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presented by Brendon Aurele Bullard

candidate for the degree of Doctor of Philosophy and hereby
certify that it is worthy of acceptance.

Signature Masahiro Morii

Typed name: Professor Masahiro Morii, Chair

Signature Carlos Argüelles Delgado

Typed name: Professor Carlos Argüelles Delgado

Signature Matthew B. Reece

Typed name: Professor Matthew Reece

Date: May 3, 2022



The first differential cross section
measurements of $t\bar{t}$ produced with a W
boson in pp collisions

A DISSERTATION PRESENTED
BY
BRENDON AURELE BULLARD
TO
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The first differential cross section measurements of $t\bar{t}$ produced with a W boson in pp collisions

ABSTRACT

Measurements of inclusive $t\bar{t}W^\pm$ production cross sections performed by the ATLAS and CMS collaborations have consistently shown excesses of 20%-70% over theoretical predictions. These observations have lead to a growth in interest from the theory community over the last several years, leading to the realization that subleading electroweak corrections involving internal $tW \rightarrow tW$ scattering can be important for differential $t\bar{t}W$ production cross section calculations. This thesis presents the first differential cross section measurements of the $t\bar{t}W$ process using 138 fb^{-1} of pp collision data at $\sqrt{s} = 13 \text{ TeV}$ collected by the ATLAS experiment. Of particular interest is the N_{jets} distribution, a key input for the measurement of $t\bar{t}H$ production in multi-lepton final states. Inclusive and differential cross sections are extracted at the particle level in $2\ell\text{SS}$ and 3ℓ fiducial regions, both separated by total charge of the leptons as well as inclusively in charge with relative charge asymmetries. Charge-asymmetric enhancement in the $t\bar{t}W$ $2\ell\text{SS}$ fiducial regions and charge-symmetric enhancement in the 3ℓ region are observed. Excesses in the $t\bar{t}W$ production cross section are localized to events with low jet multiplicity, high leptonic H_T , and high di-lepton invariant mass. Distributions are generally in good agreement with predictions of several Monte Carlo models.

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List of Acronyms

PLIV	Prompt Lepton Improved Veto	QMisID	Charge Misidentification
JVT	Jet Vertex Tagger	HF	Heavy Flavor
MM	Matrix Method	MC	Monte Carlo
TF	Template Fit	SFOS	Same-flavor opposite-sign
SR	Signal Region	SF	Scale Factor
CR	Control Region	JES	Jet Energy Scale
VR	Validation Region	JER	Jet Energy Resolution
PV	Primary Vertex	NP	Nuisance Parameter
CV	Conversion Vertex	MLE	Maximum Likelihood Estimate
SV	Secondary Vertex	POI	Parameter of Interest
RNN	Recurrent Neural Network	TaP	Tag and Probe
MIP	Minimum Ionizing Particle	ME	Matrix Element
HLT	High Level Trigger	NF	Normalization Factors
BDT	Boosted Decision Tree	PDF	Parton Distribution Functions
ECIDS	Electron Charge Identification Selector		

TO MY PARENTS.

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Part I

Theory

1

The Standard Model

1.1 ELEMENTARY PARTICLES

The Standard Model of particle physics is the most comprehensive theory of the fundamental constituents of matter and energy devised by humankind. It posits the existence of leptons and quarks that coalesce to form ordinary matter at macroscopic scales and bosons that mediate interactions.

The dynamics of the theory include the electromagnetic interaction mediated by the photon γ , the strong nuclear interaction mediated by the gluon g , and the weak nuclear force mediated by the massive $W^\pm$ and Z^0 bosons. The SM particle content and its interactions are illustrated in Figure [1.1](#).

Beyond a mere catalogue of the known elementary particles, the Standard Model (SM) describes their properties and interactions. The most common use of the SM for high energy physics is the calculation of scattering amplitudes, typically by means of a perturbative expansion in small coupling strengths. Each term in the perturbative expansion can be represented by a set of Feynman diagrams, allowing for an intuitive interpretation of the processes that mediate the scattering interaction. As an example, the s -channel diagram for $t\bar{t}$ production in pp collisions is shown in Figure 1.2. This chapter will provide an overview of the formulation of the Standard Model, highlighting its key features relevant for the work described in this thesis. This chapter draws from references [22, 23, 24] heavily throughout.

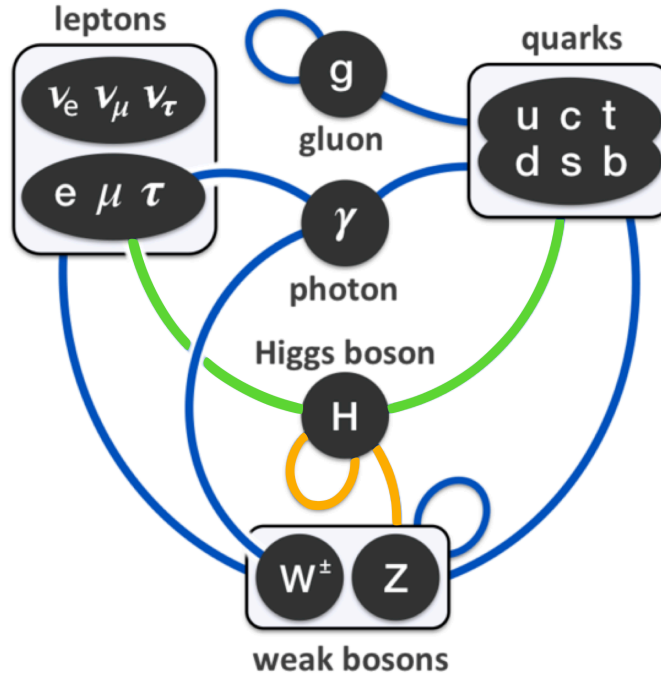


Figure 1.1: The interactions of the SM. Black ovals represent particles while lines connect particles that couple. Gauge interactions are shown in blue, while the Yukawa couplings and Higgs electroweak couplings are shown in green and orange. Based on [1].

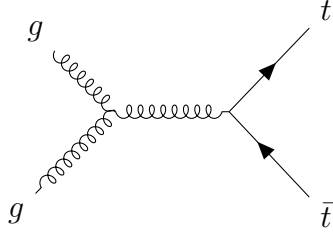


Figure 1.2: Feynman diagram for s -channel $t\bar{t}$ production at the LHC

1.2 INTERACTIONS AND SYMMETRIES

The Standard Model is a renormalizable quantum field theory composed of indivisible particles. These particles are understood as excitations in quantum fields that permeate spacetime. Particle species can be defined as the irreducible unitary representations of the Poincaré global symmetry group $\text{ISO}(1, 3)$ of Lorentz transformations. In this way, the principles of Special Relativity are fundamentally embedded in the theory. Particles are uniquely classified by their mass m , a non-negative real number, and their spin J , which can take positive half-integer values $J = 0, 1/2, 1, 3/2, 2, \dots$ ¹. The construction of the theory relies on packaging these spin states into Lorentz covariant vectors and tensors that propagate a larger number of degrees of freedom than is required for particle states. In order to remove these extra degrees of freedom, local symmetries are imposed via gauge transformations of fields that leave the SM Lagrangian invariant. The unbroken symmetry group of the SM is given by Equation 1.1:

$$G_{\text{SM}} = \text{SU}(3)_C \times \text{SU}(2)_L \otimes \text{U}(1)_{Y_W} \quad (1.1)$$

¹Additional immutable properties like color, charge, weak isospin, and weak hypercharge are added to the list of quantum numbers that uniquely define particle species when the theory describing their interactions is gauged.

This is the direct product of the symmetry groups of the strong interaction, which couples to color charge, and the electroweak interaction, which couples to weak isospin $\vec{T}$ of left-handed fermions and weak hypercharge Y_W . These local symmetries lead to the conservation of charges to which the fundamental interactions couple through Noether's theorem. Furthermore, the SM Lagrangian is invariant under $\mathcal{CPT}$ transformations, the simultaneous reversal of charge, parity, and time. Finally, the SM Lagrangian exhibits an additional set of accidental symmetries that are not embedded in the model a priori. These lead to the conservation of baryon number and the three lepton family numbers.

The SM is explicitly defined through its Lagrangian density (up to total derivative terms) and can be considered piecewise in Equation 1.2:

$$\mathcal{L}_{\text{SM}} = \mathcal{L}_{\text{QCD}} + \mathcal{L}_{\text{EW}} + \mathcal{L}_{\text{H}} + \mathcal{L}_{\text{Yukawa}} \quad (1.2)$$

Quantum chromodynamics, the theory of the strong interaction which couples to particles with color charge, is encapsulated in the first term of the SM Lagrangian:

$$\mathcal{L}_{\text{QCD}} = \sum_{\psi} \bar{\psi}_i i \gamma^\mu D_\mu^{ij} \psi_j - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} \quad (1.3)$$

Here, ψ is the 4-component Dirac spinor for each of the 6 massless quarks, $i = \{r, g, b\}$ are the three color indices, and G_μ^a is the 8-component SU(3) gauge field in the adjoint representation indexed by $a = \{1, 2, \dots, 8\}$. The covariant derivative encodes the interaction between gluons and quarks and is given by

$$D_\mu^{ij} \psi_j = \partial_\mu \delta_{ij} \psi_j - i g_s G_\mu^a T_{ij}^a \psi_j \quad (1.4)$$

where T_{ij}^a are the 3×3 Gell-Mann matrices that generate $SU(3)$. The gluon field strength tensor $G_{\mu\nu}^a$ encodes the gluon field propagation and self-interaction and is given by

$$G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a + g_s f^{abc} G_\mu^b G_\nu^c \quad (1.5)$$

where f^{abc} are the structure constants of $SU(3)$. The non-vanishing structure constants of the QCD Lagrangian is a result of QCD being a self-interacting, non-Abelian gauge theory. It is also a strongly interacting theory at energies near and below $\Lambda_{QCD} \approx 200$ MeV when the strong coupling constant g_s becomes $\mathcal{O}(\gtrsim 1)$, which spoils the perturbative calculation of scattering amplitudes and the interpretability of Feynman diagrams. It is at this scale that QCD confines quarks to colorless bound states called hadrons and an entirely different effective theory based on the Chiral Lagrangian is better suited to model their dynamics. QCD becomes a weakly interacting theory at energy scales much larger than Λ_{QCD} , as the coupling g_s becomes $\mathcal{O}(\lesssim 0.1)$. This high energy behavior of the strong interaction is known as asymptotic freedom.

The next term in the SM Lagrangian models the propagation of free fields and interactions in the electroweak (EW) sector:

$$\mathcal{L}_{EW} = \sum_{\psi} \bar{\psi} \gamma^\mu i D_\mu \psi - \frac{1}{4} W_a^{\mu\nu} W_{\mu\nu}^a - \frac{1}{4} B^{\mu\nu} B_{\mu\nu} \quad (1.6)$$

In the EW Lagrangian, ψ runs over the 2-component Weyl spinors for both quarks and leptons.

The fields B_μ and $\vec{W}_\mu = (W_\mu^0, W_\mu^1, W_\mu^2)$ are the massless $U(1)_Y$ and $SU(2)_L$ gauge fields,

respectively. The covariant derivative for the EW interaction is defined as

$$D_\mu \psi = \partial_\mu \psi + ig' \frac{1}{2} Y_W B_\mu \psi + ig \frac{1}{2} \tau_i^L W_\mu^i \psi \quad (1.7)$$

with Y_W the weak hypercharge and τ_i^L the Pauli matrices (the L superscript denotes their application to left-handed fermions only). The kinetic terms of the B_μ and $\vec{W}_\mu$ fields are defined analogously to the kinetic terms of the gluon field in the QCD Lagrangian, where the structure constants are derived from separate Lie brackets of the $U(1)$ and $SU(2)$ gauge group algebras (they vanish for the Abelian group $U(1)$).

The remaining two terms of the SM Lagrangian involve the Higgs field H , a complex scalar isospin doublet with $Y_W = +1$ written as

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} \quad (1.8)$$

The Lagrangian that describes the Higgs field and its interactions with the massless EW vector bosons

$$\mathcal{L}_H = (D^\mu H)^\dagger (D_\mu H) + V(H) \quad (1.9)$$

where the covariant derivative for the EW interaction $D_\mu H$ is defined as in Equation 1.7. The most general gauge-invariant and renormalizable Higgs potential is given by

$$V(H) = \mu^2 H^\dagger H + \lambda_H \left(H^\dagger H \right)^2 \quad (1.10)$$

The most general gauge-invariant terms that can be written for interactions between fermions and

the Higgs take the form of scalar Yukawa interactions:

$$-\mathcal{L}_{\text{Yukawa}} = y_{ij}^E \overline{e_{iR}} L_j H^* + y_{ij}^D \overline{d_{iR}} Q_j H^* + y_{ij}^U \overline{u_{iR}} Q_j H + \text{h.c.} \quad (\text{I.11})$$

where care has been taken to write explicitly the chiral-right $\text{SU}(2)_L$ singlet fields $\overline{e_{iR}}$, $\overline{d_{iR}}$, and $\overline{u_{iR}}$. The constants y_{ij} determine the coupling strengths of fermions to the Higgs and ultimately fermion masses once the Higgs field acquires a vacuum expectation value, where i, j index the three fermion generations. Note that there is a separate term for charged leptons (y_{ij}^E), up-type quarks (y_{ij}^U), and down-type quarks (y_{ij}^D), while the SM treats the neutrinos as massless.

These are the ingredients to the renormalizable SM with its unbroken electroweak symmetries. It does not feature the well-known electroweak bosons $W^\pm$ and Z^0 and fermions are massless. The next section will discuss the process of electroweak symmetry-breaking that motivated the introduction of the neutral scalar boson to the SM in the first place.

1.3 THE HIGGS MECHANISM AND FERMION MASSES

The Higgs field, subsequent Electroweak symmetry-breaking (EWSB) mechanism, and existence of an observable neutral scalar boson were proposed by Brout, Englert, and Higgs in 1964 [25, 26]. Electroweak gauge symmetry is spontaneously broken, in that the Lagrangian remains gauge-invariant but admits vacuum states that break EW gauge symmetry. Given $\mu^2 < 0$ in Equation 1.10, the Higgs field H assumes a nonzero vacuum expectation value (VEV)² The Higgs doublet then

²It is expected that the Higgs potential evolved from $\mu^2 > 0$ to $\mu^2 < 0$ in the first moments after the universe began.

takes the following form, which is unique up to $\text{SU}(2)_L \times \text{U}(1)_{Y_W}$ gauge transformations:

$$\langle H \rangle = \begin{pmatrix} 0 \\ v \end{pmatrix}, \quad \text{with } v > 0 \quad \text{and} \quad v^2 = \frac{|\mu^2|}{\lambda_H} \quad (1.12)$$

The only linear combination of the 4 generators of the unbroken EW symmetry group that annihilates $\langle H \rangle$, and therefore leave $\mathcal{L}_H$ invariant under its gauge transformation, is $I_3 + \frac{1}{2}Y_W = Q$, which is the electric charge. This implies that $\langle H \rangle$ is uncharged. Therefore the full Standard Model symmetry group given in Equation 1.1 is spontaneously broken:

$$\text{SU}(3)_C \otimes \text{SU}(2)_L \otimes \text{U}(1)_{Y_W} \rightarrow \text{SU}(3)_C \otimes \text{U}(1)_{EM} \quad (1.13)$$

This leads to the photon of the Electromagnetic (EM) interaction remaining massless and the conservation of electric charge. The symmetries of the remaining 3 linear combinations of generators are broken and lead to the absorption of the associated degrees of freedom (Goldstone bosons) to form the longitudinal modes required for massive $W^\pm$ and Z^0 fields. The relevant field definitions are given by:

$$A_\mu \equiv \sin \theta_w W_\mu^3 + \cos \theta_w B_\mu \quad (1.14)$$

$$Z_\mu \equiv \cos \theta_w W_\mu^3 - \sin \theta_w B_\mu \quad (1.15)$$

$$W_\mu^\pm \equiv \frac{1}{\sqrt{2}} (W_\mu^1 \mp iW_\mu^2) \quad (1.16)$$

where $\tan \theta_w = g'/g$. The substitution of these fields into $\mathcal{L}_{\text{SM}}$ give the familiar constants of the SM after symmetry breaking:

$$e = g \sin \theta_w \quad (\text{EM coupling strength}) \quad (1.17)$$

$$M_W = \frac{v}{2}g \quad (1.18)$$

$$M_Z = \frac{v}{2}\sqrt{g^2 + g'^2} = \frac{M_W}{\cos \theta_w} \quad (1.19)$$

The sole remaining degree of freedom of the doublet H manifests as an observable neutral scalar field h , which can be substituted into $\mathcal{L}_{\text{SM}}$. Its mass is given by $m_h^2 = 2\mu^2 = 2\lambda v^2$. Substituting $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ v+h \end{pmatrix}$ into Equation 1.11 gives mass terms for the fermions and their couplings to the state h :

$$\mathcal{L}_{\text{Yukawa}} = -\frac{1}{\sqrt{2}} \sum_i y_i v \bar{\psi}_L^i \psi_R^i + \text{h.c.} \quad (1.20)$$

$$- \frac{1}{\sqrt{2}} \sum_i y_i h \bar{\psi}_L^i \psi_R^i + \text{h.c.} \quad (1.21)$$

where i runs over the charged lepton and quark species and y_i is the Yukawa coupling strength of the fermions. Note that the fermion mass is proportional to its coupling strength to the Higgs boson h .

To summarize, the issue with the Electroweak Lagrangian of the Standard Model is that fermions and EW boson mass terms spoil gauge invariance of $\mathcal{L}_{\text{EW}}$. Therefore, the EW symmetry is spontaneously broken and masses are furnished for the EW bosons through the absorption of degrees of freedom from the Higgs field H . The fermions obtain their masses simply through Yukawa cou-

pling terms. These are two qualitatively different mechanisms, a fact that will be revisited in Chapter 2.

