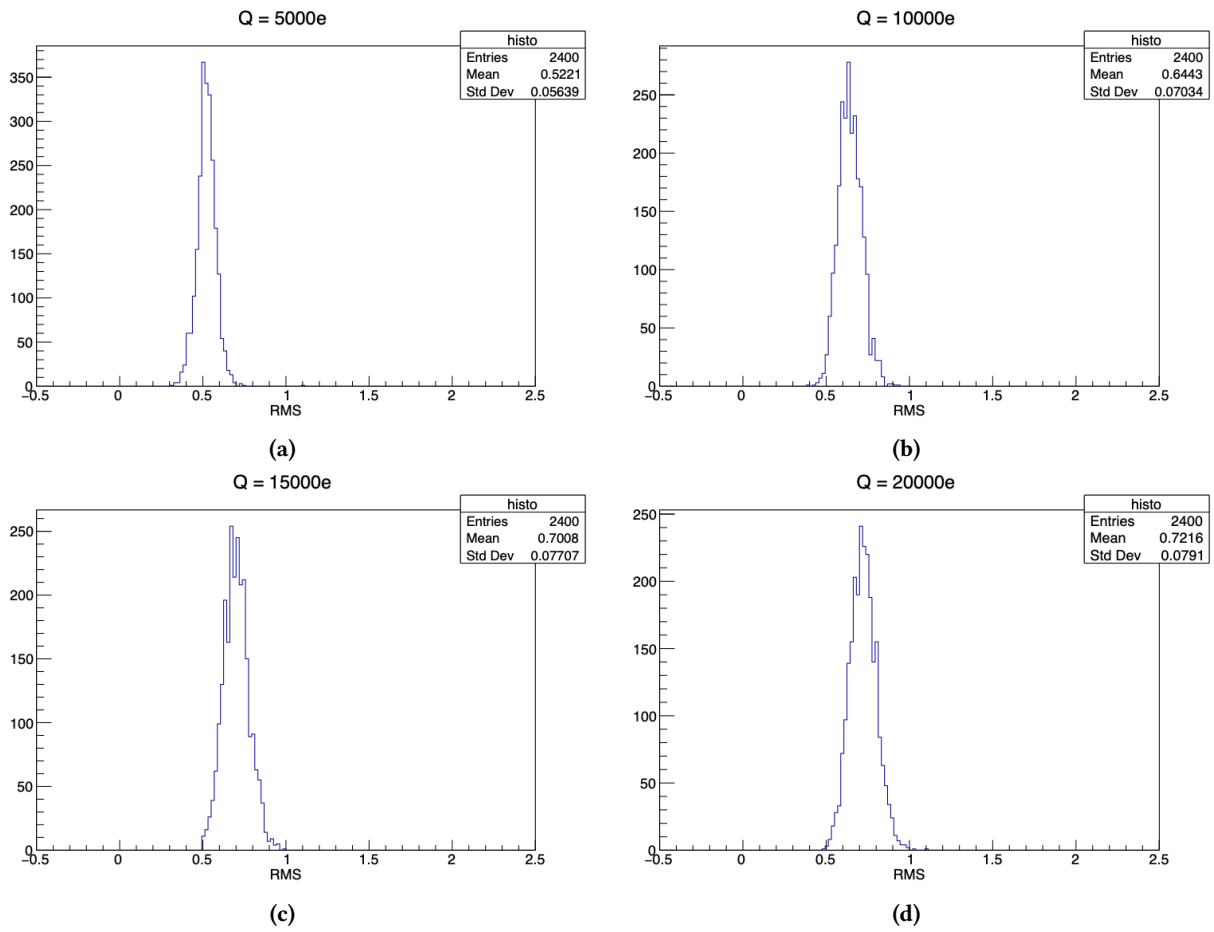


Figure 6.15: The distribution of RMS of the mean ToT across 2400 8×8 pixel submatrices for injected charges of (a) 5000 e (b) 10,000 e (c) 15,000 e (d) 20,000 e.

Injected charge	Mean ToT single 8×8 pixel matrix	Mean ToT entire pixel matrix	Relative difference
5000e	4.47	4.78	6.5%
10000e	5.78	6.22	7.1%
15000e	6.55	7.09	7.6%
20000e	7.03	7.64	8%

Table 6.1: Comparison of mean ToT values between a (left) single 8×8 pixel submatrix (bottom-left corner of the ITkPix V1.0 pixel matrix) and (right) the entire pixel matrix for various charge injections. The relative error column shows the discrepancies between the submatrix and entire matrix values.

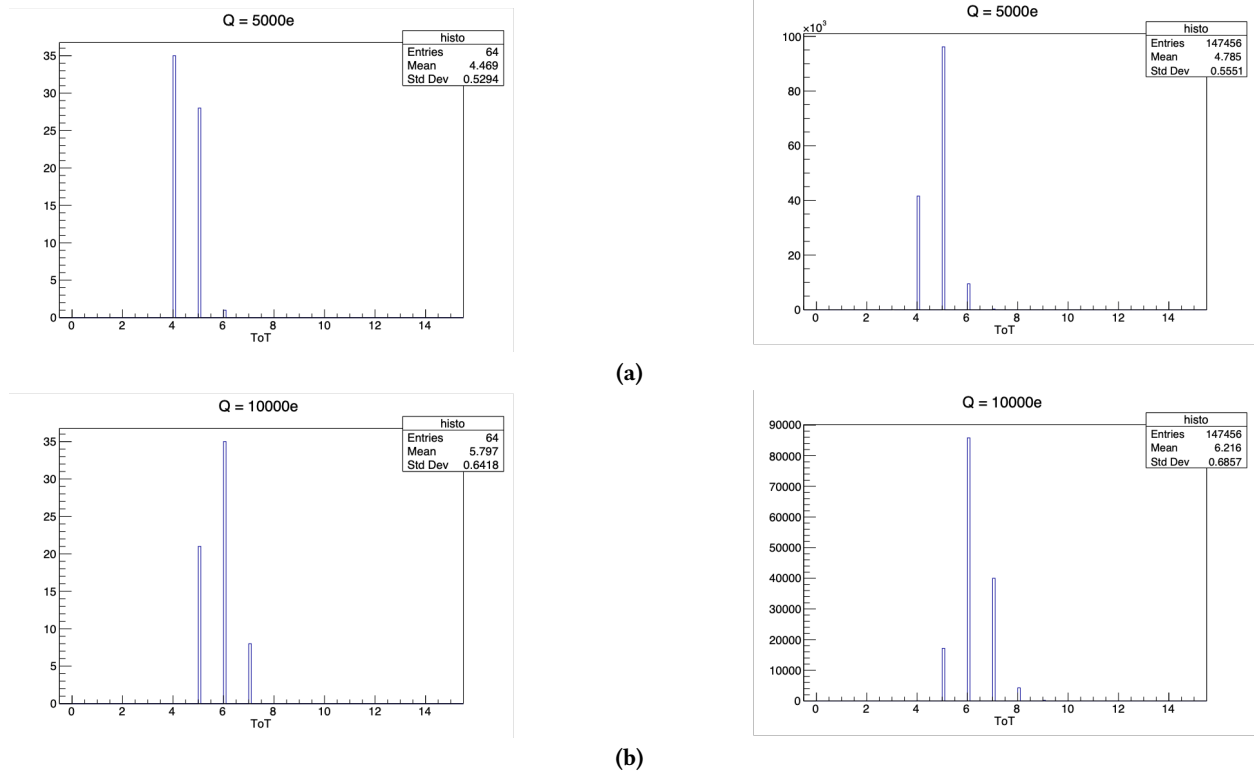


Figure 6.16: Comparison of ToT distributions: (left) for a single 8×8 pixel submatrix and (right) for the entire ITkPix V1.0 pixel matrix. The distributions are shown for injected charges of (a) 5000 electrons and (b) 10,000 electrons. The chosen 8×8 submatrix is located in the bottom-left corner of the ITkPix V1.0 pixel matrix.

Identifying the Optimal 8×8 Pixel Submatrix : Kolmogorov-Smirnov Tests

Table 6.1 compares the mean ToT from a single 8×8 pixel submatrix located in the bottom-left corner of the ITkPix V1.0 pixel matrix with the mean ToT of the entire matrix. The table also presents the relative difference between these ToT values, indicating that the mean ToT from this single submatrix does not closely match the mean ToT of the entire pixel matrix. The following section details the results of Kolmogorov-Smirnov (KS) statistical tests conducted to identify the optimal 8×8 pixel submatrix that best represents the observed ToT dispersion across the entire pixel matrix.

The KS test is a non-parametric statistical test that compares the distributions of two data sets by measuring the largest absolute difference between the cumulative distribution functions (CDFs) of the two samples. The test statistic, D , is defined as the maximum absolute difference between the CDFs of the two samples. Mathematically, this can be expressed as:

$$D = \max|F_1(x) - F_2(x)| \quad (6.1.2)$$

Here, $F_1(x)$ and $F_2(x)$ are the empirical CDFs of the two samples. In this study, the KS test is employed to identify an 8×8 pixel submatrix within the ITkPix V1.0 pixel matrix that best represents the overall distribution of ToT values. For each injected charge, the average ToT values from a candidate 8×8 submatrix are compared to those from the entire pixel matrix using the KS test. This test calculates the maximum "distance" (KS statistic, D) between the CDFs of the submatrix and the entire matrix for various injected charges. Among all candidate submatrices, the one with the smallest maximum distance (D) is considered the best representative of the overall ToT distribution. By minimizing this maximum distance across different injected charges, the selected submatrix accurately reflects the ToT dispersion observed in the entire pixel matrix. Thus, the best pixel submatrix determined from the KS test can be mathematically summarized as:

$$\text{Best Sample} = \min(\max(D_{\text{sample,original}})) \quad (6.1.3)$$

Here, $D_{\text{sample,original}}$ is the KS statistic between the submatrix (sample) and the entire pixel matrix (original). The results of the KS tests for injected charges of $2000e$ and $10,000e$ are shown in Figure 6.17. The best 8×8 pixel submatrix determined by the KS test (center) has the smallest KS distance D , and its ToT distribution is in excellent agreement with that of the entire pixel matrix (left). Conversely, the worst 8×8 pixel submatrix, identified by the largest KS distance, is illustrated on the right, showing significant discrepancies in the mean ToT compared to the full pixel matrix.

The results of the KS tests for charge injections from $2000e$ to $20,000e$ are presented in Table 6.2. This table showcases the mean ToT of the entire ITkPix V1.0 pixel matrix, the mean ToT of the best 8×8 pixel submatrix determined from KS tests, and the relative difference between the two ToT values. The largest relative difference is 1.7%, demonstrating that the KS test can successfully identify an 8×8 pixel submatrix that accurately represents the ToT dispersion in the entire pixel matrix.

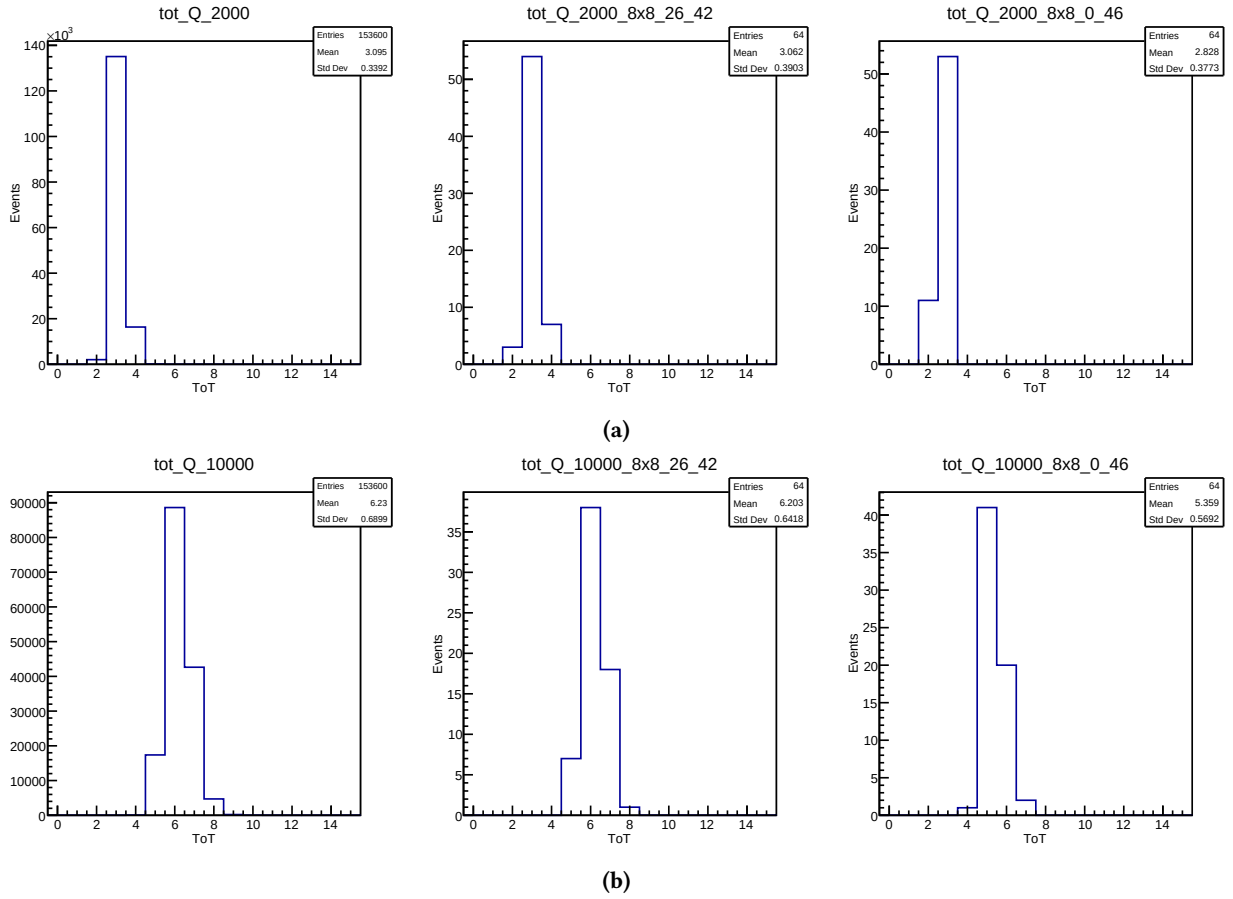


Figure 6.17: Comparison of the ToT distributions: the ITkPix V1.0 full pixel matrix (left), the best 8×8 pixel submatrix as determined by the KS test (center), and the worst 8×8 pixel submatrix based on the KS test for charge injections of (a) 2000e and (b) 10,000e.

Injected charge	Mean ToT entire pixel matrix	Mean ToT best 8×8 pixel matrix	Relative difference
2000e	3.095	3.062	1.1%
4000e	4.371	4.297	1.7%
6000e	5.119	5.109	0.20%
8000e	5.714	5.656	1.0%
10,000e	6.23	6.203	0.43%
12,000e	6.635	6.625	0.15%
14,000e	6.969	6.953	0.23%
16,000e	7.244	7.188	0.77%
18,000e	7.466	7.422	0.59%
20,000e	7.654	7.656	0.03%

Table 6.2: Comparison of the mean ToT of the entire ITkPix V1.0 pixel matrix with the mean ToT of the best 8×8 pixel submatrix determined by the KS test for various charge injections. The differences between the two ToT values are within a few percent.

6.1.5.3 Study of the Optimal Pixel Submatrix Dimensions

The studies presented thus far aim to determine the optimal 8×8 submatrix using KS-test to accurately represent the observed ToT dispersion in the ITkPix V1.0 pixel matrix. Since analog

clustering is a process significantly affected by realistic modeling of charge-to-ToT conversion, an 8×8 pixel submatrix is initially chosen for the study because 64 pixels exceed the typically observed cluster size. The results tabulated in Table 6.2 indicate that an 8×8 pixel submatrix, identified using the KS-test, can successfully model the ToT dispersion in the ITkPixV1.0 pixel matrix. Therefore, implementing a multi-LUT-based charge calibration in Athena would require storing 64 single-LUTs with a structure depicted in Figure 6.9 in the database. The following section details a study to determine the optimal pixel submatrix dimension based on the overall spread of the ToT distribution as a function of the submatrix dimension, using the KS test statistic, D , which quantifies the maximum difference between the CDFs of the submatrix and the entire matrix (see Section 6.1.5.2), as the parameter of interest.

A scan is performed for pixel submatrix dimensions ranging from 16×16 to 4×4 , and Table 6.3 tabulates the minimal KS distance D observed for each submatrix dimension. The dimension with the smallest D value corresponds to the optimal submatrix dimension, indicating the closest match between the submatrix's ToT distribution and the overall ToT distribution of the entire pixel matrix.