1.3.1 DEFICIENCIES OF THE STANDARD MODEL

While the SM has produced predictions verified by experiments to the level of parts per billion and successfully explains physics across orders of magnitude, it has several clear deficiencies that motivate the continued research in fundamental particle physics. They are given as follows:

1. While the SM can be extended to accommodate curved spacetime geometries at low energies, there is no true quantum theory of gravity within the SM.
2. Since the observation of galactic rotation curves by Rubin [27], physicists have known the existence of a stable form of matter unlike Baryonic matter that does not interact electromagnetically. Further assuming that the so-called Dark Matter is constituted by weakly interacting massive particles give rise to baryon acoustic oscillations in the early universe that explain features of the Cosmic Microwave Background [28]. The SM does not offer a candidate for Dark Matter and no particle Dark Matter has ever been detected.
3. The existence of Dark Matter and the accelerating expansion of the universe motivates the Λ CDM model, where Λ refers to the cosmological constant that can be added in Einstein's field equation to give rise to accelerated expansion of the universe. The conventional interpretation of Λ is that of a vacuum energy density. The Standard Model does not explain the origin of this vacuum energy.
4. It is a common (but perhaps incorrect) assumption that the universe began in a highly ordered state with equal amounts of matter and anti-matter. The necessary and sufficient conditions for electroweak baryogenesis to have occurred in the early universe, i.e. the creation of an imbalance of matter over anti-matter at the level of what is observed today, were given Sakharov: 1) baryon number violation, 2) C and CP violation, 3) departure from thermal equilibrium [29]. Baryogenesis requires more baryon and CP violation than explained by SM. It also requires a first order phase transition to have occurred, which is not provided by the smooth electroweak phase transition [30].
5. There is a term in the QCD Lagrangian that is controlled by a CP -violating phase θ that is observed to be very close to zero, leading to the preservation of CP -symmetry. There is

no mechanism to produce this behavior in the SM and results in an apparent fine-tuning problem. A well-known solution due to Peccei and Quinn provides a dynamical mechanism for small $\mathcal{CP}$ -violation, but predicts the existence of axions that have not been observed in nature [31].

6. The SM merely posits the form of the Higgs potential at low-energies through the sign of μ^2 , but does not provide a dynamical mechanism that causes the EW phase transition.
7. The Higgs boson mass is not protected by custodial symmetries in the SM, so its mass receives quantum corrections proportional to square of the the UV-cutoff scale Λ_{UV} at which new physics is expected to be relevant. If there is no new physics up to the Plank scale of 10^{19} GeV, the Higgs bare mass must be incredibly fine-tuned to produce a Higgs pole mass of 125 GeV. This result, due to the unnaturally different strengths of the weak force and gravity, is known as the hierarchy problem, the naturalness problem, or the gauge desert problem.
8. The Higgs mechanism allows mass terms for the fermions to be written down, but does not predict the hierarchy of fermion masses which span 5 orders of magnitude. Similarly, the structure of the Cabibbo-Kobayashi-Maskawa (CKM) matrix that relates the quark mass basis to its flavor basis is not predicted. This is known as the flavor puzzle.
9. The SM treats neutrinos as massless, which has been shown not to be the case by neutrino oscillation experiments like Super-Kamiokande and the Sudbury Neutrino Observatory [32, 33]. Moreover, since neutrinos are the only neutral fermions, it is possible that neutrinos obtain their mass not from Dirac mass terms, as for the other fermions, but from Majorana mass terms. In this scenario, the neutrino would be its own anti-particle.

Theoretical physicists have devised many extensions of the Standard Model aiming to address its many shortcomings. Unfortunately, experiments have consistently failed to find any evidence of such models. The next chapter will discuss the experimental status of Higgs physics and possible extensions of the Higgs sector.

2

Experimental Tests of the Standard Model

The Standard Model Higgs boson h is a truly unique particle. While there are several examples of scalar bosons observed in nature, most are composite states (for example the π^0 meson). The Higgs boson, on the other hand, is the only elementary scalar particle of the SM. The ultimate discovery of the Higgs boson and subsequent measurements of its properties were performed by experiments at the Large Hadron Collider, which will be discussed in Chapter 3. The discovery of a particle consistent with the Higgs came from the analysis of data taken between 2010 and 2012 at $\sqrt{s} = 7, 8$ TeV (Run I), while precision tests of the new resonance came from data collected between 2015

and 2018 at $\sqrt{s} = 13$ TeV. These subsequent measurements of its properties indicate that the resonance is indeed like the SM Higgs boson.

This chapter will summarize the status of experimental tests of the Higgs boson properties and highlight the importance of the Higgs couplings to fermions, with particular focus on the top quark. Theories beyond the Standard Model (BSM) that can be expected to alter the value of y_t will be discussed. Finally, the measurement of $t\bar{t}H$ production in multi-lepton final states and its dominant irreducible background production of $t\bar{t}W$ will be introduced.

2.1 PROPERTIES OF THE HIGGS BOSON

The SM Higgs boson h is a $\mathcal{CP}$ -even spin-0 boson, i.e. a scalar. The terms that appear in the SM Lagrangian involving h after electroweak symmetry breaking are given by:

$$\begin{aligned} \mathcal{L}_h = & -\frac{1}{2}m_h^2 h^2 - \underbrace{\frac{m_h^2}{2v}}_{\lambda_{hhh}} h^3 + \underbrace{\frac{m_h^2}{8v^2}}_{\lambda_{hhhh}} h^4 \\ & + \underbrace{\frac{2m_W^2}{v}}_{g_W} W_\mu^+ W_\mu^- h + \frac{1}{2} \underbrace{\frac{2m_Z^2}{v}}_{g_Z} Z_\mu Z_\mu h + \underbrace{\frac{m_W^2}{v^2}}_{g_{WWhh}} W_\mu^+ W_\mu^- hh + \frac{1}{2} \underbrace{\frac{m_Z^2}{v^2}}_{g_{ZZhh}} Z_\mu Z_\mu hh \\ & - \underbrace{\frac{m_f}{v}}_{y_f} \bar{f} f h \end{aligned} \quad (2.1)$$

where $m_h = \sqrt{2\lambda_H}v$. While the VEV is constrained by $v = (\sqrt{2}G_F)^{-1/2} \approx 246$ GeV, the parameter λ_H has no a priori prediction for its value and must be constrained by measuring the Higgs boson mass. The Higgs couplings to fermions and weak vector bosons are proportional to their mass and mass-squared, respectively. The Higgs trilinear coupling λ_{hhh} is also fixed by the structure of $V(H)$, providing another handle to validate the internal consistency of the EWSB mechanism of

the SM.

The mass of the Higgs boson is best measured in $H \rightarrow \gamma\gamma$ and $H \rightarrow ZZ^* \rightarrow 4\ell$, where the Higgs decay products are entirely visible and well-reconstructed [34]. The world average reported by the Particle Data Group (PDG) is $m_h = 125.10 \pm 0.14$ GeV. The spin and parity of the Higgs boson were determined by analyzing angular distributions of the Higgs decay products in $H \rightarrow WW^* \rightarrow e\nu\mu\nu$ and the aforementioned decay processes [35, 36]. The various Higgs couplings and Higgs mass determine its partial and total decay widths, and therefore its lifetime. This is an important measurement, as it gives a handle on all possible decays of h , including those to invisible and BSM final states. The total width of h is expected to be about $\Gamma_h \sim 4$ MeV and lifetime $t = \frac{\hbar}{\Gamma_h} = 1.6 \times 10^{-22}$ s. The best experimental constraints on the Higgs natural width are 95% confidence-level upper limits of $\Gamma_h < 14.4(22)$ MeV from ATLAS (CMS) measurements of off-shell $gg \rightarrow h^* \rightarrow ZZ$ production in 4ℓ and $2\ell 2\nu$ final states and 95% CL lower limit of $\Gamma_h > 3.5 \times 10^{-9}$ MeV from the measurement of flight distance in 4ℓ final states by CMS [37, 38, 39].

The production modes of the Higgs at the LHC are shown in Figure 2.1. Their cross sections and branching fractions of Higgs decays as a function of m_h are shown in Figure 2.2. The Higgs can decay through on shell pairs of particles with mass less than $m_h/2$. However, off-shell decays through VV^* are dominant modes due to the large couplings g_V . The decay of $H \rightarrow t^*\bar{t}^*$ is extremely suppressed due to the large top quark mass $m_t \approx 173$ GeV, requiring both top quarks to be highly virtual. Decays to pairs of photons and gluons are mediated by loop diagrams, as massless particles do not couple to the Higgs field. Decays to $b\bar{b}$ have the highest branching due to the combination of large y_b coupling and large phase space relative to the $H \rightarrow VV^*$ phase space.

Constraints on the couplings y_f for fermions other than the top quark are obtained from $H \rightarrow f\bar{f}$ rate measurements. Similarly, g_V is best measured through rate measurements of $H \rightarrow VV^*$. Measurements of the simultaneous production of $t\bar{t}H$ are used to determine the value of y_t , and will be discussed further in Section 2.3. Finally, the trilinear coupling λ_{hhh} can be constrained through measurements of di-Higgs production, while the quartic coupling λ_{hhhh} can be constrained through tri-Higgs production. Measuring the former is an achievable goal of the High Luminosity LHC through the 2030s, but the latter is not within the reach of the LHC due to its very small rate.

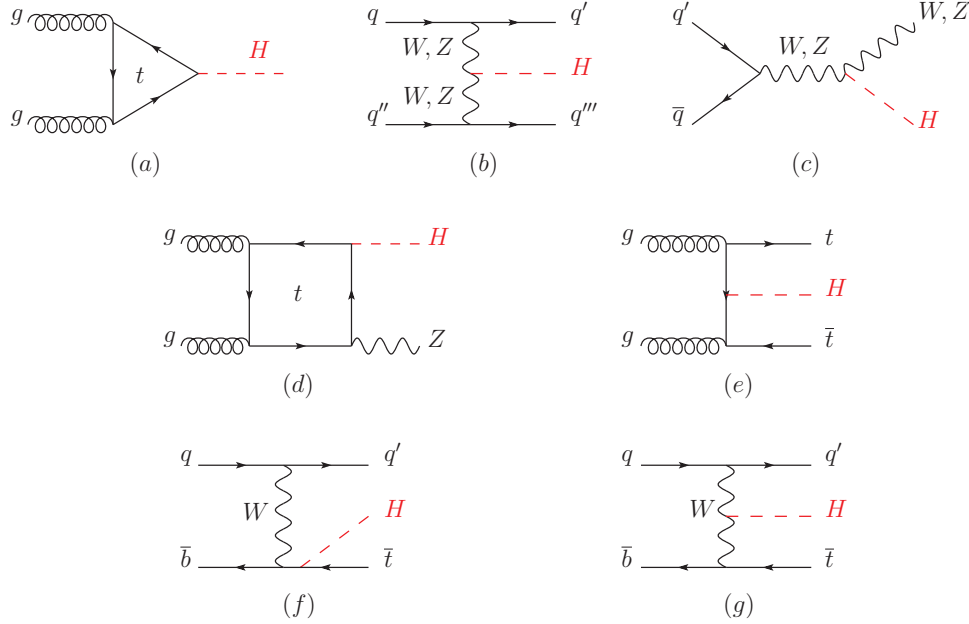


Figure 2.1: Feynman diagrams for the dominant Higgs production modes at the LHC: (a) gluon-gluon fusion, (b) vector boson fusion, (c) Higgs-strahlung (d) associated vector boson production, (e) associated production with $t\bar{t}$ pair, (f-g) interfering diagrams for single top quark associated production [23]

Deviations in the measured value of Higgs coupling strengths given in Equation 2.1 from the SM expectation can be parameterized as factors κ_F , κ_V , and κ_λ that modify the couplings to fermions, vector bosons, and the trilinear self coupling in the κ -framework [40]. By construction, any devia-

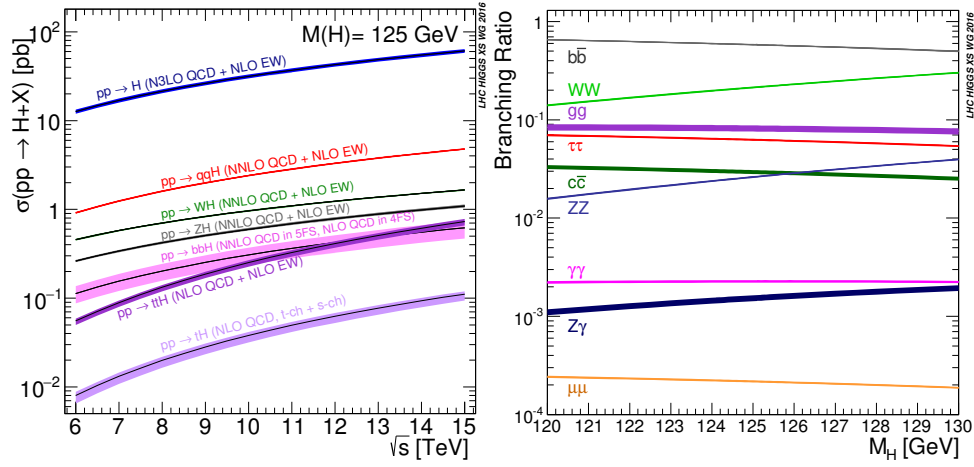


Figure 2.2: Higgs production cross sections at the LHC (left) and branching fractions as a function of m_h (right) [23]

tion from SM expectation is interpreted as non-SM Higgs couplings. Reduced coupling strength modifiers are defined for the fermions and vector bosons separately such that they are proportional to the particle's mass:

$$\tilde{y}_V \equiv \sqrt{\kappa_V} \frac{g_V}{2v} = \sqrt{\kappa_V} \frac{m_V}{v}, \quad \tilde{y}_F \equiv \kappa_F \frac{g_F}{\sqrt{2}} = \kappa_F \frac{m_F}{v} \quad (2.2)$$

This brings into focus the fundamental assumption that the Higgs field imbues mass to particles proportionally to their couplings to the Higgs boson. The measurements of these coupling strength modifiers by ATLAS and CMS are shown in Figure 2.3. The ATLAS measurement of κ_μ is derived from the measurement of $H \rightarrow \mu\mu$ production with 139 fb^{-1} [41].

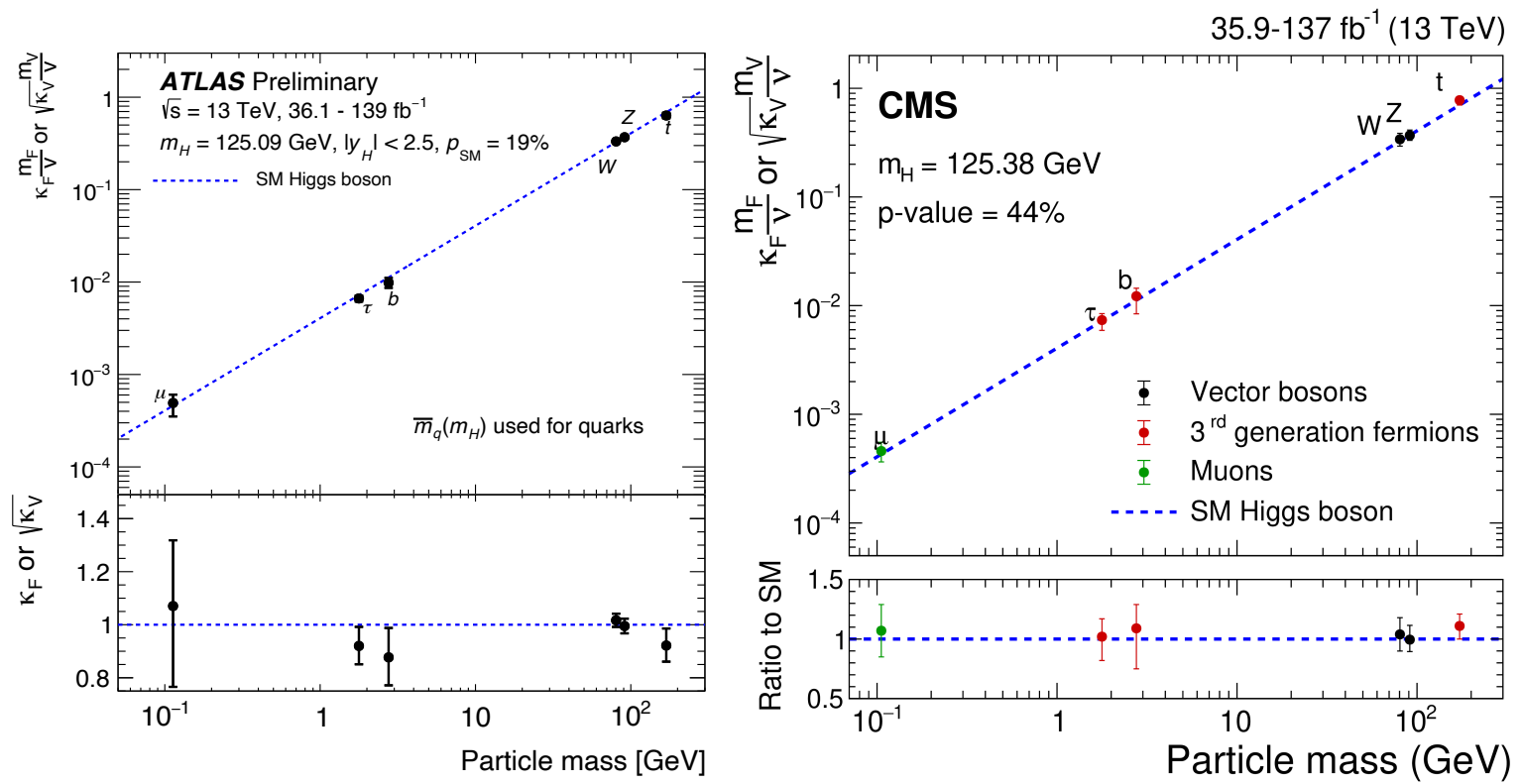


Figure 2.3: Summary of Higgs coupling measurements performed by the ATLAS and CMS experiments using partial or full Run II data [2, 3]

Measurements of Higgs couplings are generally in agreement with the SM. However, the coupling strengths of the Higgs boson to fermions is probed far less precisely than those of the weak vector bosons. Given that the mechanisms for fermions and vector bosons acquiring mass are qualitatively different, it is imperative to measure these quantities more precisely in order to test the mechanism of Yukawa mass. Various extensions of the SM may cause deviations in the apparent Yukawa couplings that could be hidden within these large uncertainties. Moreover, Yukawa couplings have only been measured at the discovery threshold to third-generation fermions (t, b, τ). The muon Yukawa coupling is the only Higgs coupling to second generation fermions that is experimentally accessible at the LHC, thanks to the high-quality reconstruction of muons achievable by both ATLAS and CMS, which compensates for the low rate from $\mathcal{BF}(H \rightarrow \mu\mu) \approx 0.2\%$. The charm quark Yukawa coupling is likely out of reach due to the low rates from $\mathcal{BF}(H \rightarrow c\bar{c}) \approx 3\%$ and the difficulty in efficiently tagging c -jets while rejecting b -jets and light quark jets. The resulting contamination of resonant $H \rightarrow b\bar{b}$ and $H \rightarrow gg$ backgrounds are particularly challenging backgrounds, with branching fractions of $\approx 58\%$ and $\approx 8\%$, respectively. It will be impossible to measure the Yukawa couplings to light quarks (u, d, s) due to their extremely low rates and inseparability from multi-jet backgrounds. While electrons can also be reconstructed with high precision, the rates are suppressed relative to muons by $m_e^2/m_\mu^2 \approx 1/40,000$ and are therefore inaccessible at the LHC.

It is important to discuss another interpretation framework for Higgs measurements before opening the discussion to specific model extensions of the SM. A more general approach to parameterizing non-SM effects than the κ -framework is through the SM effective field theory (SMEFT) formalism, where all possible gauge-invariant dimension 6 operators constructed from SM fields are added

to $\mathcal{L}_{\text{SM}}$:

$$\mathcal{L}_{\text{SMEFT}} = \mathcal{L}_{\text{SM}} + \sum \frac{c_i}{\Lambda^2} \mathcal{O}_i^{d=6} + \dots \quad (2.3)$$

These effective operators are in general non-renormalizable. The only dimension 5 operators are Majorana neutrino mass terms that violate lepton number and are generally not considered since the neutrino masses are too small to have observable effects at the LHC. The SMEFT formalism is growing in popularity due to its minimal assumption, which is simply that the energy scale of new physics Λ is sufficiently higher than the EW scale such that BSM fields integrate out to effective operators, akin to the 4-Fermi contact interaction. Deviations in data from SM expectation in inclusive and differential cross sections measurements across many signatures can then be interpreted in a single framework and provide complementary information. This is another appealing feature of the SMEFT. The SMEFT formalism is not particularly relevant for the interpretation of $t\bar{t}W$ production measurements, as will be seen in Chapter ??, but is relevant for Higgs production. The best limits on the Wilson coefficients c_i related to Higgs measurements performed by ATLAS are shown in Figure 2.4 with $\Lambda = 1$ TeV. Measurements are consistent with $c_i = 0$ for all considered operators.

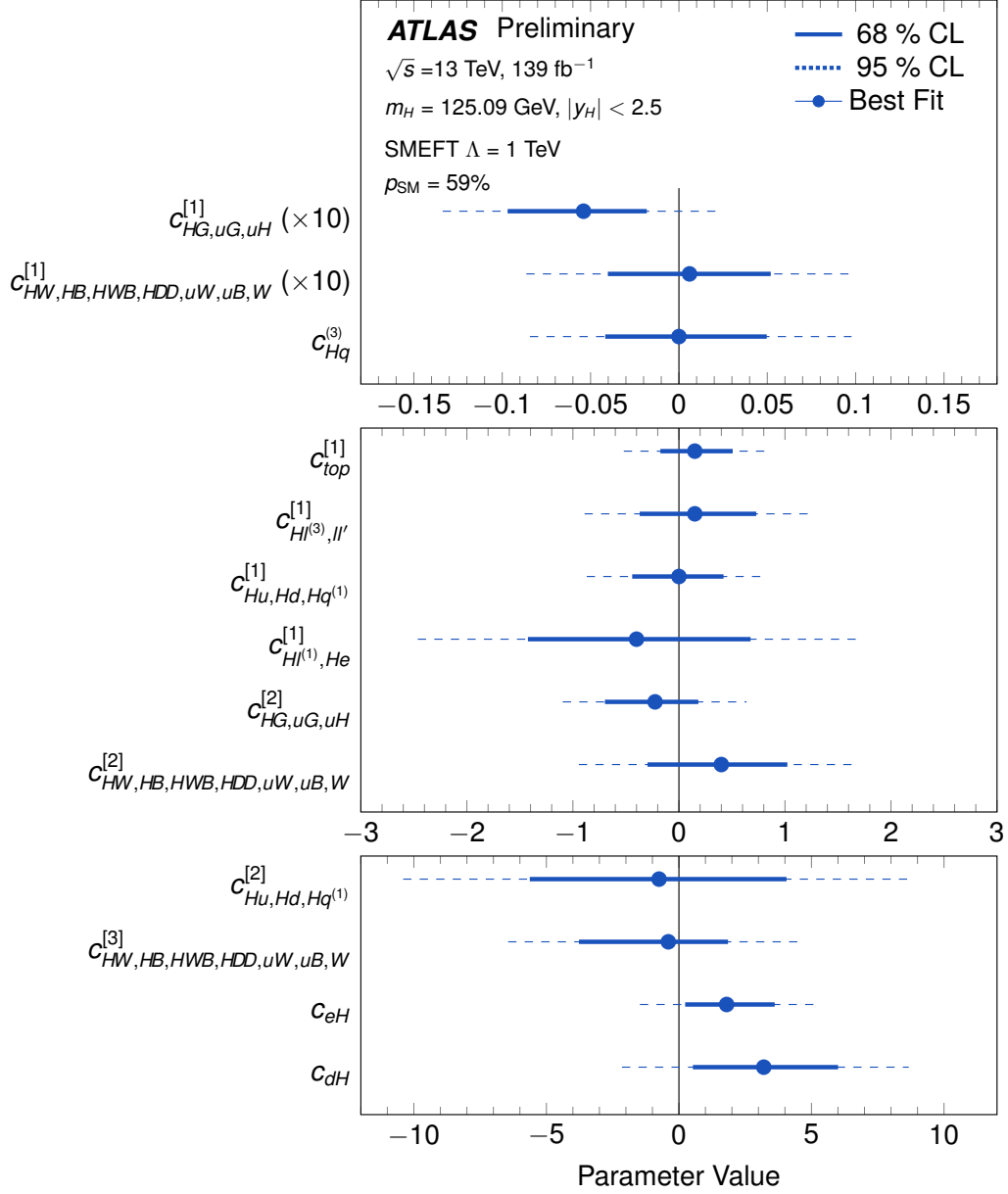


Figure 2.4: Observed measurements of SMEFT coefficients obtained from a combination of Higgs measurements performed by ATLAS [2]

2.2 EXTENDING THE HIGGS SECTOR

Interpretation paradigms like the κ -framework and the SMEFT are useful for parameterizing possible BSM effects across multiple measurements but are themselves not models of new physics.

Should generic frameworks reveal deviations from the SM expectation, follow-up measurements would be performed targeting extensions of the SM that predict those anomalous measurements.

Given that the Yukawa sector has not yet been probed precisely, we may expect to see evidence of new physics there through measurements favoring $\kappa_f \neq 1$. Extensions of the Higgs sector would be required to accommodate such a scenario and would offer new leads to follow in addressing the deficiencies of the SM.

Given that the Higgs is the only scalar boson of the SM, one may consider the following when developing model extensions of the SM Higgs sector:

1. Are there in fact no elementary scalars of the SM, and the boson h is actually a composite state i.e. a pseudo-Nambu-Goldstone boson of strong dynamics that deconfine at some high energy scale?
2. If there is one Higgs doublet in the SM, which is the minimum necessary to facilitate EWSB, is it possible that there are additional scalar fields in nature?

The first class of SM extensions are called Composite Higgs models which can feature a variety of symmetry breaking structures. Compositeness often requires the addition of new states that can mix with the Higgs and lead to modification factors to Higgs couplings to the EW vector bosons of $\left(1 - \frac{1}{2} \frac{v^2}{f^2}\right)$, where f is the symmetry breaking energy scale [42]. Such mechanisms can give a dynamical explanation for the small size of the Higgs mass, but model building finesse and tuning are required to avoid experimental limits on Higgs precision measurements and the non-observation of new states [43, 44]. The second possibility is considered in theories with additional Higgs doublets,

the simplest of which are referred to as Two Higgs Doublet Models (2HDM). Since 2HDM are simpler and less generic, they are used frequently as benchmark models against which to interpret Higgs measurements. The remainder of this section will cover the main features of the 2HDM and summarize experimental limits. For a comprehensive description of 2HDM phenomenology, see [45].

In general, 2HDM contain two doublets Φ_1 and Φ_2 with weak hypercharge ± 1 that can be parameterized as:

$$\Phi_i = \begin{pmatrix} w_i^+(x) \\ \frac{1}{\sqrt{2}} (v_i + h_i(x) + iz_i(x)) \end{pmatrix} \quad (2.4)$$

The Higgs potential in Equation 1.10 is straightforwardly extended to include both doublets, where mass mixing terms $\mu_{12}\Phi_1^T\Phi_2$ are allowed if the doublets have opposite hypercharge. In either case, both doublets may acquire VEVs $v_{1,2}$ with $|v|^2 \equiv |v_1|^2 + |v_2|^2$. A common parameterization relating the two VEVs is $\tan \beta = v_2/v_1$. Three of the eight available degrees of freedom from the two complex doublets are eaten by the EW vector bosons. What remains are two $\mathcal{CP}$ -even scalars h and the heavier H , a $\mathcal{CP}$ -odd pseudoscalar A , and two charged Higgs bosons $H^\pm$. An additional model parameter α is defined by the mixing angle that diagonalizes the mass matrix of the $\mathcal{CP}$ -even Higgs bosons obtained from the Φ_1 and Φ_2 doublets:

$$\begin{pmatrix} H \\ h \end{pmatrix} = \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \quad (2.5)$$

The alignment limit $\cos(\alpha - \beta) \sim 0$ defines the scenario where h couples to vector bosons like the SM Higgs boson. Small variations in y_f from SM expectation could be achieved in a scenario near but not exactly at the alignment limit. In order to avoid mediation of flavor-changing neutral

currents (FCNC) that have never been observed, the coupling structure of the doublets to fermions is specified in four scenarios (where Φ_2 is taken to couple to up-type quarks by convention):

Type	u, c, t	d, s, b	e, μ, τ
Type I	Φ_2	Φ_2	Φ_2
Type II	Φ_2	Φ_1	Φ_1
Type X (Lepton-specific)	Φ_2	Φ_2	Φ_1
Type Y (Flipped)	Φ_2	Φ_1	Φ_2

Note that Type II 2HDM is featured in the minimal Supersymmetric extension of the SM. Generic 2HDM and those with additional singlets can lead to experimentally discernible effects on the coupling structure of the Higgs [46]. Extensions of the 2HDM to so-called “flavorful” models posit the breaking of a flavor symmetry at the EW scale that leads to the generation of fermion mass hierarchies and the structure of the CKM matrix [47]. Experimental limits on generic 2HDM models generally favor the alignment limit, with weakening constraints to the alignment limit if $v_2 \gg v_1$. Exclusion limits at the 95% confidence level on the 2HDM parameter space obtained by ATLAS in a global fit to Higgs measurements are shown in Figure 2.5. The observed exclusion is generally similar to what would be expected under the SM-only hypothesis. The exception is in the 2HDM Type-I interpretation, where the exclusion contour is driven toward negative values of $\cos(\beta - \alpha)$ by $H \rightarrow \tau\tau$, $H \rightarrow b\bar{b}$, and $t\bar{t}H$ measurements driving the associated κ_f best fit values below unity, as seen in Figure 2.3. Since Φ_2 couples to all fermions in Type I 2HDM, it is more sensitive to coherent effects on fermions than other 2HDM scenarios.

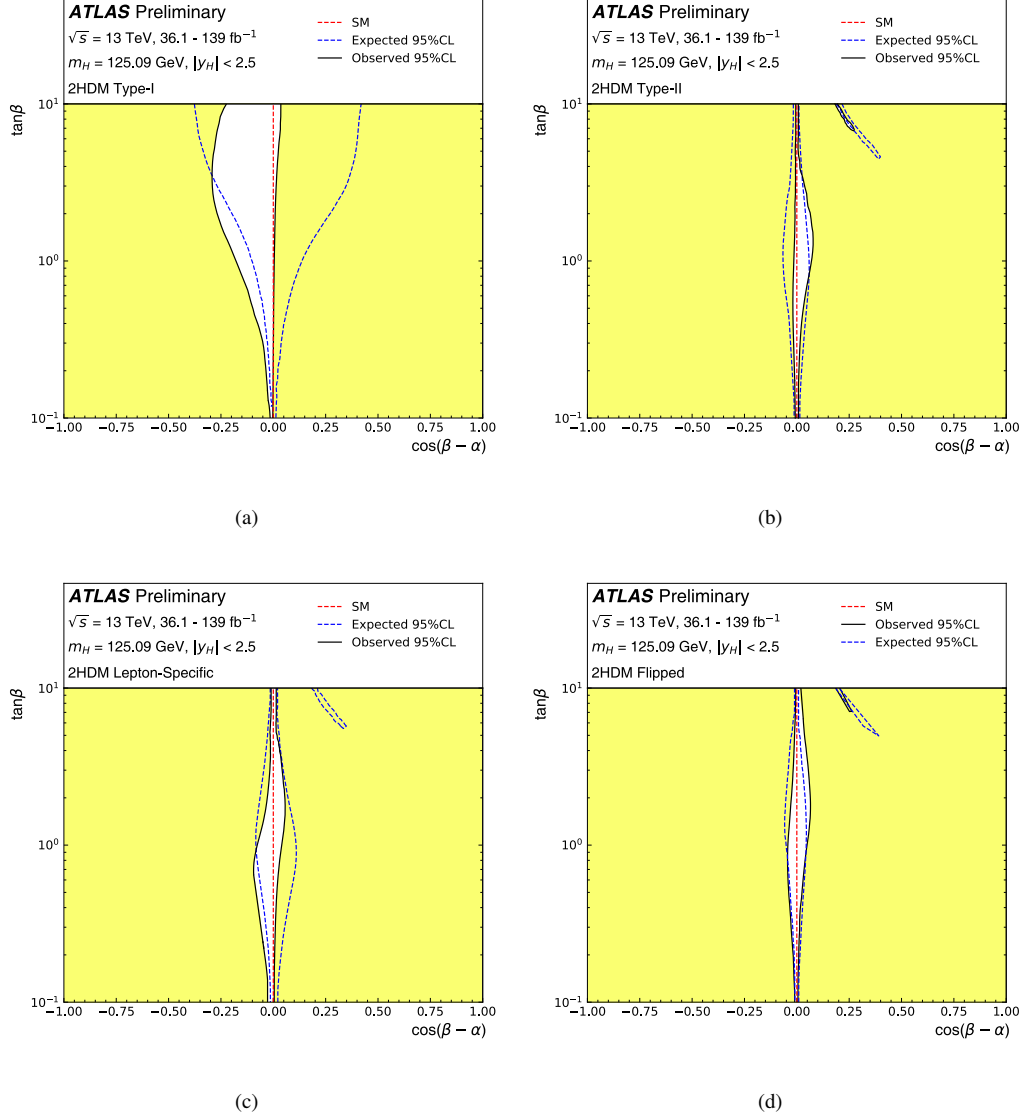


Figure 2.5: Exclusion contours at the 95% confidence level in the (α, β) phase space in the four 2HDM scenarios obtained by the ATLAS experiment [2].

2.3 MEASURING y_t IN MULTILEPTON FINAL STATES

While all Yukawa couplings can each be sensitive to a range of BSM scenarios, the Yukawa coupling of the top quark is the most consequential for the UV behavior of the Standard Model. This is due to y_t being uniquely of order unity among the SM fermions, resulting in top quark loop corrections to the Higgs mass and potential that dominate over other loop contributions. The Hierarchy problem mentioned earlier is the manifestation of these top quark loop corrections to the Higgs boson mass. These corrections also result in the destabilization of the Higgs potential at high energies, where the UV evolution causes a local minimum to occur at $V(v')$ where $v' \gg v$. It is even possible for this new local minimum to be a global minimum. In this case, the EW vacuum state is metastable and can quantum tunnel to the true vacuum state and lead to spontaneous decay of the vacuum itself. Such a scenario could radically redesign the mass hierarchy of particles within the SM and the resulting phenomenology, equating to a doomsday scenario for life in the universe. A more severe possibility is the instability of the EW vacuum if Higgs potential is unbounded from below. The stability phase diagram for the EW vacuum calculated to NNLO in the β -function of the parameter λ in $V(H)$ is shown in Figure 2.6. We evidently exist in a metastable universe given the mass of the top quark and Higgs boson. An analytical calculation for the lifetime of a false vacuum was first performed in 1977 [48, 49].