Pixel submatrix dimension	Minimum KS- distance (D)	Pixel submatrix dimension	Minimum KS- distance (D)
16×16	0.0175	12×12	0.0246
10×10	0.0350	6×8	0.0391
8×8	0.0367	5×8	0.0271
3×8	0.0450	4×4	0.0599

Table 6.3: Scan of pixel submatrix dimensions with corresponding minimal KS-test statistic, D .

The scan of the pixel submatrix dimensions presented in Table 6.3 indicate that the optimal pixel dimension, characterized by the lowest D value and thus best representing the ToT dispersion across the entire ITkPixV1.0 pixel matrix, is 16×16 . Conversely, the submatrix dimension exhibiting the largest discrepancy compared to the entire matrix is 4×4 , indicated by the highest D value. However, storing 256 LUTs corresponding to the optimal 16×16 pixel submatrix in the Athena database is expected to significantly increase the digitization time. Therefore, it is crucial to select an optimal pixel dimension that balances between accuracy and simulation time. From Table 6.3, a pixel submatrix dimension of 5×8 (40 LUTs) with a D value of 0.0271 is an optimal choice for achieving realistic modeling of charge calibration for the ITkPix V1.0 pixel readout chip in Athena.

6.1.5.4 Current Status of Multi-LUT based Charge Calibration in Athena

Based on the studies presented in Section 6.1.5.2 and Section 6.1.5.3, a realistic modeling of charge-to-ToT conversion for the ITkPixV1.0 readout chip in Athena can be achieved by storing 40 LUTs in the Athena database to accurately represent the observed ToT dispersion of the chip. A first study to store 40 single-LUTs, structured as shown in Figure 6.9, in the current Athena COOL database [314] was tested but proved unsuccessful due to the size limitations of the COOL database. As an interim solution until the new CREST [315] database is ready for use, an option to store and read the calibration constants from a text file for digitization has been implemented in Athena.

The current structure of the single-LUT, as shown in Figure 6.9, stores the calibration constants for different sensor types used in the ITk pixel detector. Storing the calibration constants for 40 such single-LUTs, corresponding to the best 5×8 pixel submatrix, in a text file results in a very large size of 192 MB. Additionally, discussions with ITkPix readout chip experts from LBNL clarified that the ToT response is driven by a mix of readout chip settings, such as threshold and feedback

current settings, rather than the sensor type. Two different threshold - 1000 e for L0 and L1 layers, 1500 e for L2-L4 layers and feedback settings - fast L0 and L1 layers and slow for L2-L4 layers are currently foreseen for the ITkPix readout chip. A MR in Athena has been implemented to restructure the format of the Look-Up Table (LUT) storing the calibration constants of the ITkPix readout chip based on the chip settings for various pixel layers, as illustrated in Figure 6.18. After restructuring the format of the LUTs, the size of the text file storing 40 LUTs for the two regions of the ITk detector (L0, L1 and L2-L4) has been reduced to 54 MB.

```
# New Format based on the feedback current and threshold settings of the ITkPixV2 chip
# L0 and L1 layers: fast feed back cureent,1000e threshold
# L2 to L14layers: slow feed back cureent,1500e threshold
# analog threshold value,noise for normal,long/ganged pixels
# Q0-Q16 charge calibration constants for normal and long/ganged pixels

calibL0andL1 = [
    [1000, 75, 1000, 75, 2080, 2957, 4000, 5163, 6824, 8700, 11285, 14709, 19600, 27500, 40400, 69500, 166400, 3000000, 999999999., 999999999.],
]

calibL2toL4 = [
    [1500, 75, 1500, 75, 2080, 2957, 4000, 5163, 6824, 8700, 11285, 14709, 19600, 27500, 40400, 69500, 166400, 3000000, 999999999., 999999999.],
]
```

Figure 6.18: Restructured format of the LUT storing the calibration constants for the two regions of the ITk Pixel detector, based on the different threshold and feedback current settings of the readout chip for various pixel layers. A threshold of 1000e is planned for layers L0 and L1, with fast feedback current settings, while a threshold of 1500e is planned for layers L2-L4, with slow feedback current settings. The numbers in the LUT correspond to the analog threshold, noise, and the optimal charges derived from a standalone script outside Athena to emulate the ToT response of the FEI3 parameterization in Equation 6.1.1.

The preliminary approach of modeling a realistic charge-to-ToT conversion using multi-LUTs in Athena involve storing 40 LUTs in a text file, as previously discussed. Subsequently, during the digitization stage, a random number m is generated between 0 and 39 with a uniform prior to select the calibration from LUT m . The aforementioned approach requires significant code restructuring of the pixel modules in Athena. Additionally, using a randomly selected LUT for digitizing each charge can lead to unpredictable pixel behavior, since a particular pixel with a given charge should have a consistent ToT response. While brainstorming new ideas, an alternative approach is currently under discussion. This approach involves using KS-test to identify the 40 most representative pixels out of the 153,600 pixels in the ITkPixV1.0 pixel matrix. For each pixel j in the ITkPixV1.0 pixel matrix with a charge Q_j , the pixel m within the set of 40 pixels in the LUT with a charge Q_m that is closest to Q_j will be chosen for charge-to-ToT conversion. However, this approach might potentially underestimate or overestimate the variations, as illustrated in Figure 6.19. In this figure, two adjacent pixels with indices 50 and 51 register charges Q_{50} and Q_{51} , which are mapped to pixels 6 and 1, respectively, in the 40 LUTs corresponding to the optimal 5×8 pixel submatrix. This example overestimates the charge variations between pixels 50 and 51, which can potentially result in incorrect modeling of the ToT variations.

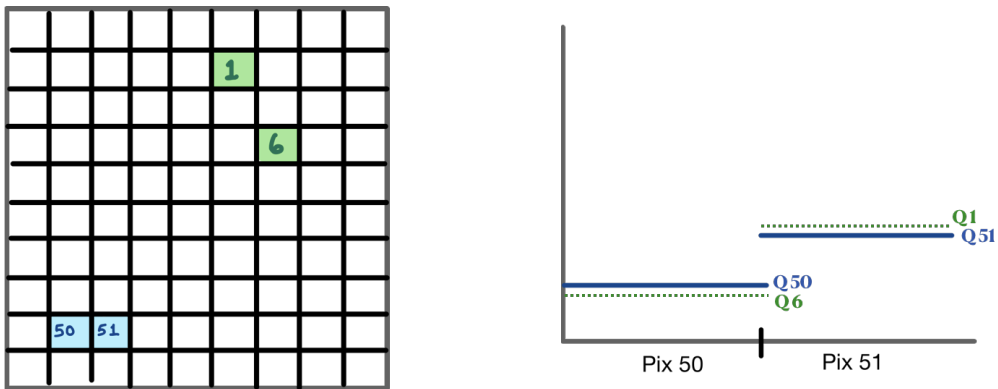


Figure 6.19: Illustration of potential inaccuracies in ToT variation modeling using multi-LUT based charge calibration in Athena.

It should be noted, however, that the final strategy for realistic modeling of charge-to-ToT conversion in Athena has not yet been finalized. Chip experts from LBNL and the University of Oregon have recently investigated the conversion of ToT back to charge for offline reconstruction at both the chip level and pixel level using LUTs with real data from an ITkPix Single Chip Module with a 3D sensor of pixel pitch $50 \times 50 \mu\text{m}^2$, tuned to a threshold of 1000e, with charges injected from 500e to 35,000e in 100e steps. The following section provides a brief summary of this study, as a proper understanding of the readout chip's operation is crucial for accurately modeling its response in Athena.

In contrast to the ITk pixel detector, the ATLAS pixel detector consists of four barrel layers, including one 4-bit ToT layer (IBL) and three 8-bit ToT layers with pixel-level tuning. This per-pixel tuning significantly enhances the ToT resolution by allowing for precise calibration of each individual pixel, leading to improved uniformity, precision, and dynamic range. In contrast, the ITk pixel detector features five 4-bit layers with only chip-level ToT tuning, resulting in less precise calibration for individual pixels. Consequently, the ITk pixel detector is expected to have an overall lower ToT resolution and a larger ToT dispersion compared to the FE of the current ATLAS Inner Detector. Figure 6.20a illustrates the mean ToT map of the ITkPix FE for an injected charge of 10,000e, while the highly non-linear ToT response of the chip is shown in Figure 6.20b.

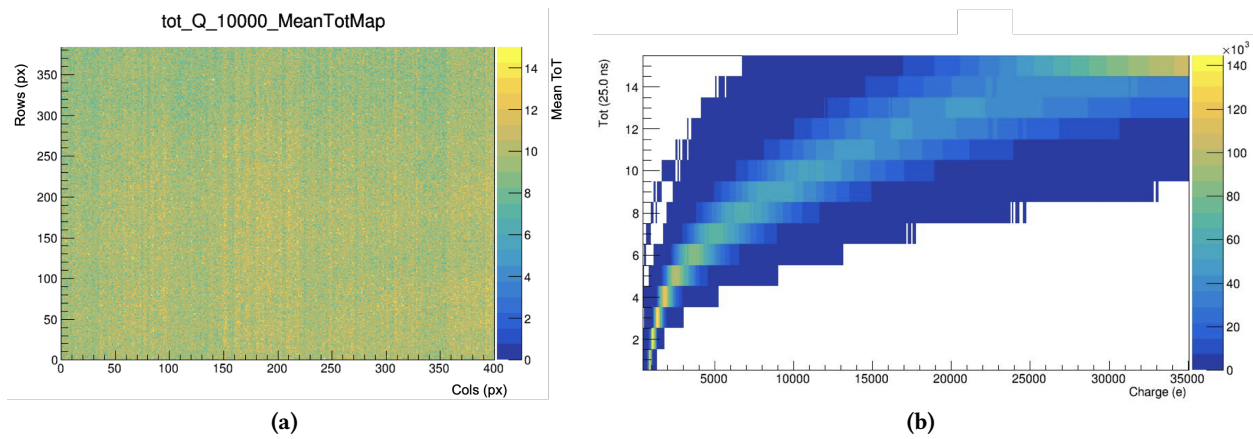


Figure 6.20: (a) Mean ToT map for an injected charge of 10,000e, and (b) ToT versus charge distribution for a Single Chip Module with a 3D sensor of pixel pitch $50 \times 50 \mu\text{m}^2$, tuned to a threshold of 1000e [313].

The per-pixel level calibration assumes a unique ToT-to-charge conversion for each pixel, with a single ToT value corresponding to a range of charges, as illustrated in Figure 6.21a. In contrast, the per-chip level calibration assumes a uniform response across all pixels on the chip, with each ToT value corresponding to the average charge over all the pixels. Figure 6.21c illustrates the per-pixel LUT converting ToT to the mean charge of each pixel, while Figure 6.21d depicts the per-chip LUT converting ToT to the average charge over all the pixels.

The conversion of ToT back to charge is limited by the 4-bit ToT resolution of the ITkPix FE. However, the per-chip level calibration is expected to lose even more charge resolution. This loss is quantified through a closure test, which plots the reconstructed charge Q as a function of the initial injected charge Q_0 , as shown in Figure 6.22. This test illustrates the impact of the ToT resolution and quantifies the uncertainty for both per-pixel and per-chip level calibration.

The results of the closure tests shown in Figure 6.22 indicate that the per-pixel calibration is significantly different from the per-chip calibration. Figures 6.22c and 6.22d demonstrate that pixel-level calibration improves charge reconstruction resolution compared to chip-level calibration. This improvement is highlighted by the distribution of reconstructed charge versus initial injected charge in Figure 6.22a and the distribution of relative charge resolution versus injected charge in Figure 6.22b, which show much larger uncertainty with chip-level calibration. The ITkPix FE experts at LBNL and the University of Oregon are currently investigating the extent to which per-pixel

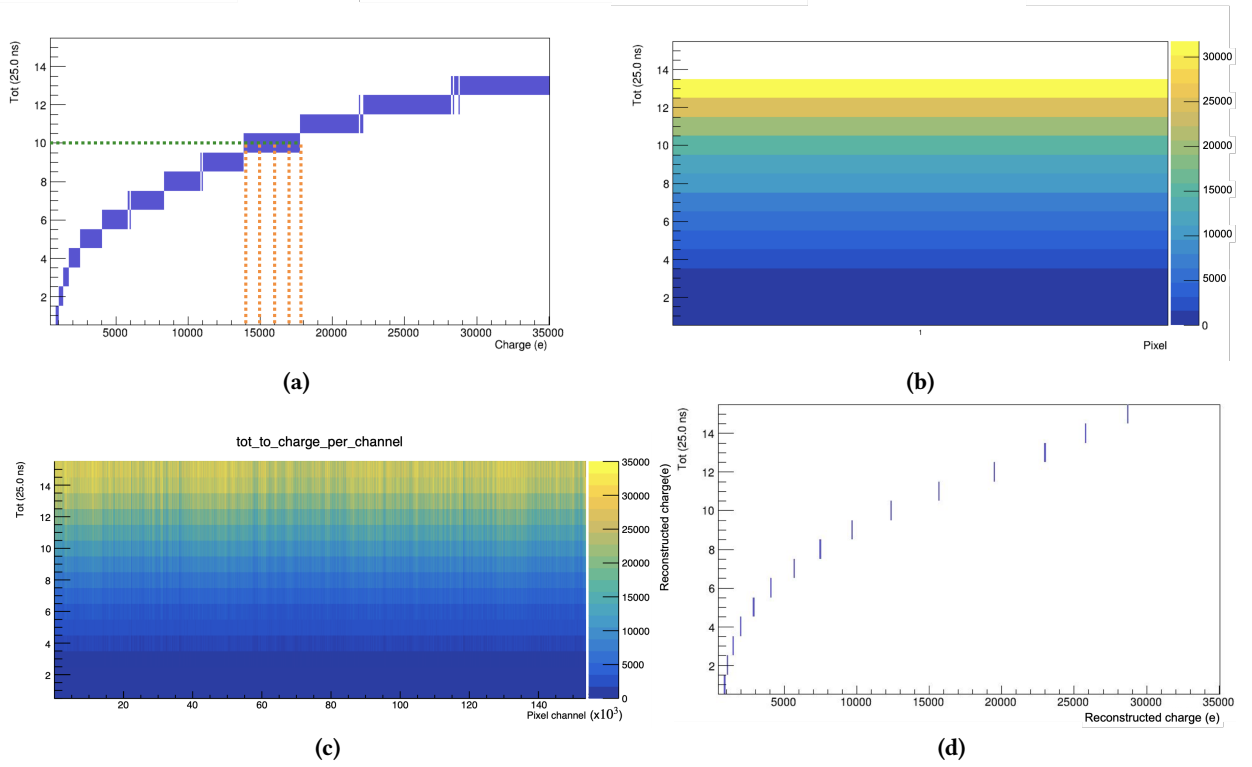


Figure 6.21: (a) ToT vs. charge distribution for a single pixel, illustrating how a particular ToT value corresponds to a range of charges (b) Map of the average charge per ToT for a single pixel (c) LUT for per-pixel ToT-to-charge calibration, where each channel on the x-axis corresponds to one pixel (d) LUT for per-chip ToT-to-charge calibration, where each ToT value corresponds to the average charge over all pixels [313].

calibration improves tracking performance. Based on their findings, an approach will be finalized for realistic modeling of charge-to-ToT conversion in Athena.

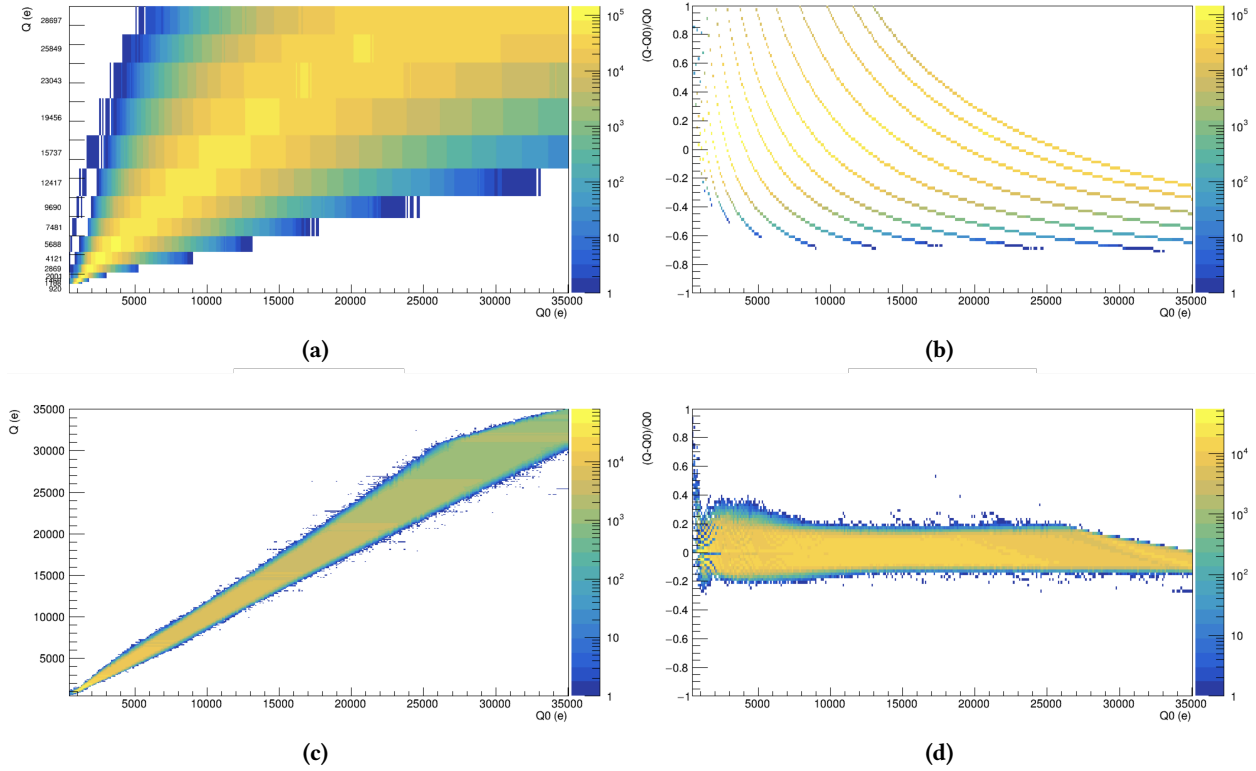


Figure 6.22: (a) Reconstructed charge Q vs. initial injected charge Q_0 for per-chip calibration (b) Relative charge resolution $\frac{(Q-Q_0)}{Q_0}$ vs. initial injected charge for per-chip calibration (c) Reconstructed charge Q vs. initial injected charge Q_0 for per-pixel calibration (d) Relative charge resolution vs. initial injected charge for per-pixel calibration [313].

6.1.6 Summary and Outlook

The studies presented in this section were conducted as part of my ATLAS qualification task. This project involved developing digitization code in Athena for realistic modeling of RD53-type readout chips, such as the various versions of the ITkPix readout chip planned for use in the ITk pixel detector, as the ITk pixel digitization in Athena was largely based on previous readout chips like the FEI3 and FEI4.

The first part of the project discussed in Section 6.1.4 presents the results of modeling Time-Walk effects, a salient feature of RD53-type readout chips and often one of the limiting factors for the time resolution of the pixel chip, thereby making its modeling in MC simulations crucial.

The second part, detailed in Section 6.1.5, involves implementing a realistic modeling of the charge-to-ToT response of the ITkPix FE in Athena, as the original implementation of charge calibration was based on a simplified parameterization used for the FEI3 readout chip. An approach similar to the current implementation of charge-to-ToT conversion for the IBL based on LUTs was suggested by the ITk Offline Software community for realistic modeling of the ITkPix FE charge calibration, accounting for the spread in pixel calibration curves across the readout chip. This study was broken down into smaller investigations, each of which is tackled individually. The studies on single-LUT based charge calibration are discussed in Section 6.1.5.1. Given the unavailability of charge calibration data from the ITkPix readout chip at the time of the study, the LUT was constructed using charges that mimic the behavior of the FEI3 parameterization, illustrated in Figure 6.11. This test ensures that the digitization based on a single-LUT works as intended. Section 6.1.5.4 provides a first look at the ITkPixV1.0 dataset for investigating multi-LUT based charge calibration. This dataset, provided by ATLAS colleagues from LBNL and the University of Oregon, corresponds

to a digital single chip card tuned to a threshold of 1000e. The novel ITkPix FE chip differs from its predecessors such as FEI3 and FEI4 due to its low ToT resolution and high ToT dispersion. While module-to-module variation in ToT is anticipated to be minimal, pixel-to-pixel variation within small regions of the ITkPix FE is expected to be significant. The optimal pixel submatrix and pixel dimensions that best capture the observed ToT variations across the entire pixel matrix are determined using Kolmogorov-Smirnov tests, detailed in Section 6.1.5.2 and Section 6.1.5.3, respectively. The current challenges, potential roadblocks, possible solutions for the implementing multi-LUT based charge calibration in Athena is discussed in Section 6.1.5.4. The studies conducted by colleagues at LBNL and the University of Oregon on converting ToT to charge, and their impact on charge reconstruction resolution using per-pixel and per-chip level calibration, are briefly discussed in Section 6.1.6. The ITkPix FE is a newly designed readout chip for the ITk pixel detector, lacking prior community knowledge on its behavior. Accurate modeling of this chip in Athena requires further understanding of its operation. Tracking performance studies are currently underway, with an approach for modeling charge calibration expected to be finalized based on these new findings in the near future.

6.2 Modeling Radiation Damage Effects in HL-LHC MC Events

At the HL-LHC (see Section 5.1), the ATLAS detector will be exposed to unprecedented levels of radiation, leading to significant radiation damage (see Section 3.5) over time. Radiation damage significantly affects the performance of silicon tracking detectors, with the pixel detector closest to the interaction point experiencing the highest fluence and, consequently, the most severe damage. The current pixel detector receives damage from non-ionizing radiation over 10^{15} 1MeV n_{eq}/cm^2 , while the pixel detector designed for the HL-LHC must cope with an order of magnitude larger fluence [316]. The most critical effect is signal reduction, making it essential to generate simulated data that accurately reflects the performance evolution with the accumulation of luminosity and, thus, fluence. The algorithm developed and implemented by the ATLAS collaboration to correct simulated MC events for radiation damage effects in Run 3, achieving impressive agreement between collision data and simulated events is briefly introduced in Section 6.2.1, with detailed discussions available in Ref [316].

In preparation for the high-luminosity operations of the LHC, the demand for a faster ATLAS MC production algorithm has become imperative due to escalating collision events, tracks, and particle hit rates, imposing stringent constraints on available computing resources. A new algorithm is proposed that is not only faster compared to the current Run 3 algorithm but also maintains the same level of precision. Section 6.2.2 introduces the philosophy behind the new algorithm for modeling radiation damage effects at HL-LHC. Section 6.2.2.2 discusses the implementation strategy using the Allpix-Squared software framework and the essential components involved. Section 6.2.2.5 presents the results of closure tests to validate the new strategy, and Section 6.2.3 concludes the study with a discussion on the first tests on computing performance. The studies presented in this chapter have been published in [317].

6.2.1 Run 3 Radiation Damage Digitizer

The following section presents the algorithm developed and implemented by the ATLAS collaboration to incorporate the effects of radiation damage on the Pixel and IBL detectors in MC events during the Run 3 operations of the LHC. The ATLAS Pixel detector (see Section 2.2.4.2) has been operational since the start of LHC Run 1, while the IBL layer (see Section 2.2.4.1) was inserted as the new pixel layer closest to the IP before the beginning of Run 2 in 2015. Both the IBL and the Pixel detector consist of hybrid pixel modules, with the IBL featuring thinner sensors. Planar

n^+ -on-n technology is used for the Pixel and IBL sensors, except in the forward regions of the IBL, where novel 3D n^+ -on-p sensors are employed for the IBL, as discussed in Section 2.2.4.1.

By the end of early Run 3 LHC operations in 2023, the IBL and B-Layer planar sensors had integrated a fluence of $1.2 \times 10^{15} \text{ n}_{eq}/\text{cm}^2$ and $1.0 \times 10^{15} \text{ n}_{eq}/\text{cm}^2$, respectively, resulting in a signal loss of approximately 30% for both detectors [318]. This signal loss and the changes in Lorentz angle (see Section 3.3.4) due to radiation damage are implemented in the digitization step of the simulation, where energy depositions of charged particles are converted into digital signals sent from the module front ends to the detector readout system. Figure 6.23 provides a schematic of the physics models integrated into the radiation damage digitizer [316]. During initialization, the digitizer acquires global details about the detector geometry (such as pixel size, type, and tilt angle) and operational conditions, including sensor bias voltage, temperature, and fluence. The digitizer computes individual charge deposits within the pixel sensor by taking inputs on the magnitude and location of energy deposited by traversing charged particles, which are derived from Geant4 simulations, and then outputs a digitized representation of the measured charge. Silvaco TCAD tool is further employed to simulate the electric field of an irradiated pixel detector. The TCAD simulations consider a limited number (2-3) [319, 320] of effective deep defects that model the modification of macroscopic variables, such as leakage current, operational voltage, and charge collection efficiency, due to radiation damage. Figure 6.24 illustrates an example of simulated electric field profiles in IBL planar sensors.

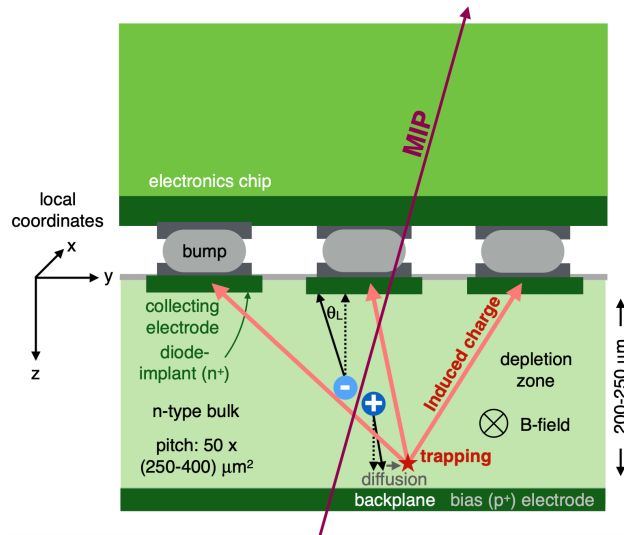


Figure 6.23: Schematic diagram of the Run3 radiation damage digitizer physics: As a MIP traverses the sensor, electrons and holes are generated and transported to the electrodes under electric and magnetic fields. Some may be trapped but still induce charge on primary and neighboring electrodes. Figure taken from [316].

The Run 3 radiation damage digitizer uses electric field maps simulated using TCAD to evaluate the time carriers will take to reach the collecting electrode. Radiation damage introduces defects that deform the electric field, creating a deep minimum in the sensor mid-plane, as shown in Figure 6.24. This deformation has two main effects: first and foremost, it reduces carrier velocity, increasing the likelihood of trapping. If the expected collection time is longer than a randomly generated fluence-dependent trapping time, the carrier is considered trapped, and its induced signal is calculated using a pre-computed weighting potential map of the sensor, also simulated with TCAD. Second, the Lorentz angle becomes dependent on the position along the bulk. These combined effects lead to reduced CCE, cluster shape deformation, and space-point resolution degradation. The Run 3 radiation damage digitizer algorithm is now the default for simulating events in ATLAS MC.

Figure 6.25 compares the charge collection efficiency (CCE) between experimental data and simulated MC events for IBL planar sensors. The comparison spans nearly two orders of magnitude of

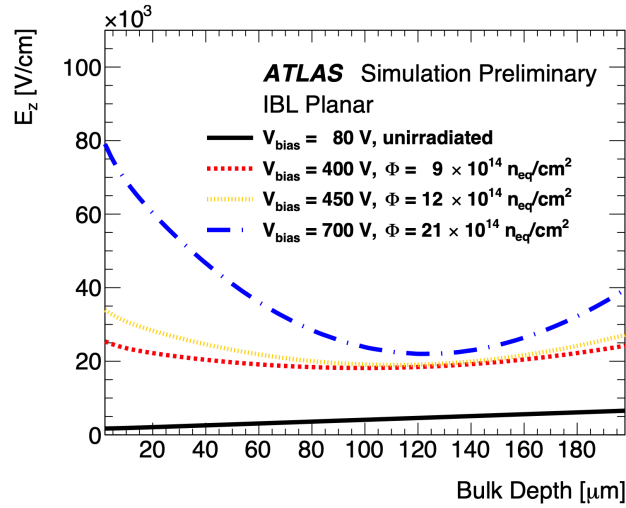


Figure 6.24: TCAD-simulated electric field profile of IBL planar sensors during Run 2 and Run 3. The electric field projection along the bulk is shown as a function of bulk depth, with electrons drifting towards lower z values. The Chiochia model [320] is used to simulate radiation damage effects. Figure taken from [318].

fluence, showing excellent agreement down to a level of 1%. This section provides a short overview of the philosophy behind the Run 3 radiation damage digitizer and its success in predicting CCE. Further details on this digitization model, as well as comparisons and validation of the simulation with collision data collected between 2015 and 2017 ($\leq 10^{15} \text{ 1 MeV n}_{eq}/\text{cm}^2$), are presented in [316, 318].

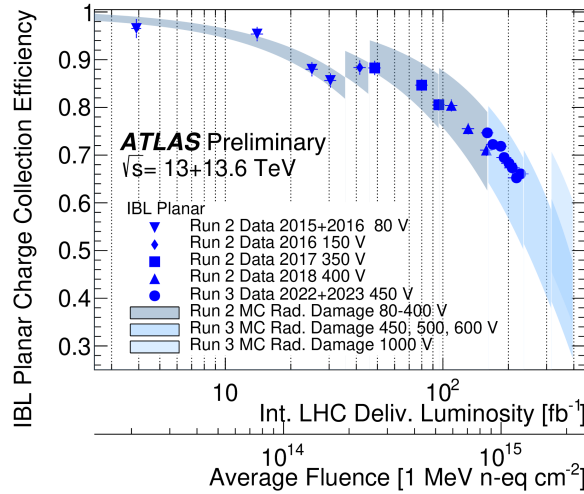


Figure 6.25: Comparison of evolution of CCE as a function of the integrated delivered luminosity and average fluence for IBL planar sensors for data (points) and the ATLAS radiation damage simulation (bands) from the beginning of Run 2. Vertical bands indicate uncertainties in TCAD radiation damage model inputs and trapping constants. Sudden increases in charge collection efficiency observed at the beginning of each year are due to changes in the operational parameters (bias voltage and thresholds). Figure sourced from [321].

The Run 3 radiation damage digitizer, despite its success, is unsuitable for modeling the anticipated radiation damage to the ITk pixel and strip detectors at HL-LHC, as the increased collision events, tracks, and particle hit rates would significantly slow down the algorithm, rendering it impractical and inefficient. Consequently, a new, faster, yet equally precise algorithm is required, which is presented in the following section.

6.2.2 Radiation Damage Digitizer Based on Look-Up Tables (LUTs) for Silicon Detectors at HL-LHC

At HL-LHC (see Section 5.1), the innermost parts of the pixel detector, located closest to the interaction point, will be exposed to unprecedented levels of radiation, reaching a non-ionizing radiation fluence of $1 - 2 \times 10^{16} \text{ n}_{eq}/\text{cm}^2$ over the expected lifetime of the ATLAS detector. This necessitates a complete replacement of the current ATLAS tracking system with an all-silicon inner tracker, the ITk, as discussed in Section 5.4. The increase in particle density at HL-LHC leads to a higher expected fluence, with $18 \times 10^{15} \text{ n}_{eq}/\text{cm}^2$ for the sensors in L0 after 2000 fb^{-1} of integrated luminosity, and $4 \times 10^{15} \text{ n}_{eq}/\text{cm}^2$ for the sensors in the L1 layer of the ITk pixel detector after 4000 fb^{-1} . The Run 3 digitizer algorithm introduced in Section 6.2.1 is notably slow and inefficient for modeling radiation damage effects in the MC events within HL-LHC environments. Consequently, a novel lightweight methodology centered on charge re-weighting from Look-Up Tables (LUTs) is explored and detailed in the subsequent sections.

6.2.2.1 LUT Methodology

The Look-Up Table (LUT) method models radiation damage effects in ATLAS MC events following the charge deposition simulated by Geant4 and preceding the signal digitization step (see Section 6.1.1). The radiation damage digitizer predicts which pixels will register signals from deposited charges and determines the magnitude of these signals. The novel LUT-based radiation damage digitizer, proposed for ATLAS data taking during HL-LHC, involves simulating ATLAS MC events with an ideal, undamaged pixel sensor and incorporating radiation damage impacts as corrections using the LUTs.

The LUT methodology draws inspiration from the 'template' method [322] developed by the CMS collaboration. Unlike the CMS approach, which corrects simulated pixel clusters, the LUT method reweighs observables of groups of drifting carriers within the silicon bulk. Therefore, the LUT method for modeling radiation damage effects in ATLAS MC events is tailored around the dynamics of charge carriers within pixel sensor bulk. Figure 6.26 illustrates this approach for planar sensors.