In addition to these phenomenological consequences of the largeness of y_t , the top quark is the only SM particle more massive than the Higgs boson. This is more than a curiosity of the top quark, though it is one that justifies interest in the relationship between the Higgs boson and the top quark. Since Higgs decays to $t\bar{t}$ is kinematically forbidden, there are only two ways to measure y_t . The first

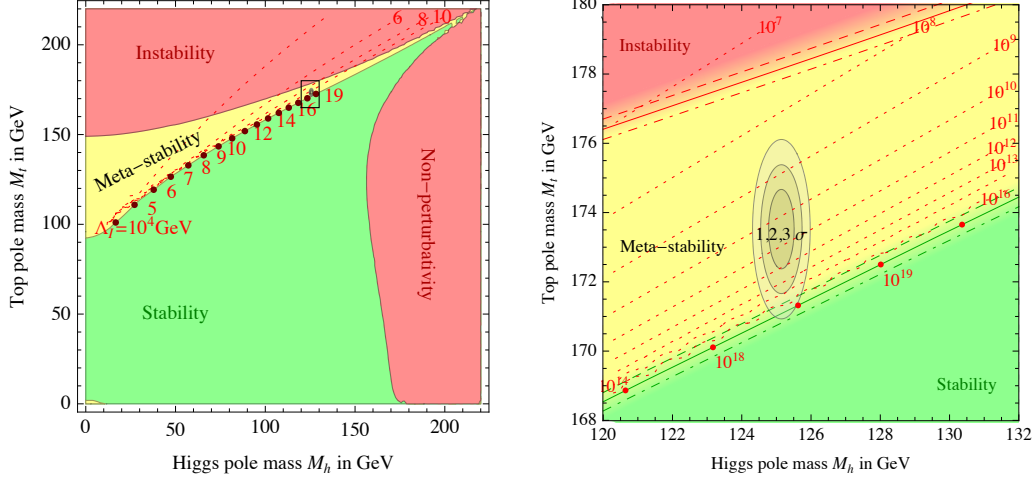


Figure 2.6: Phase diagram depicting stability regions of the EW vacuum with instability scale Λ_t shown along the stability boundary. Uncertainty bands of 1, 2, and 3 σ correspond to experimental uncertainties on m_h and m_t [4].

is indirectly through the top quark loop in gluon-gluon fusion production and $H \rightarrow \gamma\gamma$ decays, but the interpretation of y_t in this method is conditioned on the assumption that there are no BSM fields that enter into the loops. The only way to measure y_t at tree level is through the measurement of $t\bar{t}H$ and tH production cross sections. The former has a cross section of $\sigma(pp \rightarrow t\bar{t}H) \sim 530$ fb at 13 TeV computed at NLO in QCD, while inclusive tH production to equal precision has a cross section of ~ 75 fb [50]. For measurements of $|y_t|$, $t\bar{t}H$ production is unparalleled in sensitivity.

The simultaneous production of $t\bar{t}H$ was first reported at 5σ significance in 2018 through a combined measurement of Higgs decay channels by the ATLAS and CMS collaborations [51, 52]. Both collaborations analyzed events consistent with one of several Higgs decay modes:

- $H \rightarrow \gamma\gamma$. Though the branching fraction is low, photons are well reconstructed and identified. This channel achieves low systematic uncertainties through a data-driven background estimation. An analytical function is fit to data in the $m_{\gamma\gamma}$ sidebands and interpolated into the signal window around 125 GeV. The background estimation is subtracted from data

and the residual is fitted to a signal model. The measurement's total uncertainty is therefore driven by statistical uncertainties resulting from low production rates.

- $H \rightarrow \tau\tau$, $H \rightarrow WW^*$, and $H \rightarrow ZZ^* \rightarrow 4\ell$. Collectively referred to as multi-lepton final states, these channels boast higher branching fractions of Higgs decays and therefore lower statistical uncertainties than $H \rightarrow \gamma\gamma$. However, these channels suffer relatively larger systematic uncertainties due to the less cleanly reconstructed hadronic τ leptons, the incomplete visibility of the Higgs final state from the presence of neutrinos, and the reliance on simulation to model irreducible backgrounds from $t\bar{t}V$ and diboson production. As a result these channels are equally limited by statistical and systematic uncertainties.
- $H \rightarrow b\bar{b}$. The $b\bar{b}$ channel boasts the largest branching fraction of Higgs decays at about 58%. The dominant background comes from production of $t\bar{t}$ in association with additional heavy-flavor quarks through gluon emission and splitting, $g \rightarrow b\bar{b}/c\bar{c}$. Since these processes are driven by soft QCD, they are more sensitive to logarithmic resummation and come with large systematic uncertainties. As a result, the $H \rightarrow b\bar{b}$ channel is dominated by systematic uncertainties.

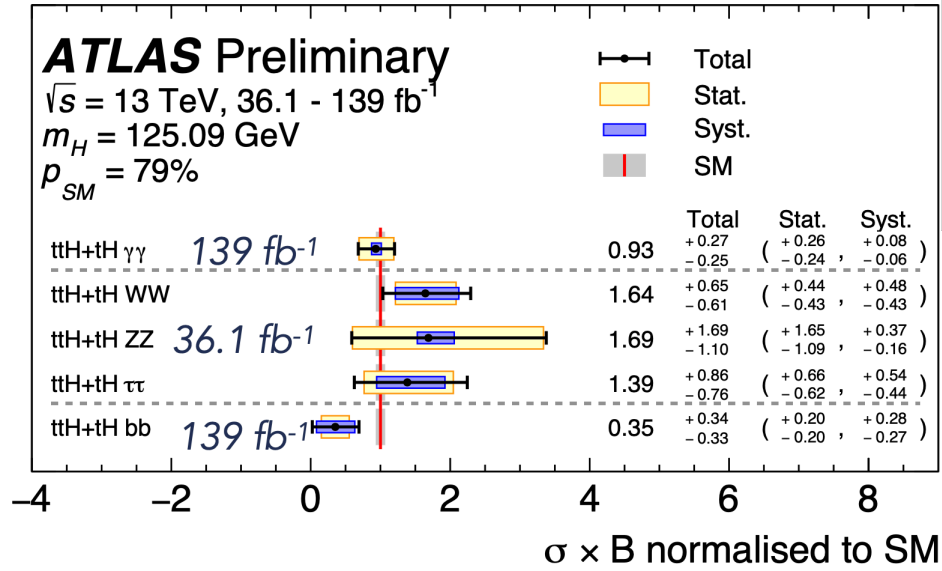


Figure 2.7: Summary of $t\bar{t}H$ measurements performed by ATLAS edited for brevity and clarity [2].

A summary of the latest published ATLAS measurements of $t\bar{t}H$ production is shown in Figure 2.7. Note that only the multi-lepton channels are lacking a measurement using the full Run II

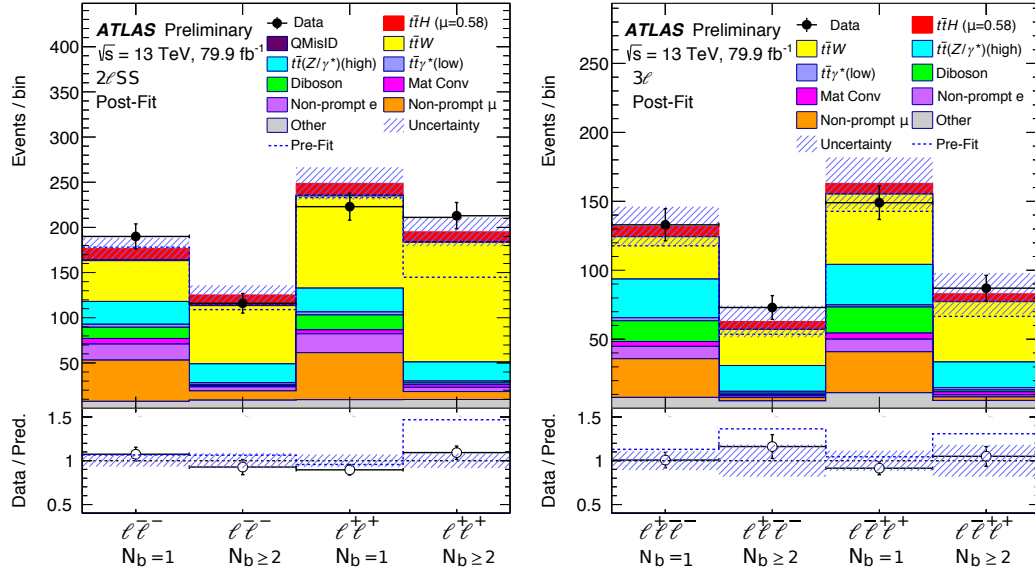


Figure 2.8: Prediction and observation in b -jet multiplicity bins for the two dominant channels of $t\bar{t}H$ multi-lepton production

dataset of 139 fb^{-1} . A preliminary measurement in the multi-lepton final state was performed using 80 fb^{-1} of data, which reported an observed (expected) $t\bar{t}H$ significance of 1.8σ (3.2σ) and a best-fit signal strength of $\hat{\mu}_{t\bar{t}H} = 0.70^{+0.26}_{-0.25}(\text{stat})^{+0.25}_{-0.22}(\text{syst})$ [53]. The analysis jointly measured the production of $t\bar{t}W$, the largest irreducible background in the multi-lepton final state. Normalization factors were applied to the $t\bar{t}W$ prediction in different regions of phase space and were pulled upwards by 20%-70%, the effect of which is shown in post-fit distributions of b -jet multiplicity in Figure 2.8. The impact of $t\bar{t}W$ -associated uncertainties is illustrated in Figure 2.9, which constitute roughly half of the nuisance parameters with the largest impact on $\mu_{t\bar{t}H}$. This $t\bar{t}W$ -like excess is consistent with previous measurements of inclusive $t\bar{t}W$ and $t\bar{t}Z$ production with 36.1 fb^{-1} of data separately by ATLAS and CMS [54, 55]. These and similar excesses observed in $t\bar{t}Z$ production are summarized in Figure 2.10.

It is clear that the precise measurement of $t\bar{t}W$ production through its entire phase space is nec-

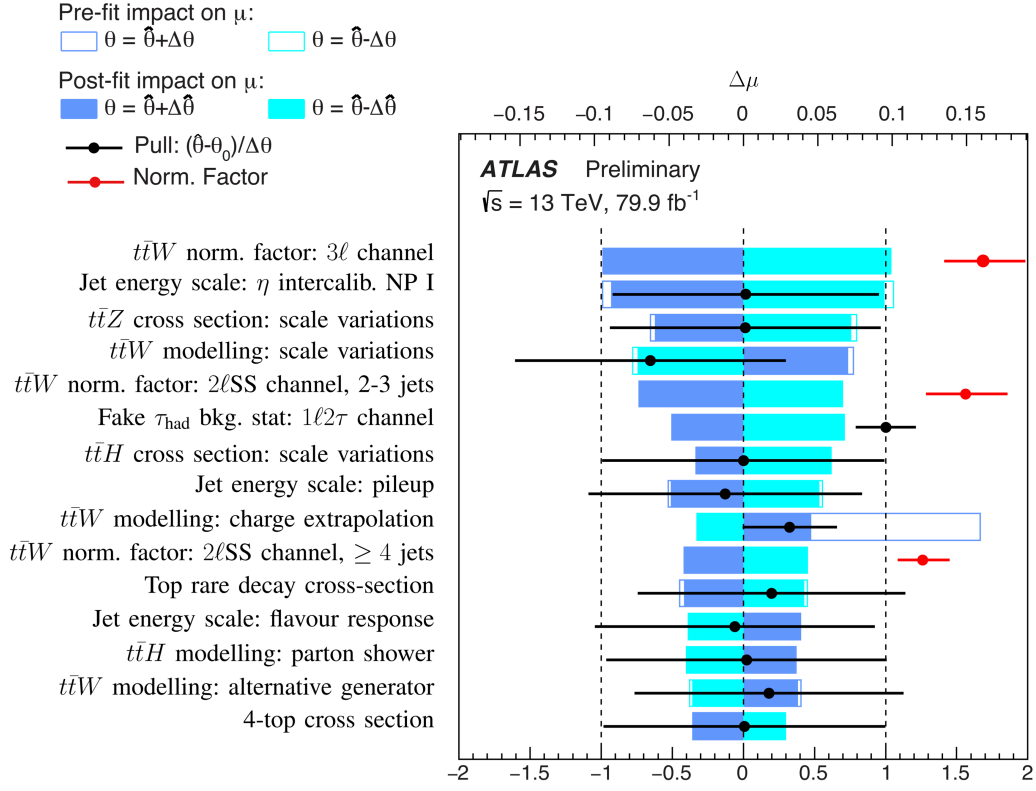


Figure 2.9: List of nuisance parameters with the largest post-fit impact on $\mu_{t\bar{t}H}$

essary before a new measurement of *t $\bar{t}$ H* production in multi-lepton final states can be performed.

This thesis will describe the inclusive and differential cross section measurement for *t $\bar{t}$ W* production using data collected by the ATLAS experiment during Run II of the LHC at $\sqrt{s} = 13 \text{ TeV}$.

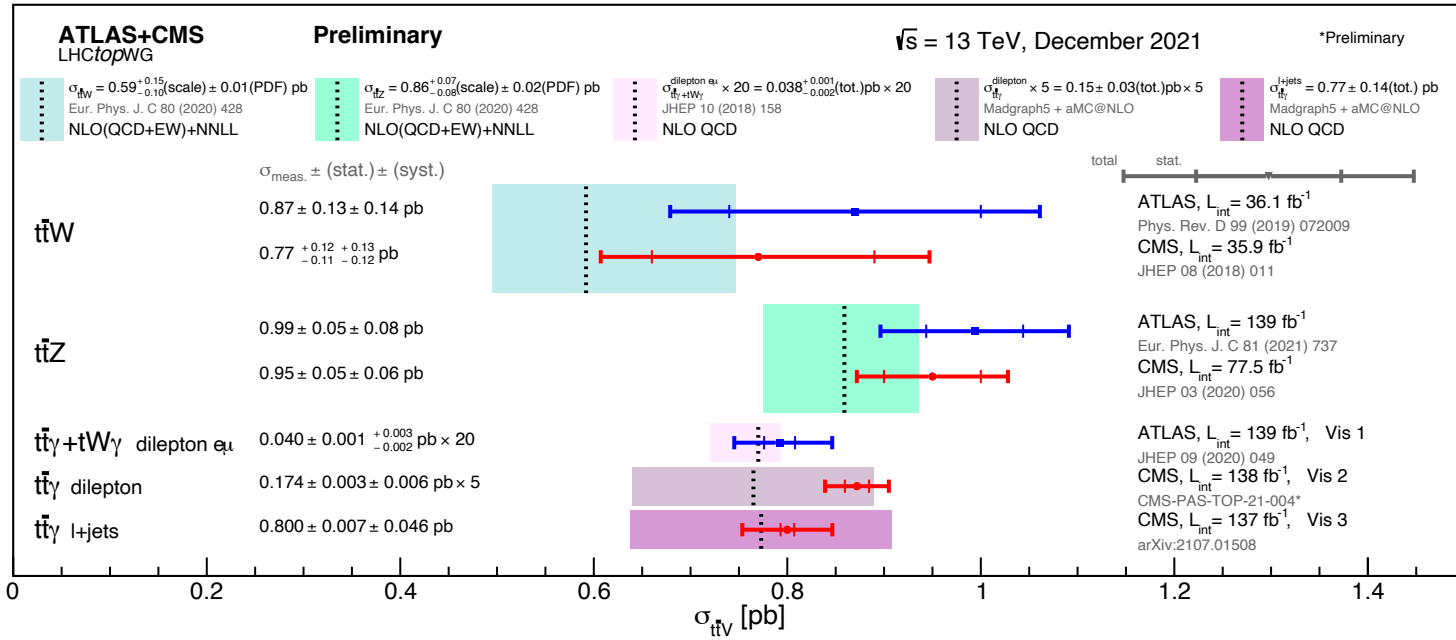


Figure 2.10: Summary plot of $t\bar{t} + V$ cross section measurements performed by ATLAS and CMS [5]

Part II

Experiment

3

The Large Hadron Collider

There is only one way to recreate the energy densities reached in the first moments after the big bang in a terrestrial experiment: high energy particle colliders. The options are further restricted to circular colliders if high luminosities are required, as particle beams can be continuously circulated to produce many interactions per beam fill. The choice of particle species to use for collisions is limited to particles that are a) electrically charged, allowing them to be accelerated and deflected by electric and magnetic fields and b) sufficiently long-lived such that a stable beam can be sustained. The list of such particles used to date is short: electrons, positrons, protons, anti-protons, and heavy

ions¹.

Heavy ions are a good choice for studying QCD dynamics in general and quark-gluon plasma in particular, while electrons and (anti-)protons are better suited for probing QCD and electroweak physics. Electron colliders (e^+e^-) have the advantage of colliding fundamental particles, so the center of mass energy of hard-scattering interactions can be finely controlled. They are better suited for precision measurements, particularly of the electroweak interaction since electrons do not feel the strong interaction. Circular electron colliders are limited in their energy due to high synchrotron radiation, making electron colliders ill-suited for searches in the highest accessible energy regimes. The LEP collider is the most notable circular electron collider from which many modern precision SM measurements have come [56]. (Anti-)protons are better suited for high energy circular colliders due to their larger masses and therefore negligible synchrotron radiation, but due to their composite nature, do not allow the energy of hard scattering between constituent partons to be controlled. Colliders producing $p\bar{p}$ interactions have the feature of higher $\sigma(q\bar{q})/\sigma(gg)$ relative to pp colliders, but suffer from the technical difficulty of producing anti-protons and therefore deliver lower luminosities; the most recent $p\bar{p}$ collider was the Tevatron at Fermilab, where the CDF and DØ experiments discovered the top quark in 1995 [57, 58].