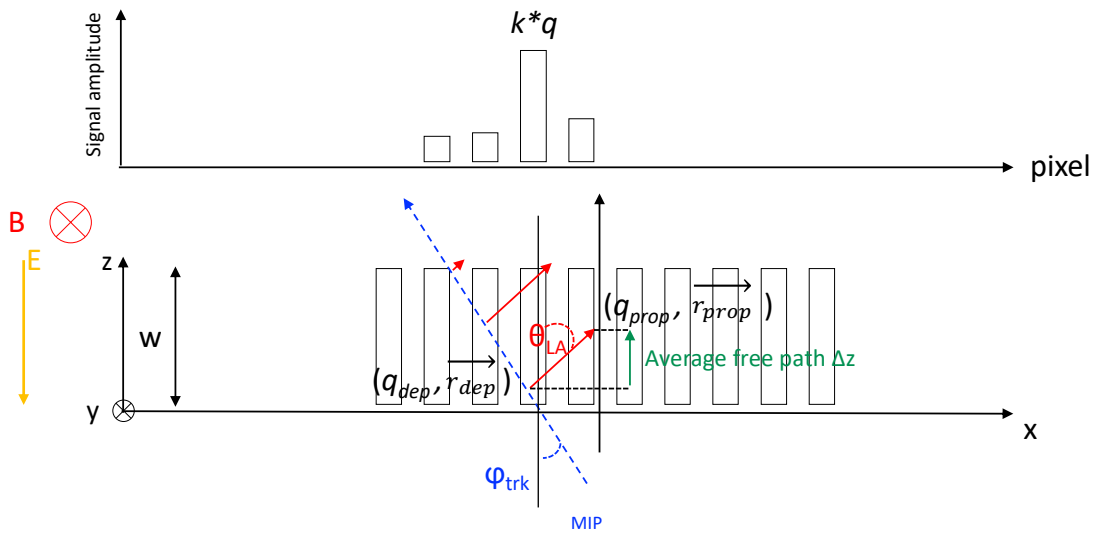


Figure 6.26: Schematic representation of carrier dynamics in silicon planar pixel sensors. As a MIP traverses the sensor at an angle φ_{trk} , electron-hole pairs are generated and drift towards respective electrodes influenced by electric and magnetic fields. Some electrons and holes may get trapped en route, yet they induce charges on both primary and neighboring electrodes [317].

Here, the sensor is assumed to be a planar pixel sensor of thickness w . The magnetic field $\mathbf{B}$ is oriented in the y -direction, and the electric field $\mathbf{E}$ is aligned along the depth axis z of the bulk. The charge carriers experience deflection in the x -direction due to the magnetic field. The electrons and holes produced by a MIP traversing the sensor thus drift toward collecting electrodes at an angle known as the Lorentz angle (θ_{LA}) with respect to the electric field.

In a pristine detector without radiation damage effects, the final position of the carriers is calculated by projecting the carrier position to the respective collecting electrode, and then smeared to account for diffusion. The LUT method is intended to apply corrections to this basic approach, where the initial position of the charge carrier is referred to as the *deposited* position $\mathbf{r}_{dep} = (x_{dep}, y_{dep}, z_{dep})$ and the final position as the *propagated* position $\mathbf{r}_{prop} = (x_{prop}, y_{prop}, z_{prop})$, as indicated in Figure 6.26.

The drifting carriers, as illustrated in Figure 6.26, can be trapped in the trapping centers formed by defects in the sensor bulk due to radiation damage before reaching the collecting electrode. In such cases, the charge carriers induce a signal that corresponds to only a fraction, $k < 1$, of their total charge, and this fraction can be calculated using the Shockley-Ramo theorem (see Section 3.3.3), which requires the initial and final positions of the carrier as input.

The distance covered by trapped charge carriers along the bulk depth direction, $\Delta z = z_{prop} - z_{dep}$, depends on their initial position $\mathbf{r}_{dep}$ due to the non-uniform electric field in the sensor bulk following radiation damage [318]. As the carriers drift, they move at an angle θ_{LA} relative to the electric field, which also varies with $\mathbf{r}_{dep}$, further reflecting the electric field's non-uniformity. The carriers' final position in the bending direction (orthogonal to both electric and magnetic fields) is displaced on average by $\Delta x = \tan(\theta_{LA}) \cdot \Delta z$. Additionally, diffusion adds dispersion to their final position, so the final x -direction position is $x_{prop} = x_{dep} + \Delta x$ in the absence of diffusion. The carrier's final position $\mathbf{r}_{prop}$ determines the amplitude of the induced signal on the electrodes, which depends on the initial position $\mathbf{r}_{dep}$ and the electric and magnetic fields. The induced signal is a fraction k of the carrier charge q , and k is also a function of the original carrier position $\mathbf{r}_{dep}$. The LUT method thus calculates the free path Δz , the Lorentz angle θ_{LA} , and the fraction of the induced signal k for each group of carriers, and these three quantities will be referred to as the *observables* in this thesis.

The Allpix-Squared [323] simulation framework (see Section 6.2.2.2) is used to determine the three observables through repeated simulations of the drift of carriers deposited at precise positions $\mathbf{r}_{dep}$ within the sensor bulk, using detailed electric field and Ramo potential maps generated by TCAD simulations.

For each simulated event, the initial position $\mathbf{r}_{dep}$ and final position $\mathbf{r}_{prop}$ of the carrier, along with the signal fraction k induced on the pixel matrix, is recorded. Ideally, the values of the three observables should be saved as a function of the initial position $\mathbf{r}_{dep}$ of the carrier. However, due to limited computing resources, the LUTs will be a function of only $z \equiv z_{dep}$. For a fixed z value, the average over all $(x_{dep}, y_{dep}) \equiv (x, y)$ positions is computed for each observable and assigned to that z value. To simplify notation, "dep" is omitted from here onward. Thus, for a single event and a single z value, the three LUTs are given by Equation 6.2.1.

$$\begin{cases} \Delta z(z)|_1 &= \sum_{x,y} \Delta z(x, y, z) / \sum_{x,y} \\ \theta_{LA}(z)|_1 &= \sum_{x,y} \theta_{LA}(x, y, z) / \sum_{x,y} \\ k(z)|_1 &= \sum_{x,y} k(x, y, z) / \sum_{x,y} \end{cases} \quad (6.2.1)$$

Using the LUTs defined in Equation 6.2.1, the propagated position $\mathbf{r}_{prop}$ and the induced signal q_{ind} of a charge q deposited at depth z in the sensor bulk are calculated as follows:

$$\begin{cases} x_{prop} &= x + [\tan(\theta_{LA}(z)) \cdot \Delta z(z)] + \Delta_x^{diff} \\ y_{prop} &= y + \Delta_y^{diff} \\ z_{prop} &= z + \Delta z(z) \\ q_{ind} &= k(z) \cdot q \end{cases} \quad (6.2.2)$$

Here, $\Delta_{x,y}^{diff}$ is a Gaussian-distributed random number added in Athena to simulate the effect of diffusion. The process of charge deposition and drifting is iteratively simulated for each r_{dep} to evaluate the dispersion in carrier dynamics. Equation 6.2.2 encapsulates the elegance of this novel LUT method, where the complex dynamics of carriers within an irradiated sensor bulk are approximated by an "average" estimator. It is noteworthy that while this thesis primarily focuses on planar pixel sensors, the same methodology can also be seamlessly applied to strip sensors. Moreover, ongoing efforts are underway to extend this methodology to 3D sensors [318].

A brief introduction to the Allpix-Squared simulation framework is presented in Section 6.2.2.2, followed by a discussion on the TCAD simulations used as inputs for the Allpix-Squared simulations in Section 6.2.2.3. A detailed description of the process of calculating the LUTs is provided in Section 6.2.2.4.

6.2.2.2 Allpix-Squared for Radiation Damage Digitizer

Allpix-Squared is a generic, open-source software framework for the simulation of silicon pixel detectors [323]. The framework allows the user to create detailed simulations of the entire experimental chain of a testbeam, from incident radiation to digitized detector response. An extensible system of modules is responsible for executing the distinct simulation steps, such as realistic charge carrier deposition using the Geant4 toolkit and the propagation of charge carriers in silicon through a drift-diffusion model. Detailed electric field maps imported from TCAD simulations can be used to model the drift behavior of charge carriers within the silicon, introducing a higher level of realism to Monte Carlo-based simulations of particle detectors.

In the studies presented in this chapter, a planar n^+ -on-p pixel sensor with a thickness of $100\ \mu\text{m}$ and a pitch of $50 \times 50\ \mu\text{m}^2$ is simulated. This sensor configuration is representative of those planned for the second-to-innermost pixel layer (L1) of the ITk pixel detector. The sensor is simulated after irradiation corresponding to a fluence of $4 \times 10^{15}\ \text{n}_{eq}\text{cm}^{-2}$ and operated at a voltage of 600 V. These conditions are anticipated for the aforementioned pixel layer at the end of the HL-LHC phase of ATLAS data taking. Figure 6.27 illustrates the simulation chain implemented for producing the LUTs, highlighting the use of electric field and Ramo potential maps from TCAD, along with the simulation of trapping effects.

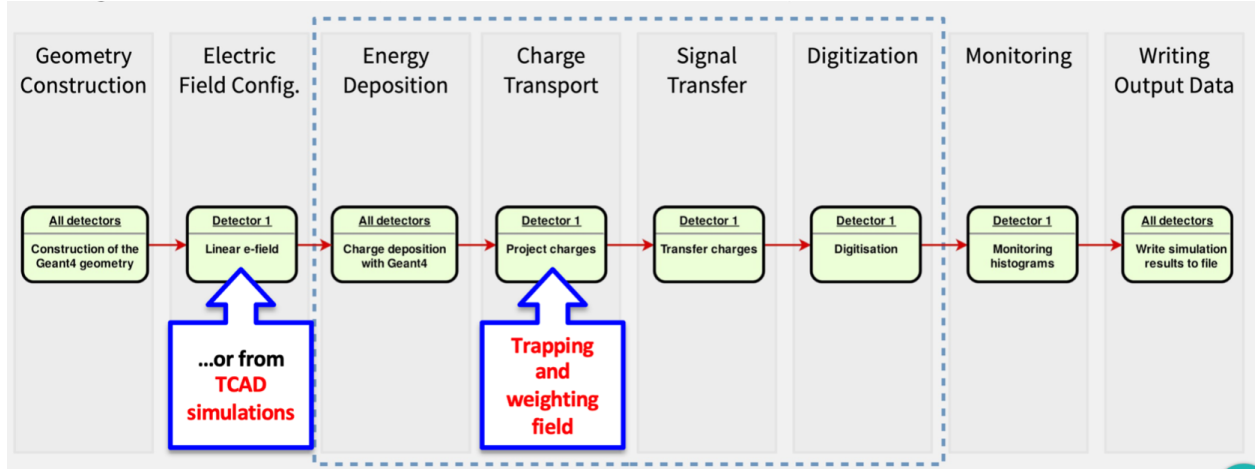


Figure 6.27: Modified Allpix2 simulation chain with a single detector for radiation damage digitizer.

6.2.2.3 Simulation Inputs

The electric field and Ramo potential maps generated using TCAD tools can be incorporated into Allpix-Squared simulations to accurately model the behavior of silicon radiation detectors, as discussed in Section 6.2.2.1. The subsequent sections detail the TCAD simulations employed to compute the LUTs in this study. All simulation results presented herein were obtained using Silvaco [324] TCAD tools.

The structure simulated in TCAD represents one-quarter of a 3×3 pixel array from a $100 \mu\text{m}$ n^+ -on-p planar pixel sensor with a pitch of $50 \times 50 \mu\text{m}^2$, as illustrated in Figure 6.28a. Simulating one pixel along with its neighboring pixels is essential for accurately modeling charge sharing via Ramo potential calculations. However, due to the design's symmetry, simulating just one-quarter of the 3×3 pixel matrix is sufficient.

The radiation damage effects are simulated using the LHCb TCAD radiation damage model [319], developed for planar n^+ -on-p pixels intended for the LHCb Velo Upgrade [325], where irradiation fluences of several $1 \times 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$ are expected. Similarly, planar n^+ -on-p pixel sensors in the ATLAS ITk detector will be exposed to comparable fluences during their operational lifetime, making the LHCb TCAD radiation damage model a suitable choice for this study. The ITk detector (see Section 5.4) will utilize planar pixels throughout, with 3D sensors employed only in the innermost section of the pixel detector. The largest anticipated fluence for planar pixels is $\Phi_{\text{max}} \sim 4 \times 10^{15} \text{ n}_{\text{eq}}/\text{cm}^2$ [326]. Electric field maps are produced using Silvaco TCAD for a sensor irradiated at the fluence Φ_{max} and polarized at the maximal operational voltage of 600 V. The extracted electric field profile along the sensor bulk depth is depicted in Figure 6.28b and Figure 6.28c illustrates the projection of the weighting field. The electric field and weighting potential maps from TCAD are integrated into the Allpix-Squared simulation chain, as illustrated in Figure 6.27, to create the three LUTs introduced in Section 6.2.2.1 for correcting the pixel response in ATLAS simulations to take into account the radiation-induced damage. The generation of the three LUTs using Allpix-Squared is presented in the following section.

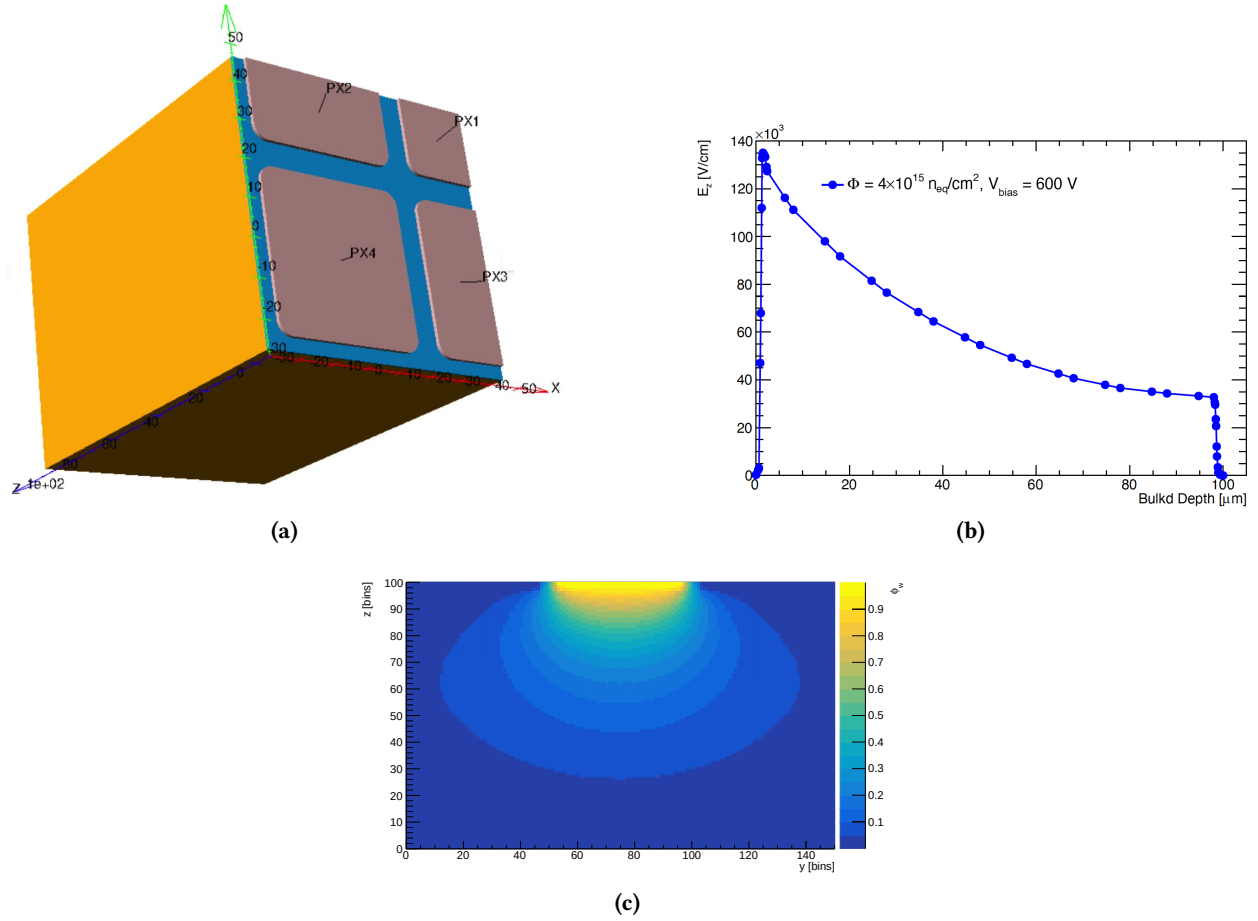


Figure 6.28: (a) One-quarter of a 3×3 pixel matrix structure simulated in TCAD (b) Extracted electric field distribution as a function of charge generation depth for the structure in Figure 6.28a, irradiated at a fluence of $4 \times 10^{15} \text{ n}_{\text{eq}}\text{cm}^{-2}$ and biased at 600 V (c) 2D projection of the weighting potential for the simulated structure [317].