Both LEP and Tevatron searched for the Higgs boson, yet neither achieved the requisite CoM energy and luminosity to reach the 3σ significance threshold for evidence, let alone 5σ for a discovery. During the 1990s, it was understood that a high energy pp collider was needed to either observe the Higgs boson or whatever new physics was guaranteed at the EW scale through the so-called *no lose theorem* [59]. The LEP tunnel was repurposed for a new pp collider and a new set of experiments

¹There is a growing interest in developing a muon collider, whose physics case motivates R&D to overcome the primary challenge of producing a stable beam of 2 microsecond lifetime particles

began development. This new collider was named the Large Hadron Collider (LHC) and the ATLAS and CMS experiments claimed the discovery of the Higgs boson in 2012 using pp collisions at $\sqrt{s} = 8$ TeV delivered by the LHC during its first data-taking period between 2010 and 2012 (Run I) [60, 61].

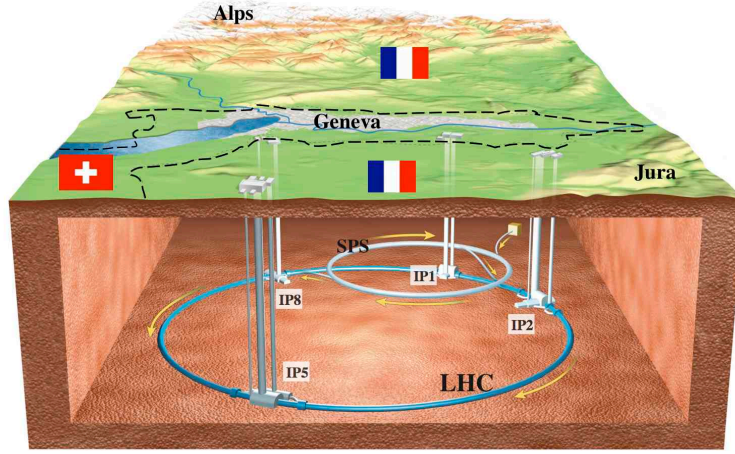


Figure 3.1: An aerial cutout of the LHC underneath the French-Swiss border facing south. The ATLAS and CMS experiments are located at IP1 and IP5, respectively.

About 17 miles (28 km) in circumference, the LHC is situated 100 meters underground and straddles the French-Swiss border around CERN in Geneva, Switzerland and is shown in Figure 3.1². The immense size of the LEP/LHC tunnel is required to maximize the achievable beam momentum and therefore center of mass energy for collisions, as $p_{max}^{beam} = erB$ where e is the fundamental charge, r is the bending radius, and B is the magnetic field strength. To reach beam momentum of 7 TeV, the LHC ring is composed of 1,232 15 meter long superconducting NbTi magnets that provide a bending field of 8.33 T to steer the beams in a circular arc. They are held below the superconducting critical temperature of 10 K using superfluid helium at 1.9 K. A cross section of the

²Figures and technical specifications for the LHC can be found in [62], where the most important aspects of the design have been restated here.

LHC DIPOLE : STANDARD CROSS-SECTION

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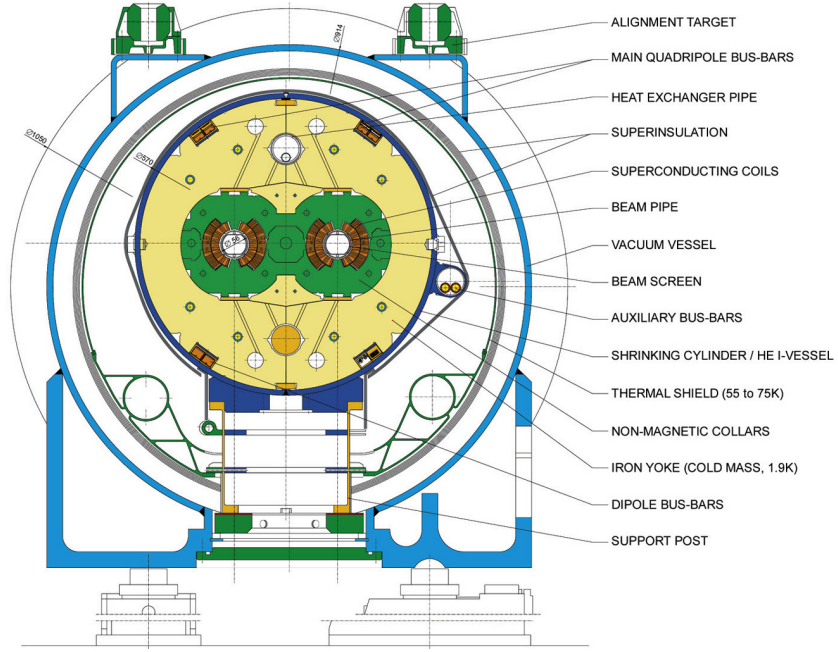


Figure 3.2: A cross section of the LHC dipole magnet cryostat

dipole magnet and its cryostat is shown in Figure 3.2.

The other key characteristic of a particle collider is its achievable instantaneous luminosity $\mathcal{L}$, measured in scattering interactions per unit area per unit time³. The luminosity of two colliding beams is given by

$$\mathcal{L} = \frac{N_1 N_2 n_b f}{A} \quad (3.1)$$

Where N_i are the number of particles in the beams, n_b is the number of particle bunches contained in each beam, f is the revolution frequency of the beams around the ring, and A is the effective beam overlap region. One very important way to increase luminosity is to minimize A , which re-

³The barn (abbreviated b) is typically used as the unit of area, which is equivalent to 10^{-24} cm^2 . One can also consider integrated luminosity, $\int \mathcal{L} dt$, which is a measure of the total luminosity delivered over time and is measured in b^{-1} .

quires strong focusing of the beams. This is achieved by local focusing of the beam by two superconducting quadrupole magnets on either side of a beam crossing point, while a total of 858 superconducting quadrupole magnets are situated around the ring to more loosely focus the beam within the accelerator aperture. Protons are guided longitudinally using radio frequency (RF) cavities with field frequency of 400 MHz. The protons settle into every 10th so-called bucket⁴, such that proton bunches are 7.55 cm long and separated by 25 ns, which fixes f to 40 MHz. The RF system is responsible for accelerating the beam from the Super Proton Synchrotron injection energy of 450 GeV to 7 TeV.

The number of collision events expected for a process with cross section σ and collision luminosity $\mathcal{L}$ is given by

$$N = \int \mathcal{L} dt \cdot \sigma \quad (3.2)$$

The cross section for a heavy resonance (e.g. Higgs boson production) increases with $\sqrt{s}$ in pp collisions. Since the number of produced Higgs bosons must be maximized to fulfill the physics goal of the LHC, it benefits from both high luminosity and $\sqrt{s}$. Table 3.1 shows a comparison of the design specifications for the LHC, as well as those for LEP2 and the Tevatron. From this, one sees that the LHC is the most energetic and luminous high-energy collider built by a wide margin⁵.

⁴Buckets are centered around rising edge of the RF field, such that protons in the back/front of the bucket are accelerated faster/slower, leading to synchrotron oscillation within bunches [63]

⁵The SuperKEKB e^+e^- collider achieved a new world record $2.22 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ on June 15 2020, surpassing the LHC. It collides electrons at $M_{\Upsilon(4S)} = 10.58 \text{ GeV}$, so can be disqualified from the comparison of high-energy colliders on a technicality.

Table 3.1: Design parameters of the LHC, LEP2, and Tevatron.

	LHC	LEP2	Tevatron
colliding beams of	p, p	e^+, e^-	$p, \bar{p}$
Momentum at collisions, TeV/c	7	0.1	0.98
Peak luminosity, $\text{cm}^{-1}\text{s}^{-2}$	10^{34} (design)	10^{32}	4.3×10^{32}
Dipole field at top energy, Tesla	8.33	0.11	4.4
Number of bunches, each beam	2808	4	36
Total beam current / beam, A	0.58	0.003	0.08
Particles / bunch, 10^{11}	1.15	4.2	2.9, 0.8
Typical beam size in the ring, μm	200 – 300	1800/140 (H/V)	500
Beam size at IP, μm	16	200 / 3 (H/V)	24
Fraction of energy lost in synchr.rad. per turn	10^{-9}	3%	10^{-11}
Total power radiated in synchr.rad., MW	0.0078	18	10^{-6}
Total energy stored in each beam, Megajoule	362	0.03	0.9
Total energy stored in the magnet system, Gigajoule	10	0.016	0.74

4

The ATLAS Detector

The LHC circulates proton bunch trains in either direction along its ring and are brought into collision at four points. Around each one of these interaction points is a particle detector that captures the products of these collisions. Each detector is comprised of several subsystems designed to perform measurements of momentum, energy, and particle identification. Not all inelastic pp collisions are worthy of the hefty computing power required to thoroughly analyze. Hardware and software-based triggering algorithms are employed to quickly decide if a given collision event is worth routing into an event reconstruction algorithm. From the raw data of channel hits processes by front-end

electronics, reconstruction algorithms determine which particles were produced along with all their trajectories as they flew away from the pp collision point. Particle trajectories can be extrapolated back towards the beampipe to infer what short-range physical processes occurred during the collision. Indeed, the lifetime of the Higgs boson is so short that it will travel a mere 100 fm before its virtually instant decay, ensuring the only way to study the Higgs is through its decay products.

Each of the four large LHC experiments (ATLAS, CMS, LHCb, and ALICE) operate in this way. LHCb is optimized to study physics of the b quark and ALICE is optimized to study heavy ion collisions. Meanwhile, ATLAS and CMS are the two all-purpose experiments which are capable of measuring and searching for a variety of signatures. While following the same general design principles, the two differ in their specific design choices and associated performance optimization. They therefore complement each other and allow for the robust discovery of new physics if observed similarly in both experiments. A description of the physics requirements that drive the features of general purpose detectors at hadron colliders and the differences between ATLAS and CMS are provided in [64].

An overview of the ATLAS detector and its subsystems are shown in Figure 4.1. It is 25 meters tall, 46 meters long, and weighs about 7,000 tons. Let it be impressed on the reader that this machine is nearly as tall as an 8-story building and as long as the width of an American football field. Despite having a mass commensurate with that of the Eiffel tower, the ATLAS detector's engineering and alignment is precise down to width of a human hair. It is a delicate beast of a machine and a marvel of modern scientific achievement¹.

¹It's not all that modern actually, much of the technology currently used in the ATLAS detector was around in 1995 when the experiment was being designed. It is upgraded every few years to keep up with the capabilities of new technology.

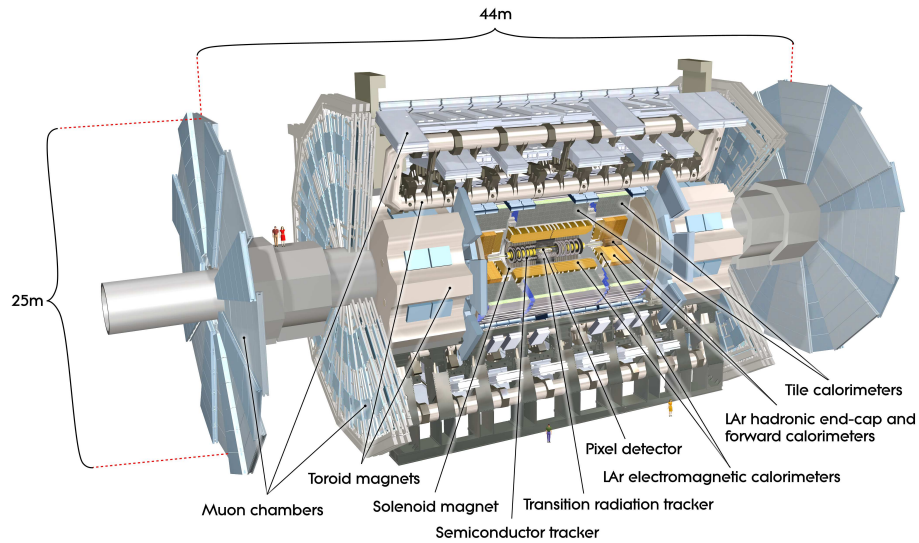


Figure 4.1: An overview of the ATLAS detector labeled by its various subsystems. A portion of the LHC beam enclosure is shown exiting the lefthand side of the largest forward muon chambers.

This chapter will outline the technical specifications of the subsystems of the ATLAS experiment. The nominal performance and coverage of each system is given in Table 4.1. Section 4.1 describes the ATLAS coordinate system used for reconstruction and analysis. Section 4.2 describes the inner tracking detector, which provides charged particle momentum reconstruction closest to the LHC beamline. Section 4.3 describes the Electromagnetic and Hadronic calorimeters, which measure the energy of electrons, photons, and hadrons. Section 4.4 will describes the Muon Spectrometer, which provides a secondary measurement of muons. Finally, Section 4.5 describes the magnet system of ATLAS, which provides the magnetic field that is essential for the measurement of charged particle momenta. The following sections reference the ATLAS overview manuscript and its Technical Design Report (TDR) [65, 66, 67].

Table 4.1: A summary of the nominal performance of each of the ATLAS subsystems.

Detector component	Required resolution	η coverage	
		Measurement	Trigger
Tracking	$\sigma_{p_T}/p_T = 0.05\% p_T \oplus 1\%$	± 2.5	
EM calorimetry	$\sigma_E/E = 10\%/\sqrt{E} \oplus 0.7\%$	± 3.2	± 2.5
Hadronic calorimetry (jets)			
barrel and end-cap	$\sigma_E/E = 50\%/\sqrt{E} \oplus 3\%$	± 3.2	± 3.2
forward	$\sigma_E/E = 100\%/\sqrt{E} \oplus 10\%$	$3.1 < \eta < 4.9$	$3.1 < \eta < 4.9$
Muon spectrometer	$\sigma_{p_T}/p_T = 10\%$ at $p_T = 1$ TeV	± 2.7	± 2.4

4.1 THE ATLAS COORDINATE SYSTEM

The coordinate system used by the ATLAS experiment is driven by the physics of pp collisions. The rectangular coordinates of the ATLAS detector are as follows: the positive x -axis points from the center of the detector towards the center of the LHC ring, the positive y -axis points vertically upwards from the center of the detector, and the z -axis is parallel to the LHC beamline to form a right-handed coordinate system. However, curvilinear coordinates are more frequently used. The azimuthal angle ϕ runs from $[-\pi, \pi]$ around the z -axis, with $\phi = 0$ aligning with the x -axis. The polar angle θ runs from $[0, \pi]$ with $\theta = 0$ aligning with the z -axis. Due to the physics of pp collisions, it is more useful to consider pseudorapidity η instead of θ , and it is defined as:

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

In the relativistic limit, this spacial coordinate is identical to rapidity y defined for both massive and massless particles:

$$y = \frac{1}{2} \ln \frac{E + p_z}{E - p_z}$$

The angular separation of reconstructed objects is defined as $\Delta R \equiv \sqrt{\Delta\phi^2 + \Delta\eta^2}$, which is invariant under Lorentz boosts along the z -axis for massless particles. *Parton Distribution Functions* (PDF) of the proton prevent the initial p_z of the hard scattering interaction between partons to be controlled, so energy and momentum are often considered in the plane transverse to the beam-line. Such variables include transverse momentum p_T and transverse energy E_T . Since the total p_T of the initial state is constrained to zero, the total transverse momentum can be added vectorially to define E_T^{miss} , which typically captures neutrinos that escape the detector undetected. The ATLAS coordinate system is shown graphically in Figure 4.2. In addition to these detector coordinates, trajectories of reconstructed particles is parameterized in terms of perigee parameters z_0 and d_0 , the distance of closest approach of a particle trajectory to the interaction point along the beam axis and in the transverse plane.

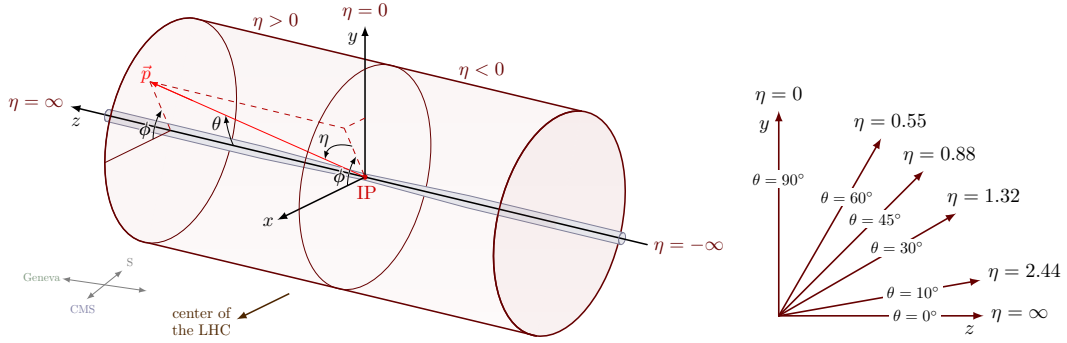


Figure 4.2: The ATLAS coordinate system (left) and select values of η and θ (right). Graphics based on [6]

4.2 THE INNER DETECTOR

This section will briefly describe the design of the inner tracking detector (ID) and will draw on the ID TDR [68, 69] and dedicated TDR for the Insertable B-layer (IBL) [70, 71]. A cutout of the ID and its mechanical design parameters are given in Figure 4.3 and Table 4.2. The goal of the ID is to

provide position measurements of charged particles as they are deflected in a strong magnetic field, allowing their momenta and trajectories to be reconstructed. This magnetic field is uniformly 2 T throughout the ID volume and is produced by a superconducting solenoid. The tracker is required to be as light as possible to minimize the degradation of calorimeter energy resolution resulting from energy loss in the ID active and support material. This has motivated the use of carbon fiber in support structure since it is strong and light. Overall tracking coverage extends to $|\eta| < 2.5$ and is composed of 3 subsystems: the inner silicon pixel tracker, the semiconductor tracker (SCT) based on silicon microstrips, and the transition radiation tracker (TRT).