6.2.2.4 Look-Up Tables Generation

Charged particles from LHC collisions uniformly ionize the volume of pixel sensors. Therefore, achieving an accurate representation of the pixel response requires studying it across all possible charge deposition locations $\mathbf{r}_{\text{dep}}$. The LUTs are generated using the "scan" mode of the "DepositionPointCharge" module in Allpix-Squared [323]. This module deposits a specified number of charge carriers at precise locations within the detector's active volume. In the studies presented herein, the scan mode is configured to deposit $q_{\text{dep}} = 1000$ electron-hole pairs every $2 \mu\text{m}$ along the z direction and every $1 \mu\text{m}$ in the other two directions for the simulated device.

After carriers have drifted to their final position $\mathbf{r}_{\text{prop}}$, the induced signal is evaluated for both the pixel cell where the carriers end up and its first eight neighbors, as depicted in Figure 6.29. It's important to note that while the propagated charge may land in the same pixel cell as the deposited charge, this isn't always guaranteed due to the Lorentz angle deflection of carriers in the transverse plane and the random diffusion of the charge carrier cloud, which can cause the charge to end up in neighboring pixels.

In the discussion following, the propagated position refer to the final position of the electrons. This assumption is made when calculating the LUTs due to the negligible impact of holes on signal "position" compared to electrons. This simplification is based on the principle known as the small-pixel effect [327]. In heavily segmented sensors such as pixel sensors, the weighting potential profile along the bulk has a steep gradient near the readout side as depicted in Figure 6.28c. Consequently, only carriers in close proximity to the pixel electrode can induce a significant signal.

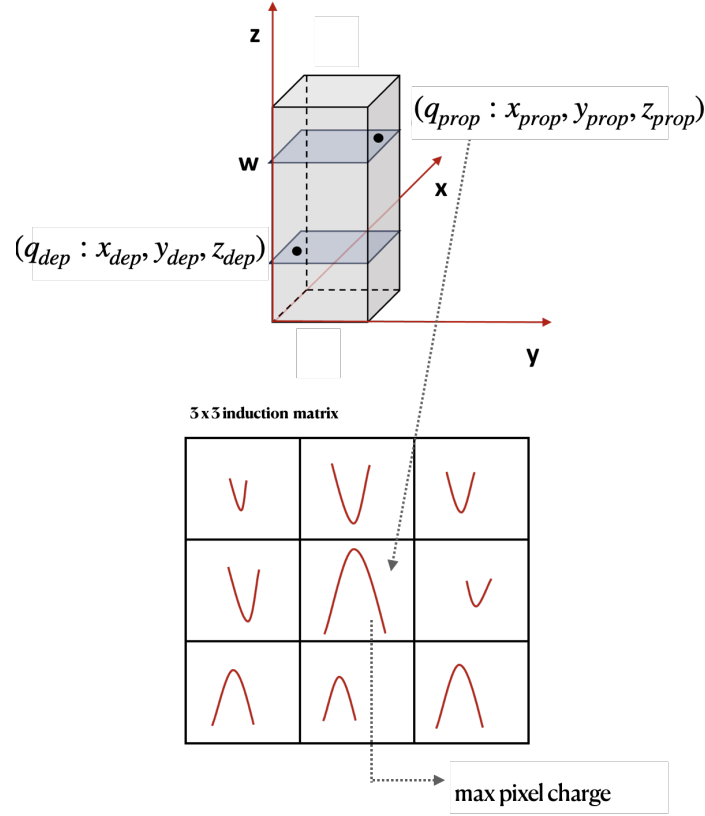


Figure 6.29: (top) Illustration of the deposited charge q_{dep} and its position $\mathbf{r}_{dep}$, along with the propagated (final) charge q_{prop} and its final position $\mathbf{r}_{prop}$. (bottom) Illustration of the 3×3 pixel matrix used to evaluate the induced signal, where the central pixel contains q_{prop} and $\mathbf{r}_{prop}$.

Since holes move away from the readout electrode, their influence on signal position can be safely neglected.

To produce the LUTs, the pixel with the largest induced signal is identified, and its position and signal q_{max} are retained for subsequent steps. The CCE for each deposition position $\mathbf{r}_{dep}$ is defined as the ratio of q_{max} to the deposited charge q_{dep} , as given by Equation 6.2.3.

$$CCE(\mathbf{r}_{dep}) = q_{max}/q_{dep} \quad (6.2.3)$$

The $CCE(z)$ is then evaluated by extracting the most probable CCE values (MPV) for each z . An example of CCE distribution for charges deposited at a z position close to the midplane is illustrated in Figure 6.30a. The $\Delta z(z)$ observable is evaluated by taking the average of the distribution of the free path traveled by the carriers as a function of the generation depth, as illustrated in Figure 6.30c. While the average over repeated simulations accurately represents the Δz distribution, as shown in Figure 6.30b, the MPV is a better estimator for the CCE distribution compared to the average. The Lorentz angle $\theta_{LA}(z)$ observable is calculated by fitting a straight line to the electron drift distribution Δx vs. Δz for each z_{dep} position across various x_{dep} and y_{dep} positions, as shown in Figure 6.30b. The slope of the fit at each z_{dep} is then extracted, and the LUT is constructed by plotting the slope ($< \tan(\theta_{LA}) >$) as a function of the generation depth, as illustrated in Figure 6.31c. The large spread of Δx values observed when electrons reach the electrode is an artifact of the simulation. At this position, electrons are already within the pixel implant and cease to diffuse further. To avoid biasing the results, the upper limit of the fit range for extracting $\theta_{LA}(z)$ is constrained to a few micrometers away from the pixel implant.

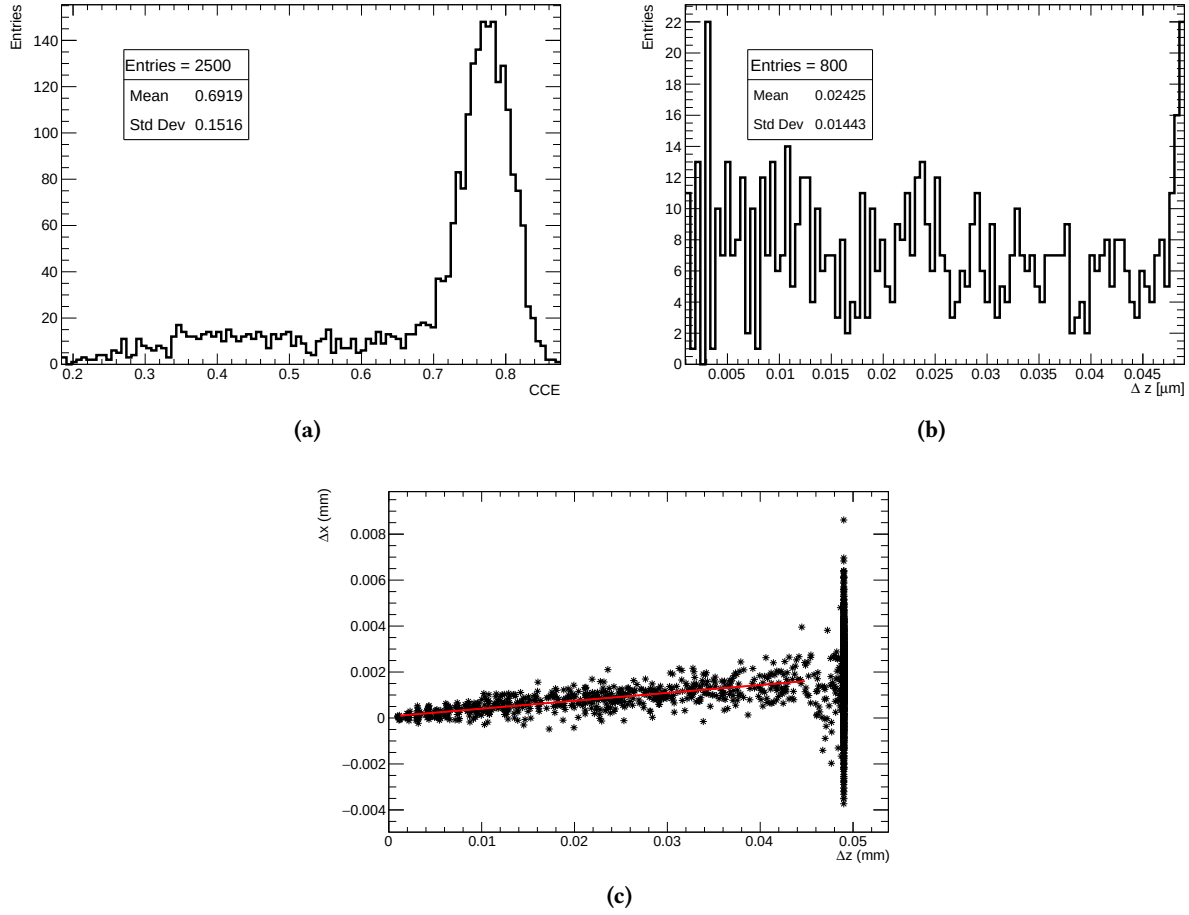


Figure 6.30: Distribution of observables for charge carriers injected near the sensor midplane. (a) Simulated CCE distribution (b) Simulated Δz distribution (c) Visualization of electron drift Δx vs. Δz towards the pixel side. The red line represents a linear fit to the electron drift data, with the average $\tan \theta_{LA}$ estimated as the slope of the fitted line.

Figure 6.31 depicts the LUTs for charge collection efficiency ($\text{CCE}(z)$), average free path ($\Delta z(z)$), and tangent of Lorentz angle ($\tan \theta_{LA}(z)$) used in this novel methodology for modeling radiation damage effects in MC events at HL-LHC. The CCE distribution peaks at over 85% at approximately $20 \mu\text{m}$ below the pixel implant. This occurs because holes created near the pixel become trapped, partially screening the signal. However, the influence of hole-trapping becomes negligible when charge is deposited farther away from the pixel electrode. The average distance Δz traveled by electrons decreases rapidly as they are generated closer to the electrode. For instance, at $z = 20 \mu\text{m}$, Δz of electrons is approximately $15 \mu\text{m}$, reflecting a 25% reduction. The Lorentz angle deflection is predicted to be very small throughout the bulk compared to its typical pre-irradiation value in ATLAS sensors, which is about 0.22 radians. This is primarily due to the large electric field inside the sensor, especially near the pixel side. The reduction in the Lorentz angle post-irradiation has already been observed in ATLAS pixel data [328]. The greatest deflection in the x direction occurs for charges deposited at the backside, amounting to just $2 \mu\text{m}$.

The following section will present the first validation of the LUT methodology.

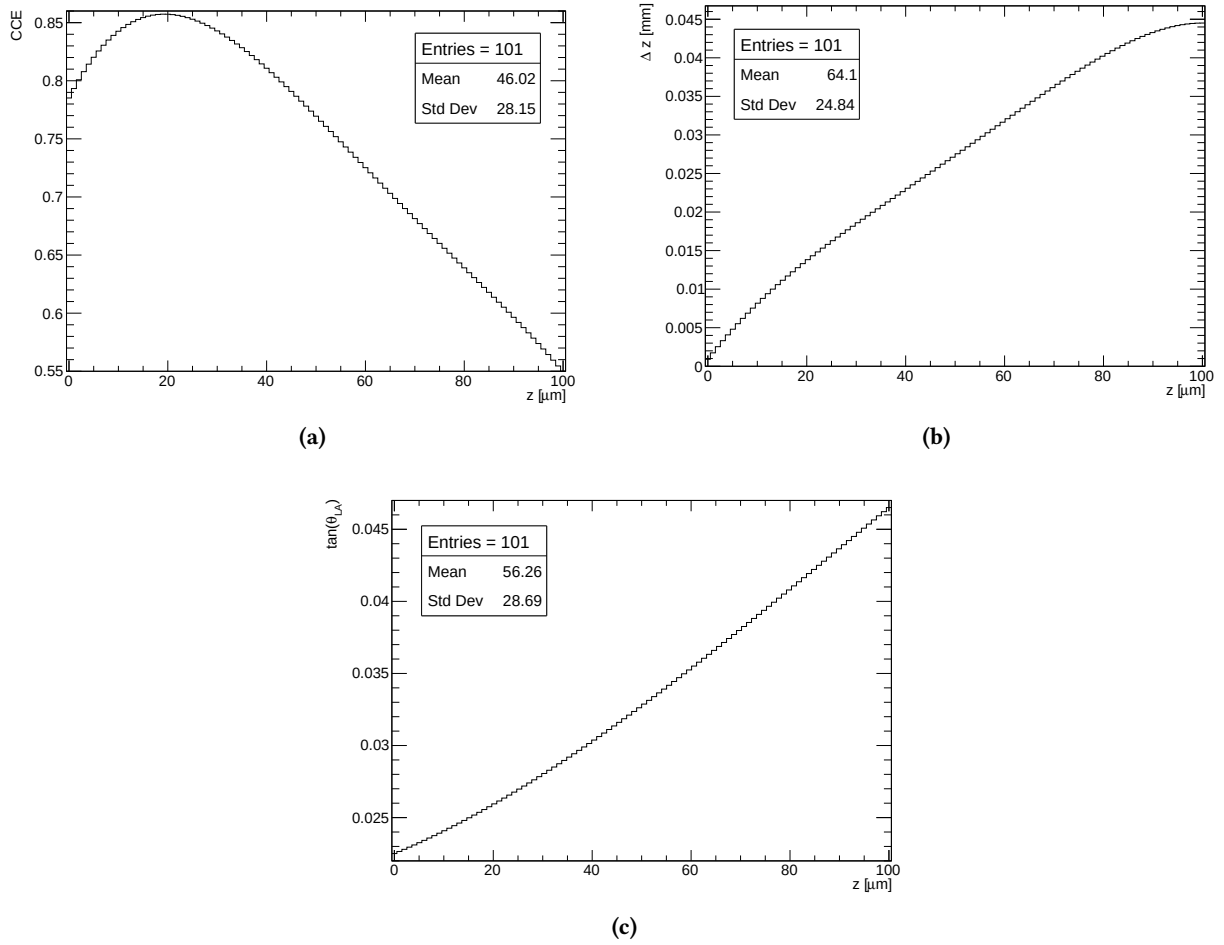


Figure 6.31: LUTs illustrating three observables. The $z = 0 \pm 100 \mu\text{m}$ corresponds to the pixel (backside) position of the sensor. (a) Charge collection efficiency ($\text{CCE}(z)$) (b) Average free path ($\Delta z(z)$) (c) Tangent of Lorentz angle ($\tan \theta_{LA}(z)$).

6.2.2.5 Internal Validation of the LUT-based Digitizer: Closure Test

A first validation of the new algorithm is performed using a closure test using the Allpix-Squared simulation chain, depicted in Figure 6.27. A new charge transport algorithm based on LUTs, the *LUT Propagator*, has been implemented in Allpix-Squared to validate this novel LUT-based methodology for modeling radiation damage effects. The core functionality of the LUT Propagator module is encapsulated in Equation 6.2.1. For each deposited electron in the sensor bulk, the induced signal and final position are evaluated using the three LUTs depicted in Figure 6.31.

The closure test presented in this section compares events simulated in Allpix-Squared using the new LUT Propagator module to fully simulated (FS) events generated by the Allpix-Squared simulation chain used to produce the three LUTs shown in Figure 6.31. Events are simulated for $100 \mu\text{m}$ thick n-in-p planar sensors with a pixel pitch of $50 \times 50 \mu\text{m}^2$, irradiated at a fluence of $4 \times 10^{15} \text{ n}_{eq}/\text{cm}^2$ and operated at 600 V — the exact same sensor type and conditions used to generate the LUTs discussed in Section 6.2.2.4. The agreement between LUT-based and full simulation events are assessed by examining cluster charge and cluster size, independently in the transverse (x) and longitudinal (y) directions. As a reminder, ATLAS uses a right-handed coordinate system with its origin at the nominal IP in the center of the detector and the z -axis coinciding with the axis of the beam pipe. The x -axis points from the IP towards the center of the LHC ring, and the y -axis points upward. Cylindrical coordinates (r, ϕ) are used in the transverse plane, ϕ being the azimuthal angle around the beam axis. The pseudorapidity is defined in terms of the polar angle θ

as $\eta = -\ln \tan(\theta/2)$.