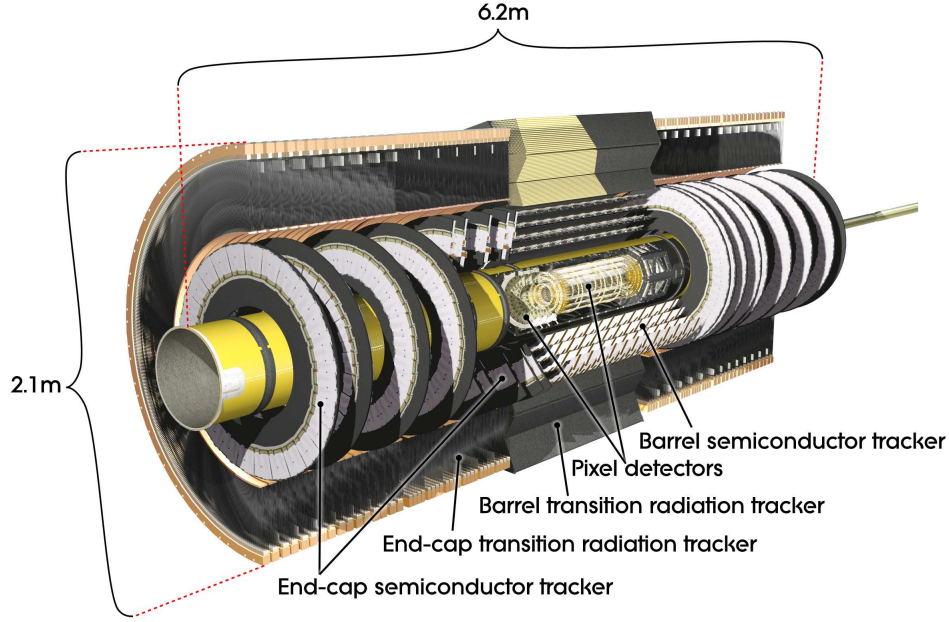


Figure 4.3: An overview of the ATLAS inner tracking detector. Note the silicon pixel, silicon strip, and transition radiation tracker subsystems

The innermost tracking layers utilize 2D channel segmentation (i.e. pixels) in order to maximize vertex reconstruction performance for primary vertex identification and suppression of pileup tracks. Secondary vertex reconstruction provided by the pixel tracker is key for tagging τ -lepton and

Table 4.2: Design parameters of the inner detector (except for the IBL).

Item		Radial extension (mm)	Length (mm)
Overall ID envelope		$0 < R < 1150$	$0 < z < 3512$
Beam-pipe		$29 < R < 36$	
Pixel	Overall envelope	$45.5 < R < 242$	$0 < z < 3092$
3 cylindrical layers	Sensitive barrel	$50.5 < R < 122.5$	$0 < z < 400.5$
2×3 disks	Sensitive end-cap	$88.8 < R < 149.6$	$495 < z < 650$
SCT	Overall envelope	$255 < R < 549$ (barrel)	$0 < z < 805$
		$251 < R < 610$ (end-cap)	$810 < z < 2797$
4 cylindrical layers	Sensitive barrel	$299 < R < 514$	$0 < z < 749$
2×9 disks	Sensitive end-cap	$275 < R < 560$	$839 < z < 2735$
TRT	Overall envelope	$554 < R < 1082$ (barrel)	$0 < z < 780$
		$617 < R < 1106$ (end-cap)	$827 < z < 2744$
73 straw planes	Sensitive barrel	$563 < R < 1066$	$0 < z < 712$
160 straw planes	Sensitive end-cap	$644 < R < 1004$	$848 < z < 2710$

B -hadron decays. Pixel segmentation is also needed to handle the high track densities typical at radii closest to the beamline. Pixel sensors in both the barrel and endcap sectors are $400 \mu\text{m}$ in z and $50 \mu\text{m}$ in azimuth. There are a total of 3 barrel layers and 3 disk layers in the endcaps, yielding 80.4 million readout channels in the pixel detector. An additional pixel layer called the IBL² and new smaller radius beampipe were installed during the first long shutdown of the LHC in 2013-2014.

The SCT layers are installed at radii beyond the pixel layers where track densities are lower. Strips in the barrel region extend nearly the full length of the sensor (6.4 cm) and have a strip pitch of $80 \mu\text{m}$. The barrel features 4 layers of silicon strip sensors oriented at a stereo angle of 40 mrad , with one sensor in each layer having strips oriented parallel to the beam axis. This improves the space-point resolution in each layer along the z axis to $580 \mu\text{m}$, while the resolution in the precision plane (azimuth) is $17 \mu\text{m}$. The end-cap features 9 layers with the same dual-sensor stereo angle design and provide similar space point resolution.

²The B-Layer name is due to its role in improving the identification of B -mesons produced in jets.

Continuous tracking at the largest radii is provided by the TRT. The TRT features 370,000 cylindrical drift tubes, each 4 mm in diameter and supporting a $31\ \mu\text{m}$ diameter gold-plated tungsten sense wire down the central axis. These tubes are referred to as straws and are filled with a gaseous mixture of 70% Xe to absorb x-rays from transition radiation, 27% CO_2 to increase electron drift velocity, and 3% O_2 to for photon quenching. Maximum electron drift time is approximately 50 ns during typical operation. The straws are oriented parallel to the beamline in the barrel and radially in the endcaps. An average of 36 hits per track are provided by the TRT. The space between straws is filled with polymer fibers (foils) in the barrel (endcap) sectors, which creates inhomogeneous material boundaries that results in the production of transition radiation by relativistic charged particles. This is typically in the soft x-ray spectrum, which can be absorbed by the Xe to produce an identifiable signal in the straws. Since transition radiation intensity depends on $\gamma = E/m$, the TRT is able to provide particle identification, particularly between $e^\pm/\pi^\pm$.

The design of the tracking detector is one of the most consequential ways in which ATLAS and CMS differ. CMS uses silicon pixel and strips to instrument the entire tracking volume, whereas ATLAS also features a continuous tracker with particle identification capabilities. CMS uses a single solenoid to provide bending in its entire volume. As a result, CMS is able to produce bending field strengths twice that of ATLAS in the tracker, giving it the edge in charged particle momentum resolution.

4.3 ELECTROMAGNETIC AND HADRONIC CALORIMETERS

This section will summarize the design of the electromagnetic and hadronic calorimeters. The comprehensive TDR for both sectors of the calorimeter and their expected physics performance can

be found in [72, 73, 74]. The purpose of the calorimeters is to destructively measure the energy of electrons, photons, and hadrons. All particles except for neutrinos and muons are absorbed within the calorimeters. The physics of electromagnetic and hadronic showers is quite different and motivates the selection of different technologies optimized to measure each (though it is not possible to strictly measure them separately).

Energy deposition of electrons and photons proceeds via bremsstrahlung and pair production to form electromagnetic (EM) showers. EM showers have a predictable shape, with 90% energy containment inside the Molière radius $R_M = 0.0265X_0(Z + 1.2)$, where X_0 and Z are the radiation length and atomic number of the material. Shower shape is then driven purely by material properties. The regularity of EM shower shape is due to the low threshold energy for pair production $E_\gamma^{threshold} = 2m_e \sim 1 \text{ MeV}$, resulting in high interaction multiplicities in EM shower evolutions. The low inherent randomness is encapsulated by the stochastic term in the energy resolution of the ATLAS EM calorimeter in Table 4.1. The radiation length X_0 characterizes both electron and photon energy loss and therefore sets the typical length scale of EM showers. Since bremsstrahlung and pair production proceed through the virtual exchange of a photon with a nucleus of charge Ze and the radiation length is inversely proportional to the interaction cross section, the rough dependence is given by $X_0 \propto 1/Z^2$. An EM calorimeter of depth $20X_0$ is typical.

Energy deposition of neutral and charged hadrons proceeds through inelastic nuclear interactions mediated by the strong force and result in hadronic showers. The length scale that describes the shower shapes is the nuclear interaction length λ_0 of a material and is typically larger than X_0 for the same material. This favors the general practice of constructing the hadronic calorimeter around the EM calorimeter. Since nuclear scattering is mediated by the exchange of massive pions,

its range is approximately given by $1/m_\pi \approx 1 \text{ fm}$, and thus direct collisions between an impinging hadron and nucleon are required. This results in a rough inverse dependence of the interaction length on material density: $\lambda_0 \propto 1/\rho \sim 1/Z$. The threshold energy for producing pions through inelastic nuclear collisions is then $E^{threshold} = 2m_\pi = 280 \text{ MeV}$. As a result, the number of interactions in a hadronic shower is small resulting in highly irregular shower shapes and a large stochastic term in the energy resolution as shown in Table 4.1.

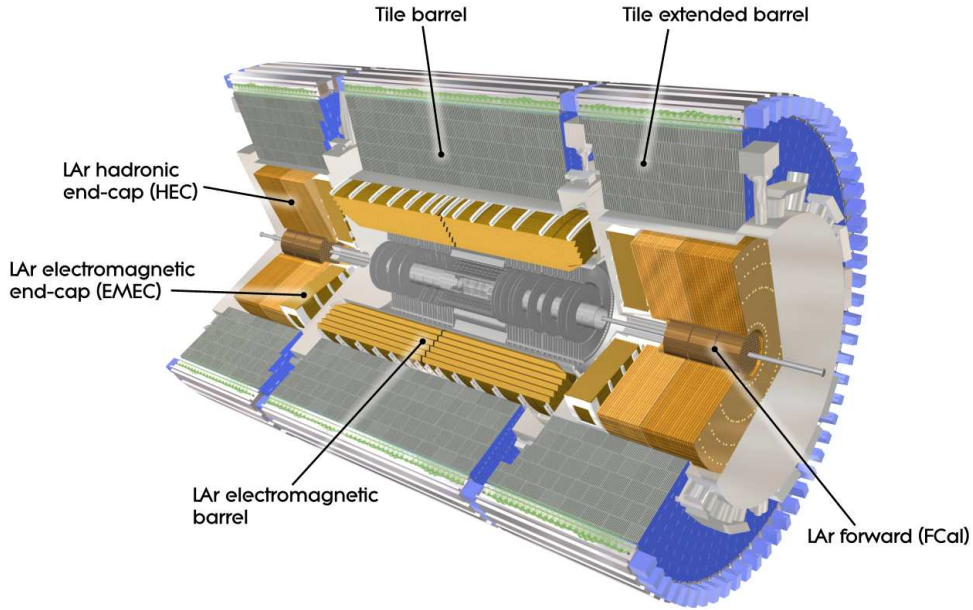


Figure 4.4: An overview of the ATLAS electromagnetic and hadronic calorimeters. Note the LAr barrel EMCal, barrel Tile HCal, and combined LAr forward calorimeter. The calorimeter surrounds the inner tracker and solenoid, which is darkened.

A cutout of the ATLAS calorimeters is shown in Figure 4.4. The barrel EM calorimeter uses alternating layers of liquid argon (LAr) with kapton electrodes and lead absorbers in an accordion geometry as shown in Figure 4.5. The use of lead for absorption maximizes the depth of the EM calorimeter in a fixed volume, providing $> 22X_0$ in the barrel ($|\eta| < 1.475$) and $> 24X_0$ in the

endcaps ($1.375 < |\eta| < 3.2$). The accordion geometry provides full coverage without azimuthal gaps. A presampling layer is instrumented in $|\eta| < 1.8$ for electron and photon energy correction and to provide identification of collimated $\pi^0 \rightarrow \gamma\gamma$ decays.

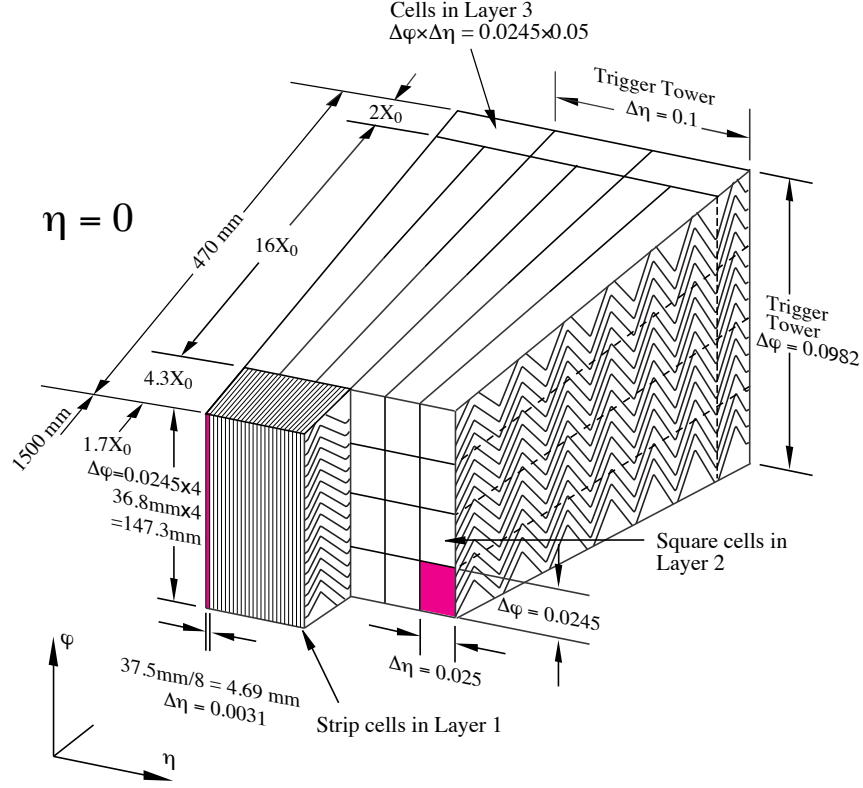


Figure 4.5: A diagram of an EM calorimeter tower with distinct accordion geometry

Outside of the EM calorimeter is the hadronic tile sampling calorimeter (TileCal) consisting of steel absorbers and plastic scintillating tiles as the active material. The barrel region covers the range $|\eta| < 1.0$ and the two extended barrel detectors cover $0.8 < |\eta| < 1.7$. The TileCal is segmented radially into 3 layers and scintillation light is collected via wavelength-shifting plastic fibers to photomultiplier tubes. A schematic of a TileCal section is shown in Figure 4.6.

The Hadronic Endcap Calorimeter (HEC) provides calorimetry in the range $1.5 < |\eta| < 3.2$ to

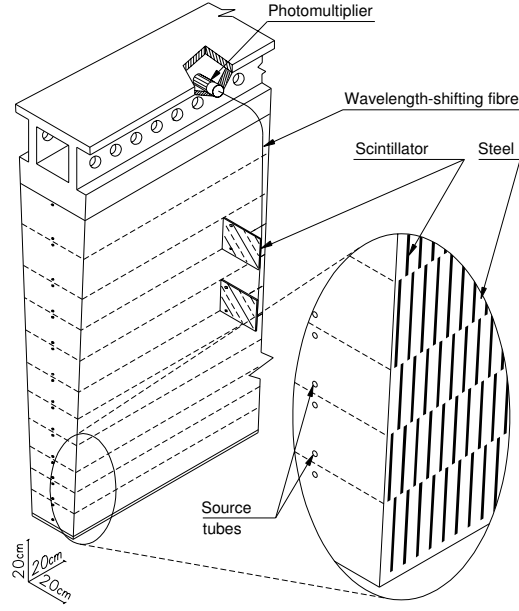


Figure 4.6: A schematic of a tile calorimeter section

ensure hermetic coverage between the most forward region of the TileCal and for forward calorimeters (FCal). The HEC is composed of wheels of copper plates alternating with active LAr. The copper layers closest to the interaction point are 25 mm thick, while plates further down the beamline are 50 mm thick. LAr active layers are uniformly 8.5 mm. Forward EM and hadronic calorimetry is provided jointly by the FCal in the region $3.1 < |\eta| < 4.9$. It is situated further away from the beamspot to reduce the high levels of radiation present close to the beamline. Due to this and the fixed constraint of the endcap cryostat, the FCal is required to be very dense to retain similar forward hadronic shower containment similar to that of the barrel. Each endcap is composed of 3 modules. The innermost layer is optimized for EM shower measurements and is made of copper, while tungsten is chosen in the remaining two layers targeting hadronic shower measurements. Figure 4.7 shows the layout of the HEC layers and recessed FCal position within 50 cm radius of the

beamline.

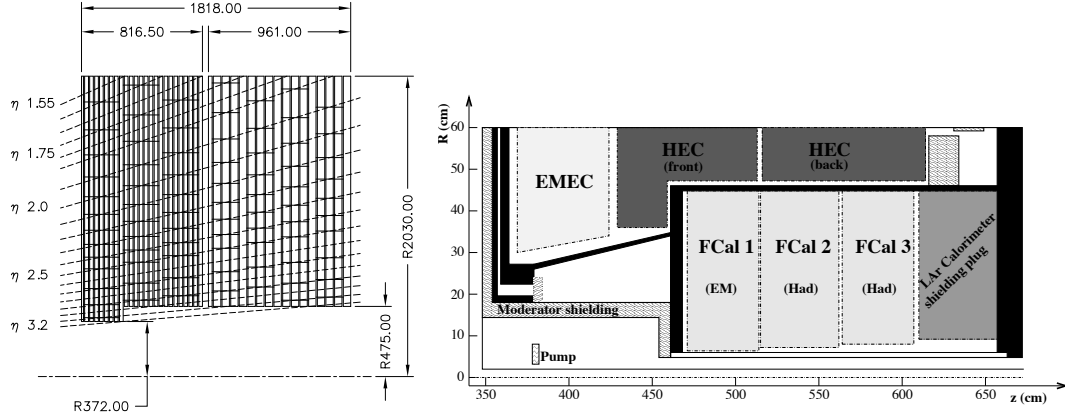


Figure 4.7: A sketch of the HEC layers (left) and positions of the 3 FCal modules (right)

4.4 THE MUON SPECTROMETER

This section will briefly describe the design of the Muon Spectrometer (MS). The comprehensive TDR for the MS can be found in [75]. A cutout of the MS is shown in Figure 4.8. As one eventually learns in the course of their work on the experiment, ATLAS is actually an acronym (or perhaps more accurately called a backronym) for A Toroidal LHC ApparatuS. The full name of the experiment, while less impressive than its abbreviated form, reveals the experiment's namesake: the toroidal geometry of the magnetic field of the Muon Spectrometer (MS). This is an important feature of the ATLAS detector and distinguishes it in design from the Compact Muon Solenoid (CMS). While the ATLAS MS field geometry features closed field lines, CMS has large volumes of iron between their MS active layers to return the solenoidal field, significantly degrading the resolution of muons reconstructed by its MS.

The MS is instrumented in 3 layers (stations) with precision tracking chambers as well as fast re-

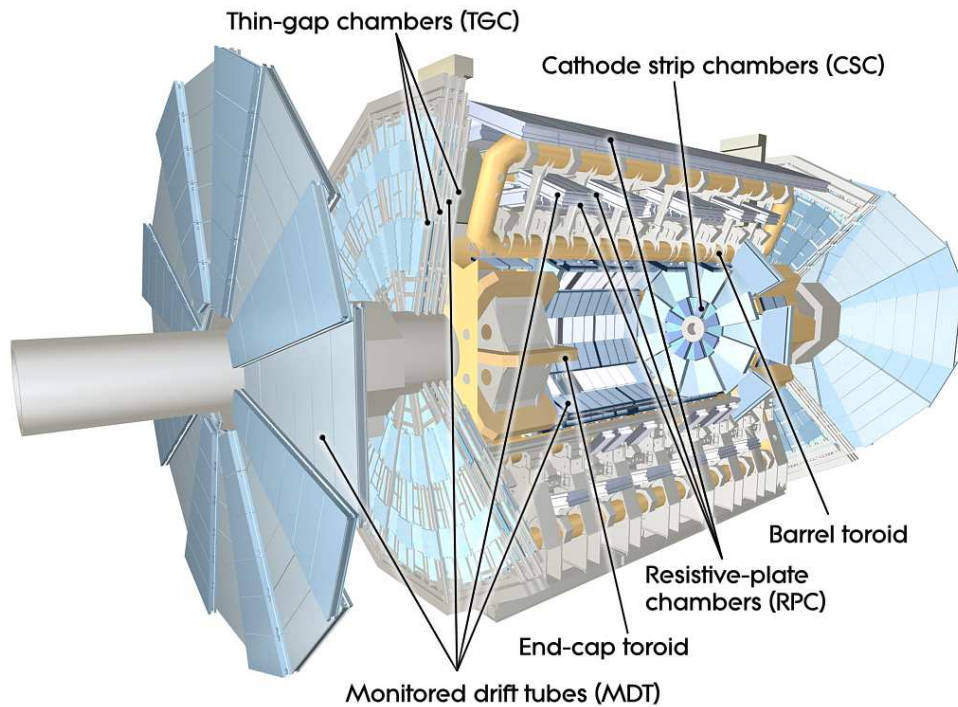


Figure 4.8: An overview of the ATLAS barrel and endcap muon spectrometer. Note the multiple detector technologies used for muon detection.

sponse trigger chambers. Monitored drift tubes (MDTs) follow similar principles as the ID straw tubes, using a gas mixture of Ar/CO₂ (93%/7%) and 50 μm gold-pated tungsten-rhenium sense wire through aluminum tubes 3 cm in diameter. Arrays of two sets of 3-4 MDTs are arranged parallel to the beam axis in 3 layers in the barrel and 2 layers in the forward region to provide precision ϕ measurement. The MDTs provide position resolution of $\sim 80\mu\text{m}$ per tube with drift times of ~ 700 ns, which is too slow for triggering.

The innermost layer of precision chambers in the forward region ($|\eta| > 2.0$) are instrumented with cathode strip chambers (CSC). The CSCs are multiwire proportional chambers with wires oriented radially and the induced charge on cathode strips are used to infer the track position. The CSCs are required for this region of the MS where flux rates are largest because hit positions can

be measured in 2D from orthogonal cathode strips on either side of the CSC chambers. Resistive plate chambers (RPC) and thin gap chambers (TGC) are instrumented for muon triggering and secondary coordinate reconstruction in the central region ($|\eta| < 1.05$) and forward regions ($1.05 < |\eta| < 2.7$). Response time for these chambers is < 1 ns with signal digitization yielding triggerable signals within 4 ns. Internal and external alignment of the MS chambers is provided via an optical system and toroid-off data-taking runs for straight muon track reconstruction. A summary of the MS instrumentation coverage is given in Table 4.3.

Table 4.3: Summary of the instrumentation coverage for the MS

Monitored drift tubes	MDT
- Coverage	$ \eta < 2.7$ (innermost layer: $ \eta < 2.0$)
- Number of chambers	1088 (1150)
- Number of channels	339 000 (354 000)
- Function	Precision tracking
Cathode strip chambers	CSC
- Coverage	$2.0 < \eta < 2.7$
- Number of chambers	32
- Number of channels	31 000
- Function	Precision tracking
Resistive plate chambers	RPC
- Coverage	$ \eta < 1.05$
- Number of chambers	544 (606)
- Number of channels	359 000 (373 000)
- Function	Triggering, second coordinate
Thin gap chambers	TGC
- Coverage	$1.05 < \eta < 2.7$ (2.4 for triggering)
- Number of chambers	3588
- Number of channels	318 000
- Function	Triggering, second coordinate

4.5 THE MAGNET SYSTEMS

This section will provide an overview of the ATLAS magnet systems, while the full TDR can be found in [76]. A rendering of the ATLAS toroidal magnet system and a photograph of the installed

barrel toroid cryostats are shown in Figure 4.9. The magnetic field in the ID is provided by a superconducting solenoid which shares its cryogenic housing with the LAr calorimeter. The toroidal field is provided by 8 air-core superconducting coils in each of the barrel and two endcap regions. While the field is approximately toroidal, its nonuniformities (particularly near the coils) must be taken into account for precision muon reconstruction. To this end, 1,800 Hall probes are installed throughout the detector volume to continuously monitor the magnetic field. A finite-element simulation of the coils and conducting elements is used to produce magnetic field maps down to arbitrary precision. The positions and orientations of the coils are floated within their known precision and their resultant field predicted by the Biot-Savart law is fitted to Hall probe measurements. Slices of the magnetic field map are shown in Figure 4.10.

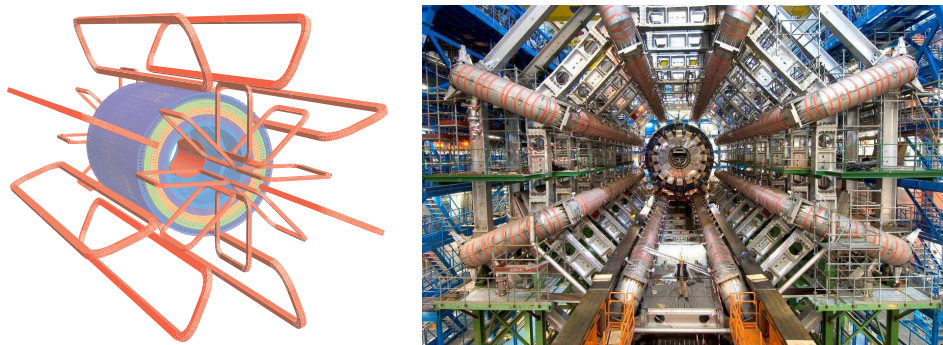


Figure 4.9: A rendering of the ATLAS magnet system (left) and a photograph of the barrel toroidal magnet cryostats. Note the 8-fold symmetry of the magnet geometry.

The endcap cryostats containing the endcap toroids will shift position after initial placement due to magnetostatic forces. Position sensors were installed onto the surface of the endcap cryostats during the first long shutdown of the LHC. A shift in position of approximately 2 mm was observed, which is larger than the position uncertainties after initial commissioning. This information was used in an updated fit for the magnetic field. My qualification task for the ATLAS experiment was

to evaluate the change in muon reconstruction performance as a result of updating the map from the Run I configuration to the improved Run II configuration. Updating the map results in a shift to the muon momentum scale and improvement in the momentum resolution of standalone (combined) muons by 0.8% (0.3%) in the forward region [77].

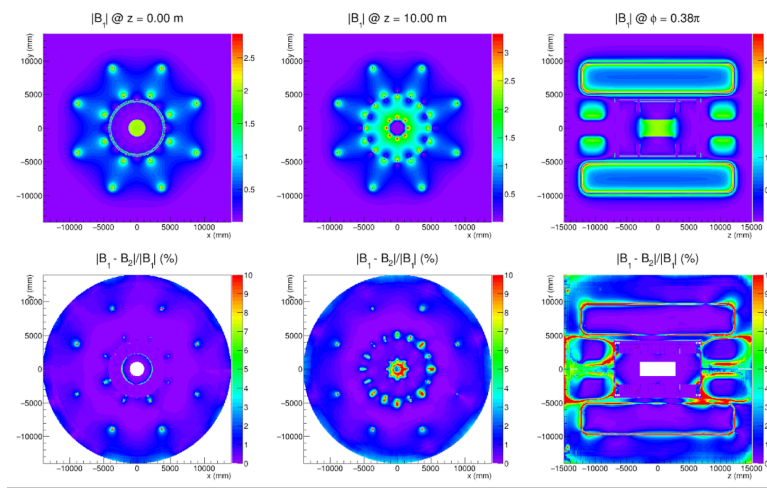


Figure 4.10: Transverse (left, center) and longitudinal (right) slices of magnetic field map and the corresponding difference between Run I and Run II detector conditions

The key characteristic of the magnets is bending power, defined as the bending component of the field integrated from the center of the detector radially outward to infinity: $\int B_\phi dr$. Bending strength in the barrel ranges between 1.5 and 5.5 T·m ($|\eta| < 1.4$) and between 1 and 7.5 Tm in the endcap regions ($1.6 < |\eta| < 2.7$). The intermediate transition region suffers from reduced bending power and can be seen in Figure 4.11.

4.6 TRIGGER AND DATA ACQUISITION

The LHC delivers proton bunches collisions to ATLAS at a rate of 40 MHz. The equivalent data rate would be on the order of 100 PB/s if the detector data was readout at every bunch crossing,

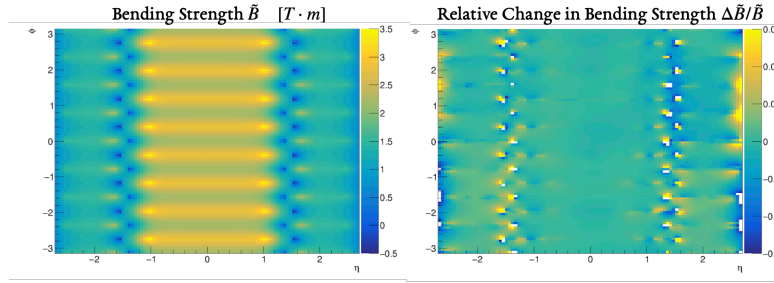


Figure 4.11: Bending strength during Run I (left) and difference in Run II conditions (right)

which is 8 orders of magnitude higher than can be processed and stored. Most of this data is uninteresting, as the most interesting hard scattering processes are very rare. ATLAS employs a two step trigger flow consisting of a hardware-based level 1 (L1) trigger and software-based high-level trigger (HLT) coupled to a data acquisition (DAQ) pipeline to capture only interesting collision events. An overview of the ATLAS trigger and DAQ stream is shown in Figure 4.12.

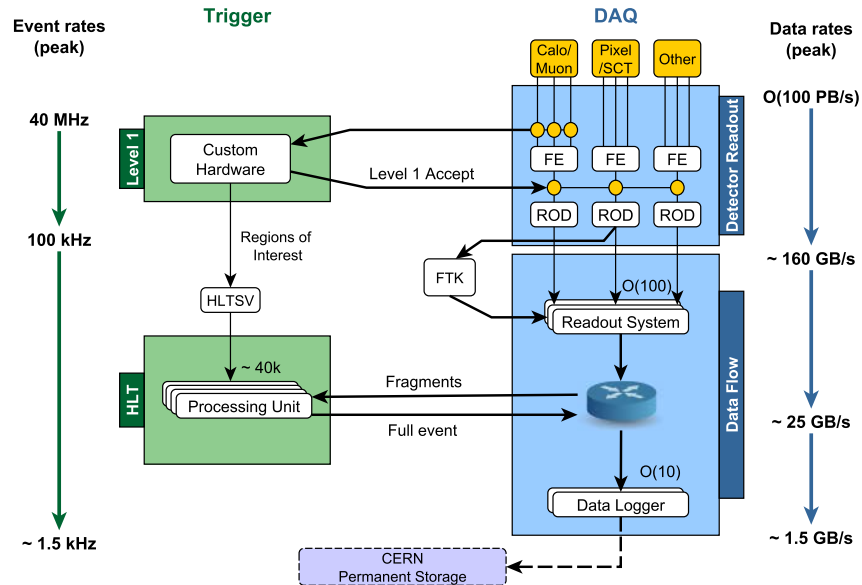


Figure 4.12: Schematic diagram of the ATLAS trigger and DAQ flow in Run II

The L1 trigger decision is formed based on limited information from calorimeters and muon trigger chambers, each of which are processed independently by dedicated trigger processors built on

custom hardware located in the ATLAS cavern [78]. Calorimeter triggers are fired based on a coarse-grained thresholding algorithm of cell deposits and muon triggers are fired based on coincidences of hits in multiple layers of MS trigger chambers consistent with muons produced near the IP. An OR of these trigger items defines an *L1 Accept* (L1A) signal that is sent to a collection of hardware-based *readout drivers* (ROD) that process detector data to the central readout system. An L1A decision is processed in under $2.5 \mu\text{s}$ and are fired at 100 kHz, reducing the data rate to 160 GB/s. The L1 trigger also defines *regions of interest* (ROI) that seed the HLT. Event fragments are transmitted via fiber optic cables to a CPU farm of 40,000 cores housed in the USA15 service hall. Software algorithms analyze event fragments to form HLT decisions based on more fully reconstructed muons, electrons, photons, and jets in $\approx 200 \mu\text{s}$. The HLT reduces the event rate down to 1.5 kHz/1.5 GB/s. Events that pass the HLT are written to tape and sent off to a tiered global computing system for offline reconstruction.

Part III

Modeling and Reconstruction

5

Monte Carlo Simulation

There are many physical processes at play in high-energy pp collisions. Most, in fact, are not characterized by a high momentum transfer scale $q^2 \sim s$. Part of this is due to the choice of colliding hadrons instead of fundamental particles like electrons, where quarks and gluons are confined at an energy of $\mathcal{O}(1 \text{ GeV})$. The universal factorization of low-energy processes internal to the proton and the high-energy scattering interactions of its constituent partons is essential for the tenability of theoretical calculations. Additional complexity arises from the transition of QCD from an asymptotically free to a confining interaction as q evolves downward toward Λ_{QCD} as final state particles

propagate away from the interaction point. Finally, myriad particles propagate through the detector volume and undergo random material interactions, creating discernible hits that are digitized and passed through a reconstruction algorithm. The processes that govern pp collisions and the stable particles that ultimately pass through a detector are drawn in Figure 5.1.

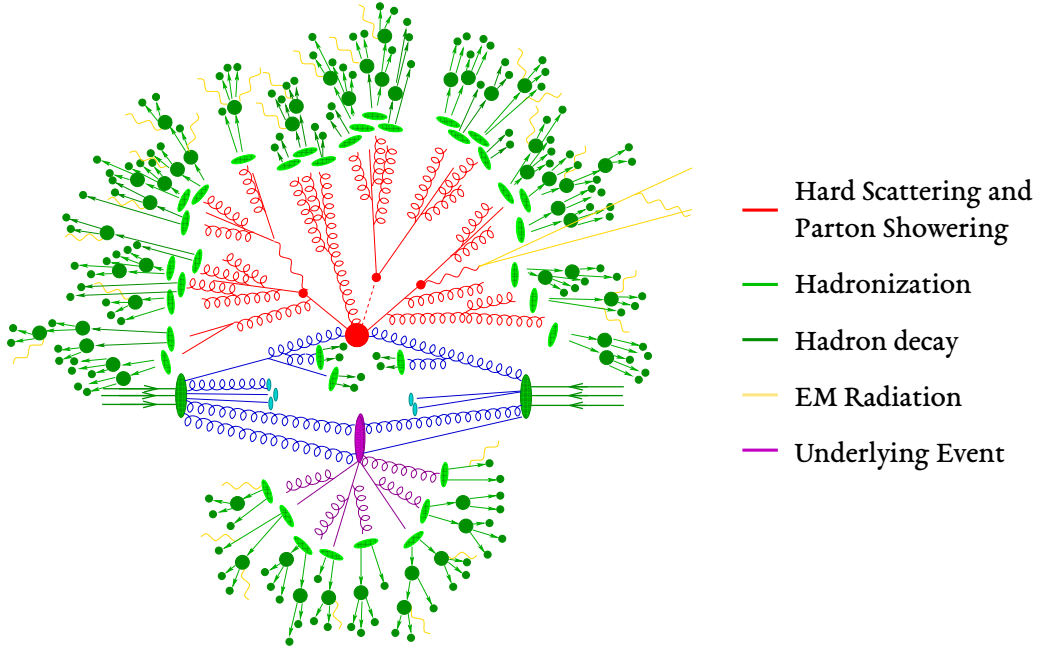


Figure 5.1: Cartoon of a pp collision event [7]

Constructing an analytical model to predict multi-dimensional probability distributions for data coming from such an experiment is impossible. For instance, a probability distribution function for the number of jets produced in an event would minimally require the integration over millions of detector channels whose hits are reconstructed to form jet objects. Collider experiments instead heavily rely on the method of Monte Carlo (MC) simulation, whereby events are probabilistically generated according to distributions that can be sampled step-by-step and fed forward through the

simulation chain. In this way, the theoretical model can be handled more like data. The successful implementation of MC methods in particle physics relies on the low cost of generating random events made possible by modern computer technology. This chapter will summarize the principles underlying MC simulation techniques and highlight specific aspects that are relevant to the most precise predictions for the $t\bar{t}W$ process. For a more detailed overview of MC methods in collider physics, see references [79, 80].