The charge deposition step is simulated using pion beams with three distinct energies, corresponding to transverse momentum (p_T) values of 1, 10, and 100 GeV/c. The pixel modules in the ITk detector are tilted around the beam axis by 0.25 radians to compensate for the spread in the charge carrier cloud drifting to the collection electrode due to the Lorentz force. To achieve the most realistic simulation of the pixel detectors under actual experimental conditions, Allpix-Squared simulations are run with this tilt and over various η values, ranging from 0 (normal incidence) to 1.4.

The following sections present the results for cluster charge and cluster size for $p_T = 1$ GeV/c. A summary of the results for all p_T values, along with a brief discussion, is provided in Section 6.2.2.5.

Results of the Closure Test on Cluster Charge

The cluster charge distributions from simulated events for $p_T = 1$ GeV/c pions are shown in Figures 6.32-6.34 for η values of 0, 1, and 1.4, respectively, for both the full simulation and the LUT-based simulation. The level of agreement between the FS and LUT simulations is remarkable, with the mean values of the two distributions differing by less than 5%. Similar results are observed for p_T values of 10 and 100 GeV/c.

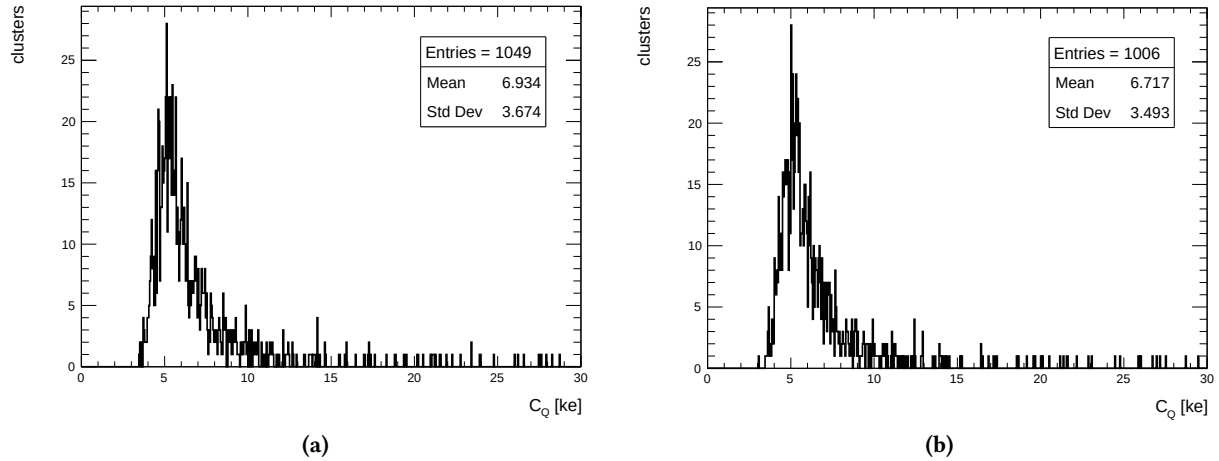


Figure 6.32: Cluster charge distribution for pions with $p_T = 1$ GeV/c impinging at $\eta = 0$. (a) Full simulation (b) LUT-based simulation.

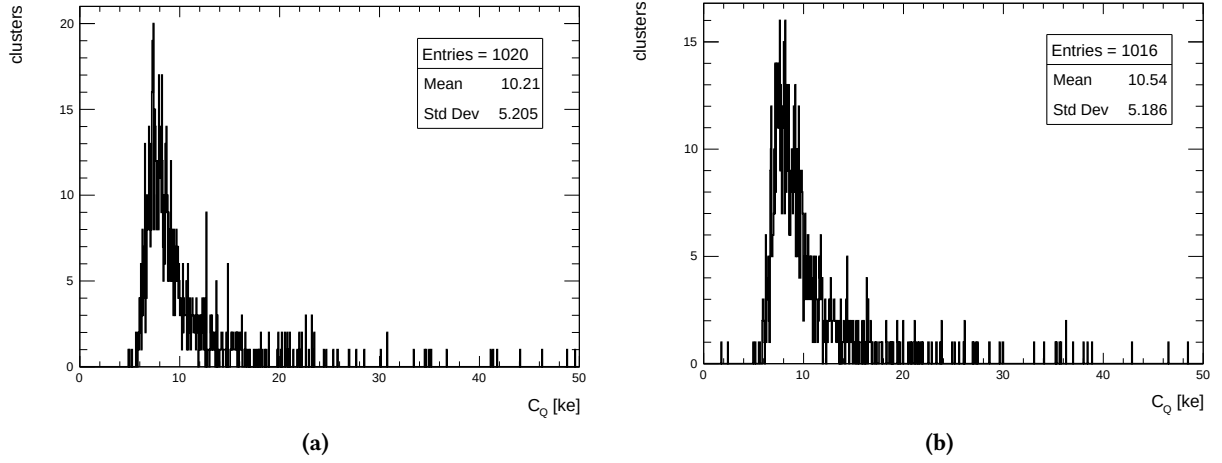


Figure 6.33: Cluster charge distribution for pions with $p_T = 1$ GeV/c impinging at $\eta = 1$. (a) Full simulation (b) LUT-based simulation.

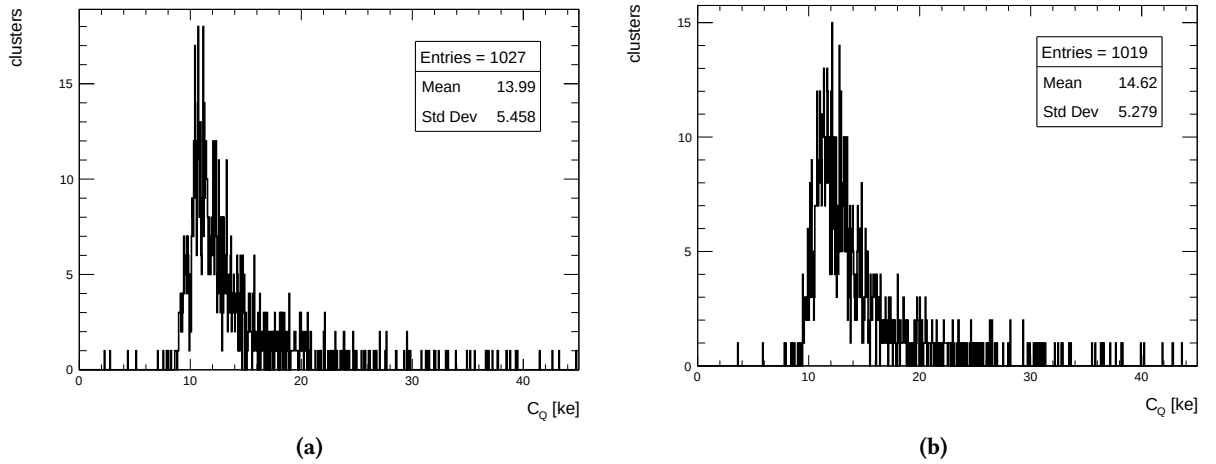


Figure 6.34: Cluster charge distribution for pions with $p_T = 1$ GeV/c impinging at $\eta = 1.4$. (a) Full simulation (b) LUT-based simulation.

Results of the Closure Test on Cluster Size

The cluster size distributions in the transverse direction from simulated events for $p_T = 1$ GeV/c pions are shown in Figures 6.35-6.37 for η values of 0, 1, and 1.4, respectively, for both the full simulation and the LUT-based simulation.

Despite the overall good agreement between the mean values of transverse cluster size distributions from the FS and LUT-based simulations, there is some discrepancy in the transverse cluster size distribution for $\eta = 1$, as illustrated in Figures 6.36. This difference is approximately 18%, while for the other η values, the agreement is within a few percent, similar to the closure test results on cluster charge shown in Figures 6.32 - 6.34. A similar discrepancy in the transverse cluster size distribution is observed for p_T values of 10 and 100 GeV/c.

The cluster size distributions in the longitudinal direction from simulated events for $p_T = 1$ GeV/c pions are shown in Figures 6.38-6.40 for η values of 0, 1, and 1.4, respectively, for both the full simulation and the LUT-based simulation. The mean values of the longitudinal cluster size distribution show excellent agreement between the full simulation and LUT-based simulation.

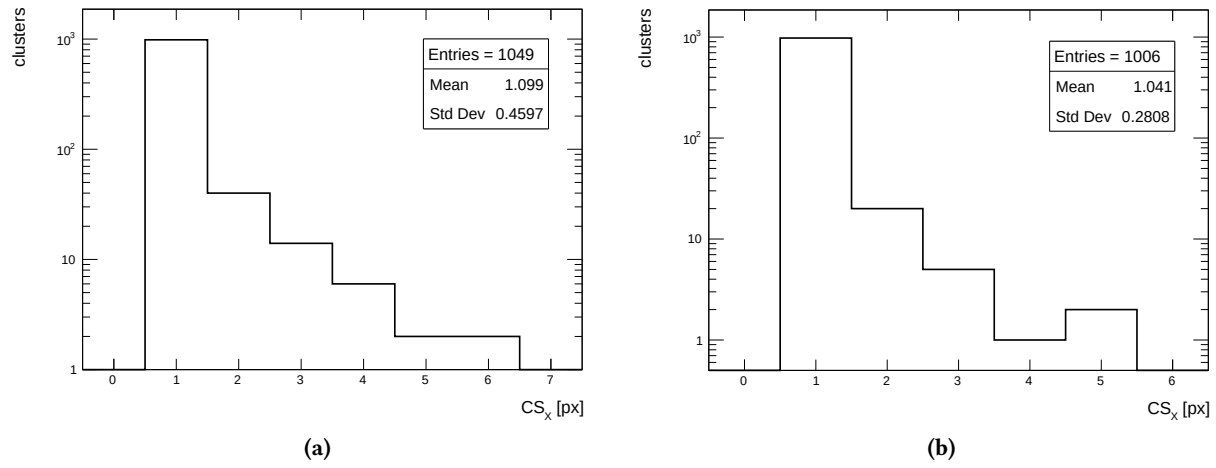


Figure 6.35: Cluster size distribution in the transverse direction for pions with $p_T = 1$ GeV/c at $\eta = 0$: (a) Full simulation (b) LUT-based simulation.

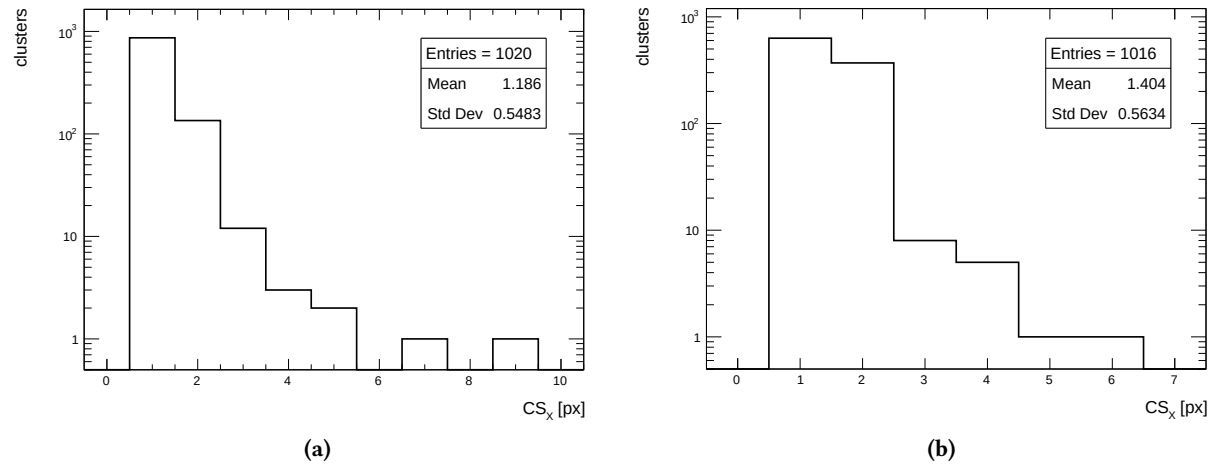


Figure 6.36: Cluster size distribution in the transverse direction for pions with $p_T = 1$ GeV/c at $\eta = 1$: (a) Full simulation (b) LUT-based simulation.

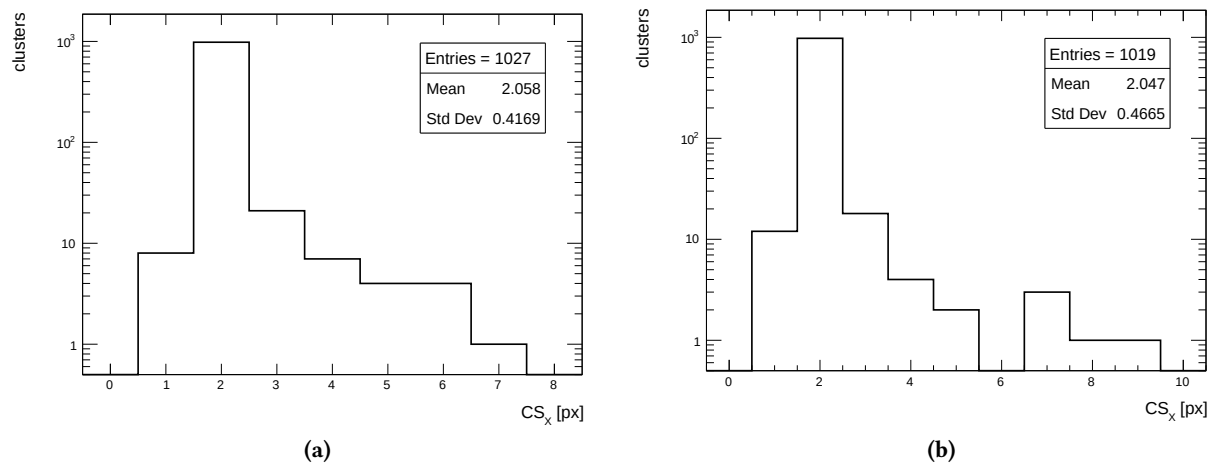


Figure 6.37: Cluster size distribution in the transverse direction for pions with $p_T = 1$ GeV/c at $\eta = 1.4$: (a) Full simulation (b) LUT-based simulation.

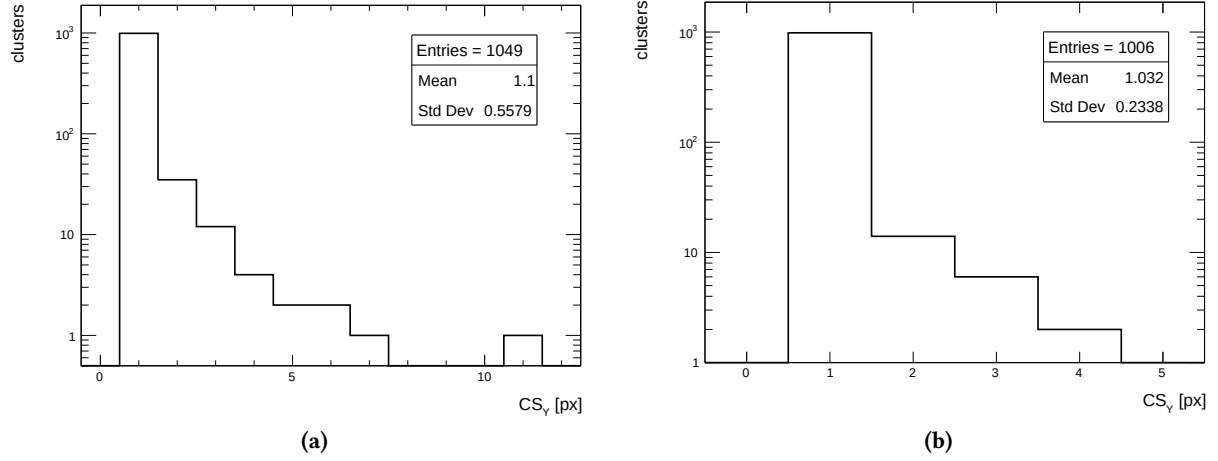


Figure 6.38: Cluster size distribution in the longitudinal direction for pions with $p_T = 1$ GeV/c at $\eta = 0$: (a) Full simulation (b) LUT-based simulation.

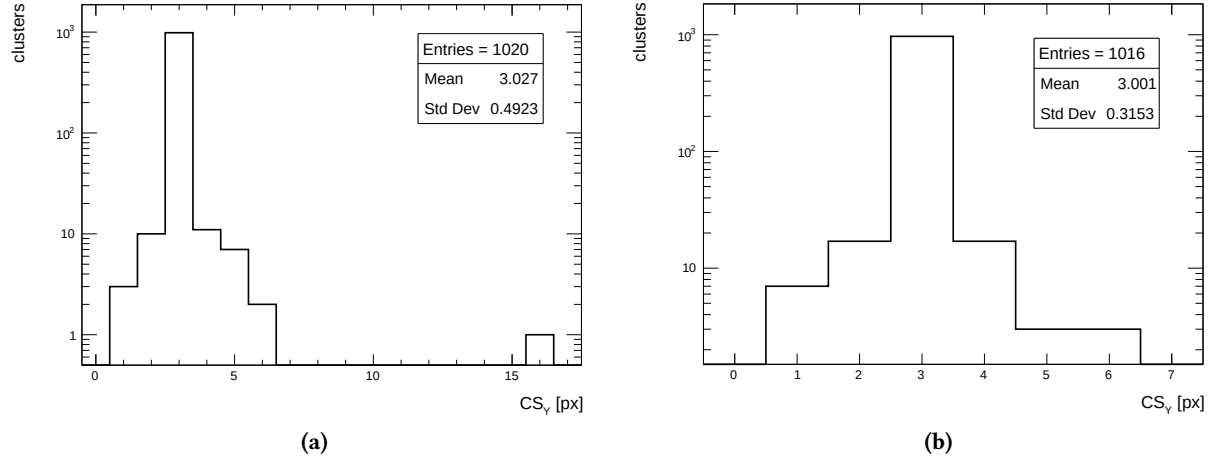


Figure 6.39: Cluster size distribution in the longitudinal direction for pions with $p_T = 1$ GeV/c at $\eta = 1$: (a) Full simulation (b) LUT-based simulation.

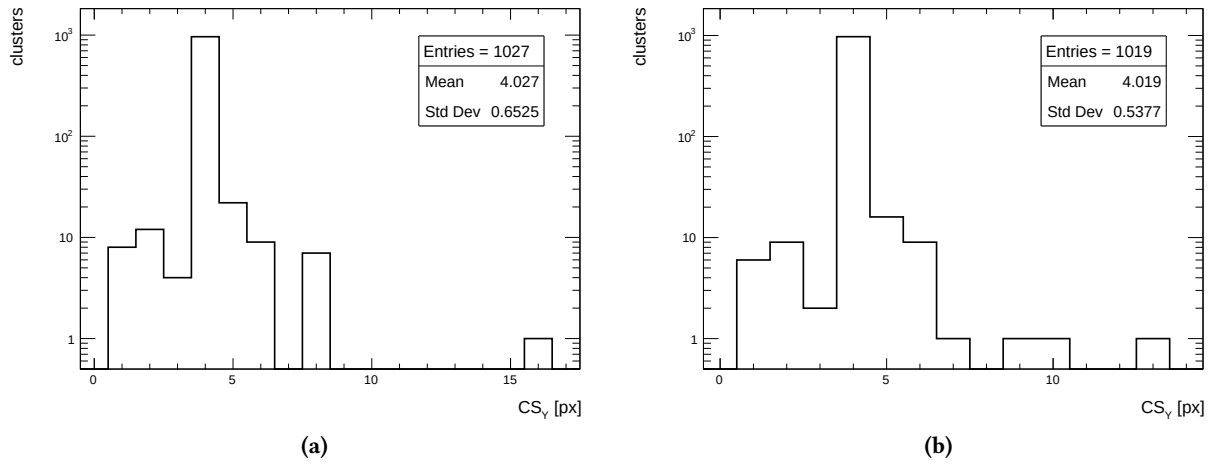


Figure 6.40: Cluster size distribution in the longitudinal direction for pions with $p_T = 1$ GeV/c at $\eta = 1.4$: (a) Full simulation (b) LUT-based simulation.

Summary and Discussion on Closure Test

Tables 6.4 - 6.6 present a summary of the closure test results for all quantities and pseudorapidities for pions with p_T values of 1, 10, and 100 GeV/c, respectively.

Table 6.4: Average cluster size in the transverse (CS_X) and the longitudinal (CS_Y) direction, along with average cluster charge (C_Q) for FS- and LUT-based events across different pseudorapidity values η and $p_T = 1$ GeV/c. The relative difference between FS and LUT, denoted by ϵ , is also presented.

η	CS_X			CS_Y			C_Q [ke]		
	FS	LUT	ϵ [%]	FS	LUT	ϵ [%]	FS	LUT	ϵ [%]
0	1.099	1.041	5.3	1.1	1.032	6.2	6.957	6.741	3.1
1	1.186	1.404	18.38	3.027	3.001	0.86	10.25	10.54	2.8
1.4	2.058	2.047	0.53	4.027	4.019	0.20	13.99	14.62	4.5

Table 6.5: Average cluster size in the transverse (CS_X) and the longitudinal (CS_Y) direction, along with average cluster charge (C_Q) for FS- and LUT-based events across different pseudorapidity values η and $p_T = 10$ GeV/c. The relative difference between FS and LUT, denoted by ϵ , is also presented.

η	CS_X			CS_Y			C_Q [ke]		
	FS	LUT	ϵ [%]	FS	LUT	ϵ [%]	FS	LUT	ϵ [%]
0	1.097	1.055	3.8	1.082	1.04	3.9	7.229	7.006	3.1
1	1.217	1.422	16.8	3.023	2.988	1.2	10.37	10.95	5.6
1.4	2.07	2.046	1.2	4.015	3.989	0.65	14.29	15.05	5.3

Table 6.6: Average cluster size in the transverse (CS_X) and the longitudinal (CS_Y) direction, along with average cluster charge (C_Q) for FS- and LUT-based events across different pseudorapidity values η and $p_T = 100$ GeV/c. The relative difference between FS and LUT, denoted by ϵ , is also presented.

η	CS_X			CS_Y			C_Q [ke]		
	FS	LUT	ϵ [%]	FS	LUT	ϵ [%]	FS	LUT	ϵ [%]
0	1.079	1.042	3.4	1.075	1.033	3.9	7.334	7.252	1.1
1	1.243	1.424	14.5	3.011	3.013	0.07	10.39	10.68	2.8
1.4	2.068	2.053	0.72	4.022	3.986	0.89	14.29	14.76	3.3

The discrepancy noted in Section 6.2.2.5 is apparent for $\eta = 1$ across all studied p_T values in the transverse cluster size CS_X . The comparison between FS and LUT-based simulations is extended to include additional pseudorapidity values such as $\eta = 0.4, 0.8$, and 1.2 to investigate the observed discrepancies for pions at $p_T = 100$ GeV/c, as summarized in Table 6.7.

Table 6.7: Average cluster size in the transverse direction (CS_X) for various pseudorapidity values (η) for pions incident at $p_T = 100$ GeV/c. The relative difference between FS and LUT, denoted by ϵ , is also presented.

CS_X			
η	FS	LUT	ϵ [%]
0	1.079	1.042	3.4
0.4	1.09	1.047	3.9
0.8	1.117	1.073	3.9
1	1.243	1.424	14.5
1.2	2.042	2.018	1.2
1.4	2.068	2.053	0.72

The difference in the transverse cluster size CS_X between FS and LUT-based events for the new pseudorapidity data points remains consistently within 1 – 4%. These results suggest that the observed discrepancy at $\eta = 1$ is confined to a very narrow range around this value. To investigate further, the divergence of the beam for simulations at $\eta = 1$ was increased to ± 10 mrad, corresponding to a pseudorapidity range of $\eta \in [0.99, 1.01]$. The outcomes of this investigation are summarized in Table 6.8.

Table 6.8: Average cluster size in the transverse direction (CS_X) for different beam divergences at $\eta = 1$ and $p_T = 100$ GeV/c. ϵ indicates the relative difference between FS and LUT.

CS_X			
Beam Divergence (x, y) (mrad)	FS	LUT	ϵ [%]
0, 0	1.224	1.428	17
10, 0	1.344	1.449	8
0, 10	1.547	1.551	0.2
10, 10	1.548	1.554	0.4

When increasing the beam divergence in the y direction, the agreement between LUT and FS events improves significantly, with discrepancies consistently below 1% as indicated in Table 6.8. Simulations with increased beam divergence generally exhibit improved agreement across all observables, achieving approximately 2% difference in CS_Y and less than 0.1% in C_Q . Given that charged particles from LHC collisions are uniformly distributed in η from -2 to $+2$, the localized discrepancies observed pose no significant concern overall.

6.2.3 Conclusions and Outlook

The extreme data rates and fluences anticipated at the HL-LHC impose stringent constraints on both detectors and computing resources. Radiation damage effects will significantly impair the performance of silicon pixel detectors in the ATLAS Inner Tracker. Therefore, it is crucial to accurately replicate such degradation in MC events, as demonstrated by the current pixel detector and the existing radiation damage digitizer discussed in Section 6.2.1.

The pursuit of a faster digitizer for the HL-LHC, while maintaining the current high level of precision, led to the development of the LUT-based radiation digitizer introduced in Section 6.2.2. A closure test was devised (see Section 6.2.2.5) to validate this LUT methodology by implementing a new charge transport model based on the LUTs (*LUT Propagator*) in Allpix-Squared. This test results demonstrated excellent agreement with data from the Allpix-Squared full simulation chain across all ranges of pseudorapidity and transverse momentum, as discussed in Section 6.2.2.5. A discrepancy in the transverse cluster size at $\eta = 1$ was observed but was understood to be confined to a range of less than 1% in pseudorapidity, as detailed in Section 6.2.2.5.

In the near future, data from ITk pixel modules equipped with the new readout chip will become available, enabling the comparison of LUT-based simulation predictions with test beam data. The LUT method can be readily applied to strip sensors and will also be extended to 3D sensors [318]. For 3D sensors in the barrel layer of the ITk detector, a single LUT of CCE as a function of the radial distance from the central electrode should suffice, as the Lorentz deflection is negligible due to the parallel alignment of the electric and magnetic fields. For 3D sensors in the rings, the Lorentz force causes carriers to drift along a curved path and preliminary results indicate that this effect is also negligible.

A preliminary speed test in Athena was conducted using dummy LUTs for an unirradiated pixel sensor with $k = 1$, $\Delta z = w - z$, and a constant $\tan \theta_{LA}$. The results indicate that the LUT-based radiation damage digitizer operates as quickly as the digitizer without radiation damage corrections. This result is inline with expectations, as the LUT-based method only applies additive and multiplicative corrections to the standard radiation damage digitizer without altering the underlying algorithm, as shown in Equation 6.2.2. The results also confirm that reading values from LUTs does not significantly impact computing load, ensuring no speed reduction when using LUTs for irradiated pixel sensors.

The LUT method for simulating radiation damage effects achieves both the precision of full simulation methods and the speed comparable to algorithms that do not model radiation damage. This novel methodology is thus expected to become the default for generating MC events during the HL-LHC phase of ATLAS.

Summary and Outlook

The pursuit of understanding the fundamental nature of the universe is a monumental and collaborative endeavor. In high-energy particle physics, this quest involves not only the design and construction of sophisticated experiments and accelerators over many years but also the integration of diverse expertise. From cutting-edge detector technology to advanced data analysis, the contributions of numerous specialists converge to drive progress. This quest is exemplified by the LHC and its experiments, such as ATLAS, and it continues to evolve with the forthcoming HL-LHC program. The HL-LHC aims to uncover new physics beyond the Standard Model by probing rare TeV-scale interactions, addressing key questions such as the origin of dark matter, baryogenesis, the hierarchy problem, and the integration of gravity with other fundamental forces. The projects undertaken in this PhD thesis encompass studies related to the ATLAS detector and the analysis of collision data collected by it, with a primary focus on the upgrade activities for the ATLAS Inner Tracker in preparation for the HL-LHC.

Measurement of $H \rightarrow \gamma\gamma$ fiducial cross-section in pp collisions at $\sqrt{s} = 13.6$ TeV

The first part of this thesis presents the first measurement of Higgs boson cross-sections at a center-of-mass energy of 13.6 TeV via the two-photon decay channel, utilizing $\approx 30\text{fb}^{-1}$ of pp collision data collected by the ATLAS experiment at the LHC in the first year (2022) of Run 3 (see Chapter 4).

Run 3 of the LHC is currently underway with smooth machine performance, and according to the latest schedule, it is expected to continue until November 2026. Following this period, Long Shutdown 3 (LS3) will commence, during which the ATLAS detector will undergo a comprehensive upgrade in preparation for the HL-LHC era. The 2024 data-taking period has proven to be the most successful to date, surpassing both the delivered luminosity by the LHC and the recorded integrated luminosity by the ATLAS detector compared to the Run 2 luminosities. The cross-section measurements in the $H \rightarrow \gamma\gamma$ channel and the combined measurement with the $H \rightarrow ZZ^* \rightarrow 4\ell$ channel, using early Run 3 pp collision data of 31.4fb^{-1} and 29.0fb^{-1} respectively, recorded by the ATLAS detector in 2022, enable the evaluation of ATLAS detector performance under the new data acquisition conditions of LHC Run 3 and facilitate the study of Higgs boson physics at the unprecedented energy of 13.6 TeV.

The cross-section is measured inclusively across different production modes and is obtained through an analytic fit to the reconstructed di-photon invariant mass spectrum. To minimize model dependence, the measurement is restricted to a kinematic phase space of the Higgs boson decay products defined at the particle level, closely matching the selection criteria used at the reconstruction level, and is corrected for detector effects. The measurements thus are performed within a fiducial region defined by the detector acceptance $|\eta| < 2.37$, excluding the range $1.37 < |\eta| < 1.52$. Selected photons must also meet identification and isolation criteria and are required to have transverse momentum greater than 35% and 25% of the di-photon invariant mass. The measured inclusive fiducial cross-section times branching ratio is $\sigma_{\text{fid},\gamma\gamma} = 76^{+14}_{-13} \text{ fb}$, which is consistent with the Standard Model prediction of $67.5 \pm 3.4 \text{ fb}$. Assuming the Standard Model acceptance and di-photon branching fraction, the fiducial measurement is extrapolated to the full phase space, resulting in a total cross-section of $\sigma(pp \rightarrow H) = 67^{+13}_{-12} \text{ pb}$ at 13.6 TeV. Additionally, combining this with measurements from the $H \rightarrow ZZ^* \rightarrow 4\ell$ channel yields a total cross-section of $\sigma(pp \rightarrow H) = 58.2 \pm 8.7 \text{ pb}$, compared to the Standard Model prediction of $59.9 \pm 2.6 \text{ pb}$.

Upgrade of the ATLAS tracking detector for HL-LHC

The central focus of this thesis, described in the second part of this dissertation, is on three studies related to the upgrade activities of the ATLAS Inner Tracker for the high-luminosity era of the LHC. The first study details my ATLAS qualification task (see Section 6.1), focusing on the implementation of the digitization module for the ITk pixel detector within the Athena software framework. The digitization of the ITk pixel detector in Athena is initially based on the FEI4 readout chip, which is currently employed in the IBL layer of the ATLAS Inner Detector. For the HL-LHC, the plan is to transition to an RD53-type readout chip (ITkPix), which is optimized for operation in the high-radiation environment expected at the HL-LHC. This qualification task addresses two central aspects of ITk pixel digitization. Section 6.1.4 details the implementation of time-walk correction, a key feature of the RD53-type readout chip. Section 6.1.5 focuses on the realistic modeling of the charge-to-Time-over-Threshold (ToT) response of the readout chip in Athena using Lookup Tables (LUTs). Preliminary data from the ITkPix V1.0 readout chip, provided by ATLAS collaborators at the University of Oregon and Lawrence Berkeley National Laboratory, is used to evaluate the feasibility of a multi-LUT approach for accurate charge-to-ToT modeling of the readout chip.

The ITkPix FE is a newly designed readout chip for the ITk pixel detector, with no prior community knowledge of its behavior. Compared to its predecessors, such as FEI3 and FEI4, this chip exhibits lower ToT resolution and greater ToT dispersion. Section 6.1.5.4 outlines the current challenges, potential roadblocks, and proposed solutions for implementing a realistic charge calibration using a multi-LUT approach in Athena. Accurate modeling of this chip in Athena necessitates a deeper understanding of its operation. Ongoing tracking performance studies aim to finalize an effective charge calibration model based on these new insights.

The second study further investigates aspects of the ATLAS Inner Tracker upgrade, focusing on the modeling of radiation damage effects (see Section 6.2). Radiation damage has a significant impact on the performance of silicon tracking detectors in LHC experiments like ATLAS and CMS, with signal reduction being a critical consequence. While adjusting sensor bias voltage and detection thresholds can help mitigate these effects, it is essential to generate simulated data that accurately reflects the performance changes as luminosity and radiation fluence accumulate. The ATLAS collaboration has developed and implemented algorithms to correct simulated MC events for radiation damage effects in both Run 2 and Run 3, achieving an impressive agreement with collision data, reaching within 1% in Run 3 (see Section 6.2.1). Despite the tremendous success of the Run 3 radiation damage digitizer, the preparation for HL-LHC necessitates a faster ATLAS MC production algorithm. This is crucial due to the increasing rates of collisions, events, tracks, and particle hits, which impose stringent constraints on available computing resources. The goal of the radiation damage digitizer is to estimate which pixels will register a signal from deposited charges and the magnitude of this signal. To achieve this for ATLAS data collection during the HL-LHC, a new strategy based on LUTs generated with Allpix-Squared is proposed and detailed in Section 6.2.2. Initially, ATLAS MC events will be simulated using an ideal, undamaged pixel sensor, with radiation damage effects subsequently incorporated through LUT-based corrections. Closure tests conducted across various pseudorapidity and transverse momentum ranges show that the events simulated with the new algorithm agree with fully simulated events within a few percent. In the near future, data from ITk pixel modules equipped with the new readout chip will be available, enabling a comparison between LUT-based simulations and test beam results.

Lastly, the third contribution to the ITk upgrade activities described in this thesis involves the assembly of quad modules at the Laboratoire de Physique Nucléaire et de Hautes Énergies (LPNHE) in Paris. Section 5.4.4.1 provides an overview of the stages involved in the quad module assembly process for the ITk Pixel Detector. This work was undertaken as a part of the site qualification process for the production of ITk quad modules.

Appendix

Measurement of the $H \rightarrow \gamma\gamma$ Fiducial Inclusive Cross-sections

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A.1 NNLOPS vs MINLO differences

The generation of Run 2 ggF samples (h027) is performed first at NLO and then re-weighted to NNLO. In contrast, the production of Run 3 ggF samples (h029) is done exclusively at NLO. The photon kinematic differences between the two types of samples are studied through the following steps:

- Derive the ratio (NNLO/MINLO) as a function of Higgs p_T from the Run 2 ggF samples, where both the NNLO and MINLO weights were stored. According to Figure A.1a, the differences in the reconstructed-level $m_{\gamma\gamma}$ distributions for the Run 2 ggF samples are within the resolution systematics.
- Conduct a closure test on the Run 2 ggF sample by applying the weights from the ratio function to MINLO in h027. The p_T distributions, both without reweighting and with reweighting, are depicted in Figure A.2.
- Apply the NNLO/MINLO weights to the Run 3 ggF samples and conduct a comparison of the reco-level $m_{\gamma\gamma}$ distribution for h029 using nominal (MINLO) and NNLOPS weights. The discrepancies between MINLO and NNLOPS for Run 3 ggF samples in the reco-level $m_{\gamma\gamma}$ distribution, as shown in Figure A.1b, are quite minor and fall well within the resolution systematics.

Thus, there is no need to introduce additional systematic uncertainties to account for the differences between Run 2 and Run 3 ggF samples.

A.1.1 DSCB fits to MinLo and NNLOPS Run 3 ggF samples

DSCB function fits to the reconstructed $m_{\gamma\gamma}$ distributions in MINLO and NNLOPS Run 3 ggF samples are depicted below:

The difference in the DSCB mean is 0.001%, while the difference in the DSCB width is 0.2% between MINLO and NNLOPS samples. These differences are negligible compared to the experimental uncertainties.

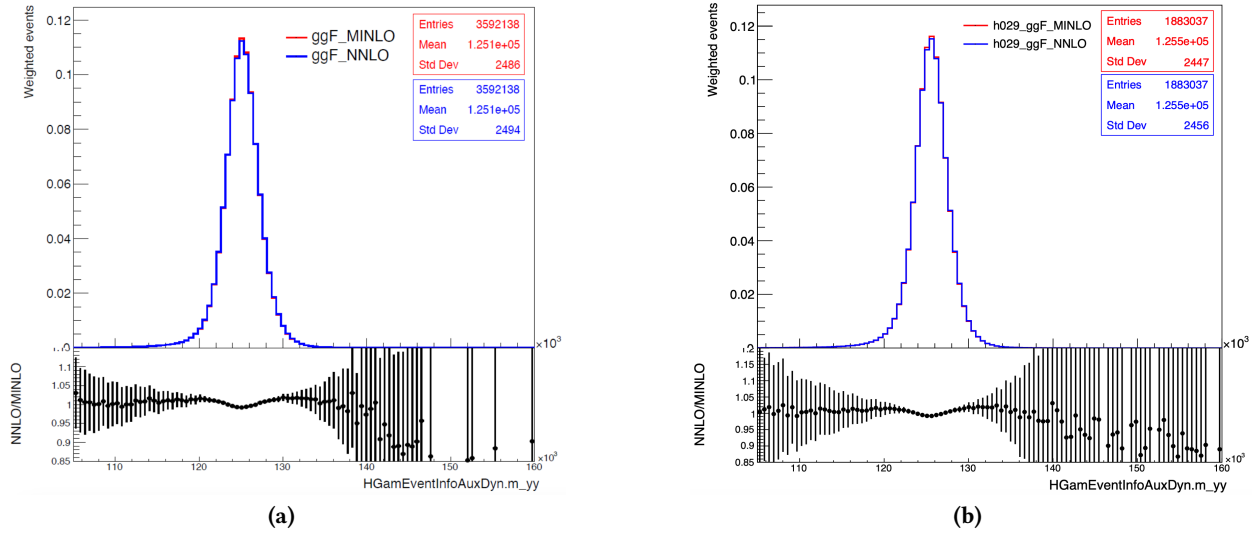


Figure A.1: Reco-level $m_{\gamma\gamma}$ distributions for (a) Run 2 (h027) ggF sample (b) Run 3 (h029) ggF sample.

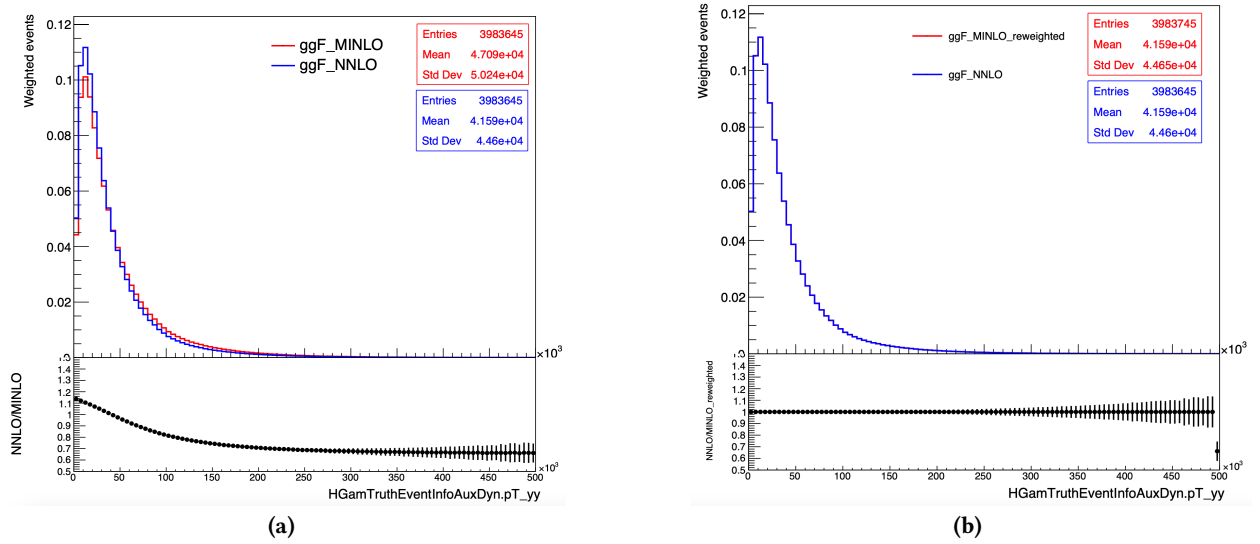


Figure A.2: Reco-level $pT_{\gamma\gamma}$ distributions for Run 2 (h027) ggF sample: (a) before reweighting; (b) after reweighting

A.1.2 Inclusive correction factor $\mathcal{C}_{\mathcal{F}}$ for MinLo and NNLOPS Run 3 ggF samples

The correction factor, $\mathcal{C}_{\mathcal{F}}$, is defined as the ratio of the signal events selected at the reconstruction level to the number of signal events selected at the particle level after applying the selection criteria described in Section 4.3.1. Figures A.4a and A.4b illustrate the truth (blue) and reconstructed (red) $pT_{\gamma\gamma}$ distributions of h029 MINLO and NNLOPS ggF samples. The values of $\mathcal{C}_{\mathcal{F}}$ are indicated in the insets of the figures.

The correction factor is 1% lower from MINLO to NNLOPS (from 71.5% to 70.7%).

A.1.3 Acceptance factor $\mathcal{A}$ for MinLo and NNLOPS Run 3 ggF samples

The signal acceptance, $\mathcal{A}$, is the fraction of signal events that passes the particle-level (fiducial) selection described in Section 4.3.1.4. Figure A.5a and A.5b illustrate the fiducial (blue) and full-phase space (red) truth $pT_{\gamma\gamma}$ distributions of h029 MINLO and NNLOPS ggF samples. The values of $\mathcal{A}$ (fiducial/full-phase-space), are indicated in the insets of the figures.

The acceptance is 0.4987 for MinLo and 0.4986 for NNLOPS.

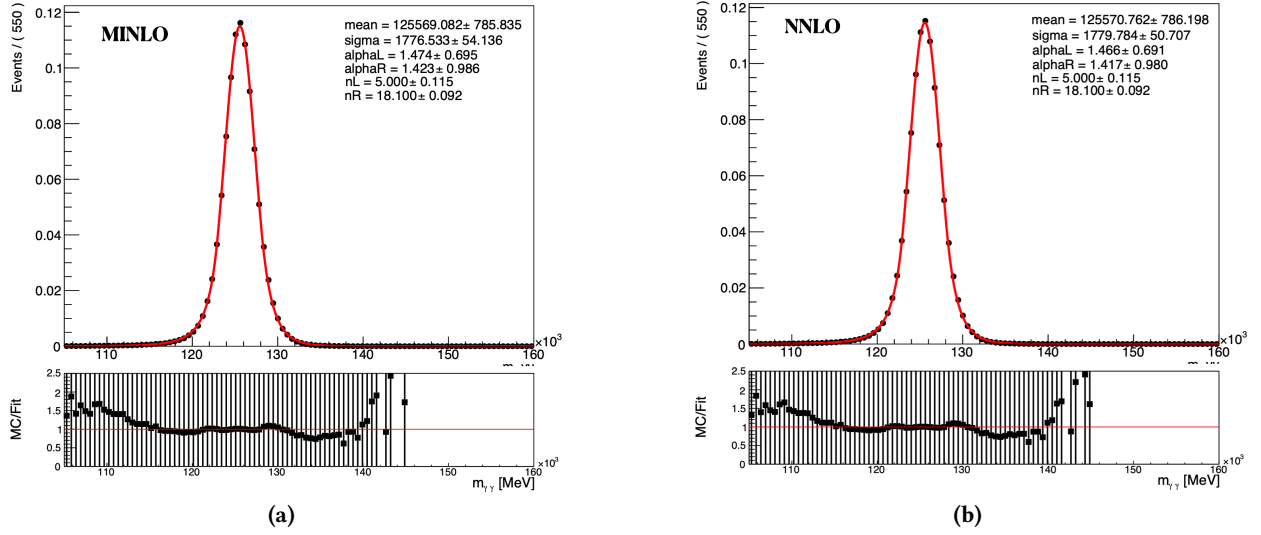


Figure A.3: DSCB fits to the reconstructed $m_{\gamma\gamma}$ distributions in (a) MINLO and (b) NNLOPS Run 3 (h029) ggF samples

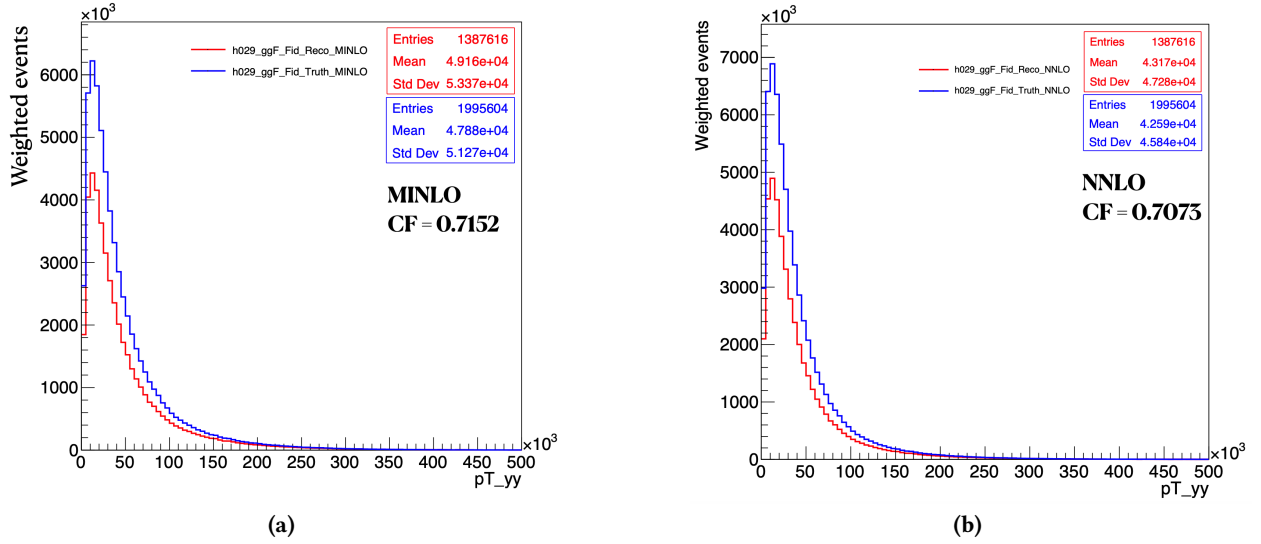


Figure A.4: $\mathcal{C}_{\mathcal{F}}$ of (a) MINLO and (b) NNLOPS Run 3 (h029) ggF samples.

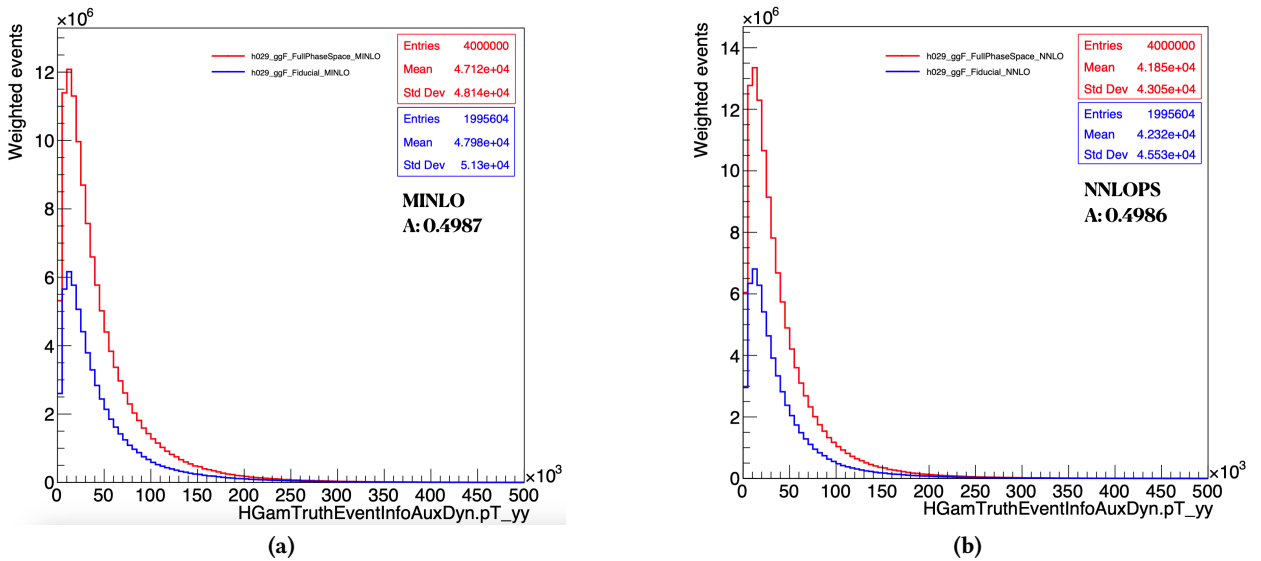


Figure A.5: $\mathcal{A}$ of (a) MINLO and (b) NNLOPS h029 ggF samples.

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