5.1 HARD SCATTERING INTERACTIONS

The probability that a hard scattering interaction occurs between individual quarks or gluons within colliding protons is determined by the magnitude of its associated cross section. This can be calculated inclusively and differentially as a function of some final state kinematics. The general expression for a $2 \rightarrow N$ scattering cross section of initial state particles ab is given by

$$\sigma_{ab \rightarrow N} = \int_{V_N} d\Phi_N \left| \sum_{n=0}^{\infty} \mathcal{M}_n(\Phi_N; \mu_R) \right|^2 \quad (5.1)$$

where $d\Phi_N \equiv \prod_{\text{final states } j}^N \frac{1}{(2E_a)(2E_b)|\vec{v}_a - \vec{v}_b|} \frac{d^3p_j}{(2\pi)^3} \frac{1}{2E_{p_j}} (2\pi)^4 \delta^4(\Sigma p)$

Here, the matrix element (i.e. scattering amplitude) $\mathcal{M}_{ab \rightarrow N}$ is written as a perturbative expansion, where $\mathcal{M}_n \propto \alpha^n$ and α is a generic coupling constant $\alpha < 1$. The matrix element is approximated by the fixed order calculation achieved by truncating the summation. The fixed order calculation must be renormalized through the introduction of a non-physical scale μ_R , which is normally fixed to some energy scale relevant to the process at hand (e.g. $\mu_R = M_Z$ for $q\bar{q} \rightarrow Z \rightarrow e^+e^-$). While the amplitude $\mathcal{M}$ calculated to all orders in perturbation theory should not depend on μ_R ,

the fixed-order calculation may retain a dependence. Theoretical uncertainties on the fixed order calculation are estimated by varying μ_R from some nominal value. The inclusive cross section for the process $ab \rightarrow X$ can be obtained through a summation over all possible final states.

The integration in Equation 5.1 is not trivial, as the $3N$ -dimensional integral is impossible to perform analytically for most processes of interest at the LHC. It is here that we encounter the first use of MC techniques. The form of Equation 5.1 can be identified with $I[f] = \int_V d^n x f(\mathbf{x})$. This expression is the definition of the average over V and can be estimated with the sample mean $\bar{f}_N \equiv \frac{1}{N} \sum_{i=1}^N f(\mathbf{x}_i)$, with N points randomly sampled over V . By the central limit theorem, this estimator has variance inversely proportional to N :

$$\text{Var}(\bar{f}_N) = \sqrt{\frac{\text{Var}(f)}{N-1}}.$$

This method is powerful as it does not suffer the curse of dimensionality, as the accuracy of the estimation can be made arbitrarily precise by increasing the sample size.

The sample size required to reach a fixed error $E[\bar{g}_N] < E_0$ can be decreased by effectively decreasing the numerator $\text{Var}(f)$ through the method of importance sampling. Instead of sampling N points $\{\mathbf{x}_i\} \in V$ uniformly, a coordinate transformation can be made by mapping $\mathbf{x} \rightarrow \mathbf{y}(\mathbf{x})$ with Jacobian $\left| \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \right| = g(\mathbf{x})$. The integral of interest can now be written as $I[f] = \int_V d^n x h(\mathbf{x})$, where $h(\mathbf{x}) = f(\mathbf{x})/g(\mathbf{x})$. If the coordinate map is chosen such that $\text{Var}(h) < \text{Var}(f)$, then the MC approximation converges more rapidly with additional samples. The method of importance sampling can be thought of as simply smoothing out the function f over its domain so that denser regions of $\mathbf{x}$ are dispersed into less dense regions.

In practice, one would like to generate events sampled from the phase space V according to probability $f(\mathbf{x})$ rather than only calculate cross sections as above. The simplest method for doing so is dubbed the “hit-or-miss” method and proceeds as follows:

1. Pick a constant value $f_{max} \geq \max_{\mathbf{x} \in V} f(\mathbf{x})$
2. Pick a point $\mathbf{x}$ in V and a (pseudo-)random number $R \in [0, 1]$
3. If $Rf_{max} \leq f(\mathbf{x})$, accept the event, otherwise reject it. Repeat from 2 until the desired sample size is obtained

This process may have a low generation efficiency and therefore slower generation speed, so instead one can save all events and an associated weight given by $f(\mathbf{x})$.

After nearly 15 years of LHC operation and decades of development in aspects of theoretical computation, there exist several general-purpose MC event generators that can automatically generate Feynman diagrams and compute integrals for arbitrary processes up to next-to-leading order (NLO) or even NNLO precision. Commonly used generators will be discussed in Section 5.4.

5.2 SOFT QCD FACTORIZATION

The above discussion of partonic cross sections $\hat{\sigma}_{ab \rightarrow X}$ can be extended to cross sections of proton collisions $\sigma_{pp \rightarrow X}$ of interest at the LHC using the Factorization Theorem:

$$\sigma_{pp \rightarrow X} = \sum_{a,b} \int dx_a dx_b f_a(x_a; \mu_F^2) f_b(x_b; \mu_F) \hat{\sigma}_{ab \rightarrow X}(x_a p_a, x_b p_b; \mu_R^2, \mu_F^2) \quad (5.2)$$

Here, a and b label the scattering partons of protons a and b , the Bjorken- x parameters $x_{a,b}$ determine the fraction of the proton momentum $p_{a,b}$ is carried by the respective parton, and $f(x; \mu_F^2)$ is the set of universal parton distribution functions (PDF) [81]. The factorization scale μ_F is a large

momentum transfer scale that characterizes the hard scattering interaction. It can be interpreted as the momentum scale that separates the hard scattering process, which is accounted for by the partonic cross section $\hat{\sigma}_{ab \rightarrow X}$, and the low-energy dynamics of the proton, accounted for in the PDFs. Like the unphysical μ_R , there is no dependence on μ_F when Equation 5.2 is performed to all orders in perturbation theory. Uncertainties on fixed-order calculations are obtained by varying μ_F from its nominally chosen value. Equation 5.2 is pictorially represented in Figure 5.2.

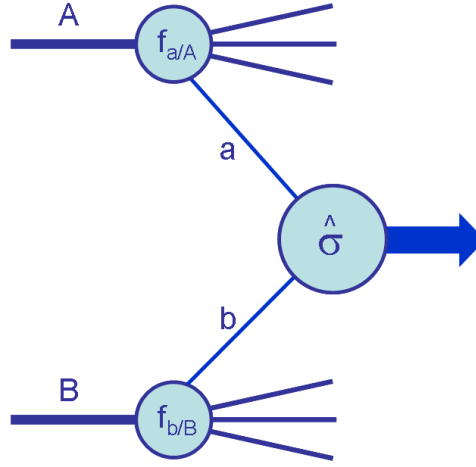


Figure 5.2: Diagram depicting the factorization theorem

The parton distribution functions absorb divergent logarithms that result in non-perturbative QCD processes. Their forms at various Q^2 are provided by hadron collider and deep inelastic scattering (DIS) experiments such as ZUES and H1 at the HERA ep collider [82]. Measurements from HERA have probed $f(x; Q^2)$ across many orders of magnitude in the (x, Q^2) plane, as shown in Figure 5.3.

The interpolation between and extrapolation beyond measurements in the (x, Q^2) plane follow

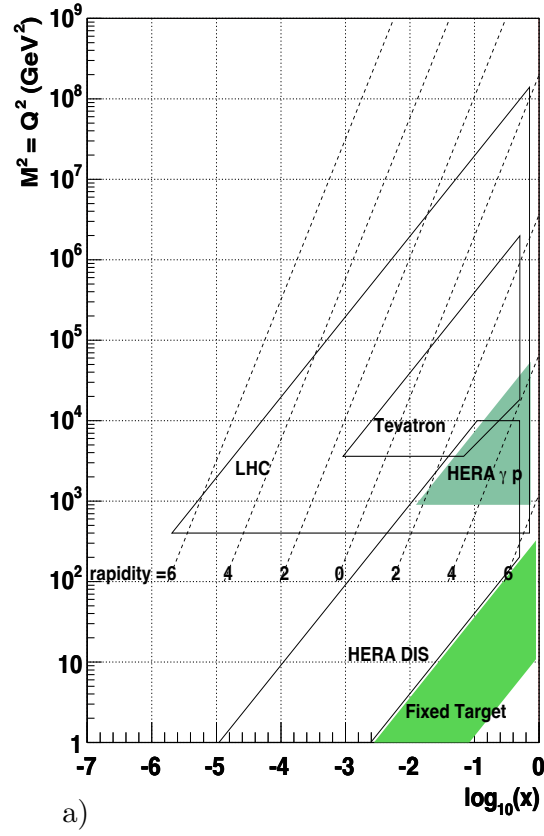


Figure 5.3: Regions in the (x, Q^2) kinematic plane probed by HERA, fixed target experiments, and hadron collider experiments [8]

from the Dokshitzer–Gribov–Lipatov–Altarelli–Parisi (DGLAP) evolution equations [83, 84, 85]:

$$Q^2 \frac{d}{dQ^2} \begin{pmatrix} f_i(x, Q^2) \\ f_g(x, Q^2) \end{pmatrix} = \frac{\alpha_s}{\pi} \sum_j \int_x^1 \frac{dz}{z} \begin{pmatrix} P_{q_i q_j}(\frac{x}{z}) & P_{q_i g}(\frac{x}{z}) \\ P_{g q_j}(\frac{x}{z}) & P_{g g}(\frac{x}{z}) \end{pmatrix} \begin{pmatrix} f_j(z, Q^2) \\ f_g(z, Q^2) \end{pmatrix} \quad (5.3)$$

The splitting functions $P_{ba}(z)$ represent the probability of a parton a splitting into parton b with

momentum fraction z . They are given at leading order in Equations 5.4 - 5.6 [86]:

$$P_{gq}(z) = C_F \left[\frac{1 + (1+z)^2}{z} \right] = q \longrightarrow \begin{array}{c} \nearrow g(z) \\ \longrightarrow q(1-z) \end{array} \quad (5.4)$$

$$P_{qg}(z) = T_R [z^2 + (1-z)^2] = g \begin{array}{c} \nearrow q(z) \\ \longleftarrow \bar{q}(1-z) \end{array} \quad (5.5)$$

$$P_{gg}(z) = 2C_A \left[\frac{z}{1-z} + \frac{1-z}{z} + z(1-z) \right] = g \begin{array}{c} \nearrow g(z) \\ \longleftarrow g(1-z) \end{array} \quad (5.6)$$

Global determination of parton distribution functions using the DGLAP equations are provided by the CTEQ and NNPDF collaborations [87, 88]. Representative examples of PDFs at low and high Q^2 provided by CTEQ are shown in Figure 5.4. One can see that at low Q^2 the valence quarks u and d contribute most dominantly in hard scattering interactions (where the difference in u/d PDFs is due to the uud quark content of the proton). At higher Q^2 , the contribution of gluons to hard scattering interactions at moderate x becomes very large and the sea (anti-)quarks become important. It should be noted that extrapolations of PDFs to high Q^2 and low x using Equation 5.3 typically incur large systematic uncertainties. This is a limiting factor for some LHC searches for heavy resonances, for example, but not for the present measurement described in this thesis.

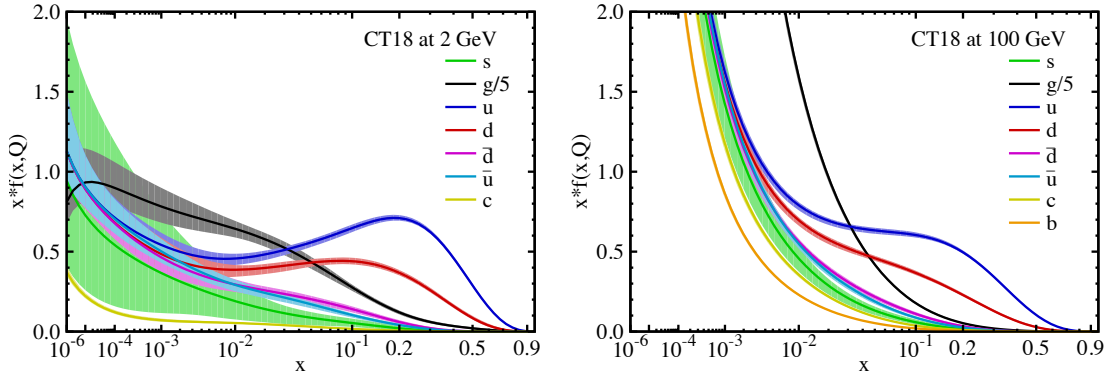


Figure 5.4: Parton distribution functions provided by CTEQ at $Q = 2$ GeV (left) and $Q = 100$ GeV (right) [9]

5.3 PARTON SHOWERING AND HADRORIZATION

A fixed-order matrix element calculation for a process $pp \rightarrow X$ at the n^{th} order can include a mix of corrections with l internal loops and k additional external field lines, with $n = l + k$. Representative Feynman diagrams corresponding to these types of corrections are shown in Figure 5.5. The k real emissions (i.e. legs) can be accounted for most precisely in the matrix element calculation but can also be accounted for in the parton showering step, whereby the matrix element calculation is modified by a semi-classical Monte Carlo algorithm. Parton showering includes photons and gluons and is responsible for evolving the event from the hard scattering energy scale $Q \sim 100$ GeV to

$Q \sim \Lambda_{QCD}$ at which hadronization occurs.¹

¹Parton showering is an alternative method to resummation, which is an all-orders approach in which the largest logarithms across all perturbative orders are summed. The precision of these calculations is characterized by the number of leading logarithms that are included. The splitting functions of Equations 5.4 - 5.6 demonstrate the soft and collinear divergences of QED and QCD radiation that must be regularized. In other words, the splitting functions cannot be integrated over the full phase soft and collinear phase space. From a theoretical point of view, this is justified by the finite granularity of a particle experiment's space and momentum resolution.

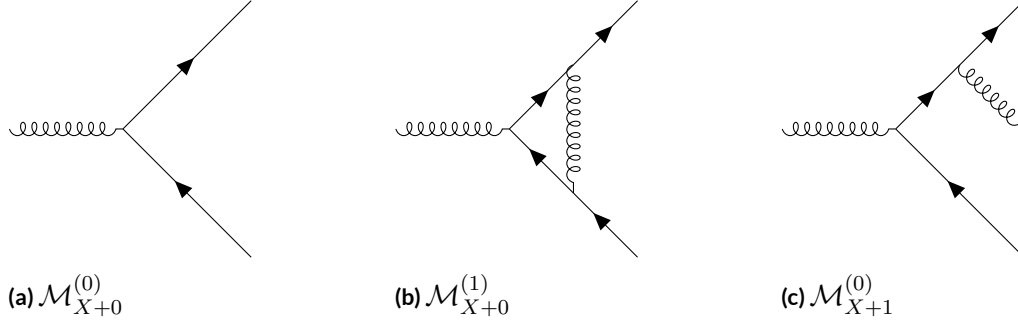


Figure 5.5: Representative Feynman subdiagrams for $pp \rightarrow q\bar{q}$ at LO and additional corrections from internal loops or real final state emission

The implementation of a parton shower relies on the Sudakov form factor:

$$\Delta_i(t_0, t_1) = \exp \left[-\frac{\alpha_s}{2\pi} \sum_j \int_{t_1}^{t_0} \frac{dt}{t} \int_0^1 dz p_{ji}(z) \right] \quad (5.7)$$

It represents the probability that a parton i of virtuality t_0 evolves to t_1 without fragmentation, at which point a parton j with momentum fraction z is emitted. The stochastic parton showering algorithm is sketched in the following steps:

1. Sample pseudo-random number r_t from $[0, 1]$ and calculate t_1 where $\Delta_i(t_0, t_1) = r_t$
2. Sample pseudo-random number r_z from $[0, 1]$ and calculate z where

$$\int_0^z dy p_{ji}(y) \Big/ \int_0^1 dy p_{ji}(y) = r_z$$

3. Split $i \rightarrow j$ with virtuality t_1 and momentum fraction z . Repeat until all partons have virtuality $t_i \sim 1 \text{ GeV}$

The Sudakov factor accounts for large logarithms characteristic of QCD divergences, so the parton shower (PS) is reliable for predictions of collinear radiation. It is ill-suited for hard and wide-angle emissions, which should be included in the matrix element (ME) calculation. Matching and merging schemes are defined in order to combine the predictions of matrix element and parton

showers (ME+PS) without double-counting $\mathcal{M}_{X+l}$ amplitudes. Specifically, matching is a procedure to combine ME and PS calculations for $\mathcal{M}_{X+0}^{(n)}$ amplitudes, while merging is a procedure to combine multi-leg NLO ME and PS calculations for $\mathcal{M}_{X+1,2}^{(n)}$ amplitudes.

After the parton shower has evolved the event to near Λ_{QCD} , color-charged particles are transformed into color singlet hadrons. Hadronization algorithms are not supported by the same theoretical underpinnings as parton showers because of the non-perturbativity of QCD in this regime.

Figure 5.6 illustrates the two classes of phenomenological models for hadronization:

- The cluster model, where the central objects are clusters of quarks. This is motivated by considering a hadron as a cluster of bound quarks (e.g. π^+ as $u\bar{d}$)
- The Lund string model, where the central objects are strings that connect bound states of quarks. This is motivated by virtual gluon flux tubes of constant energy density that form between quarks.

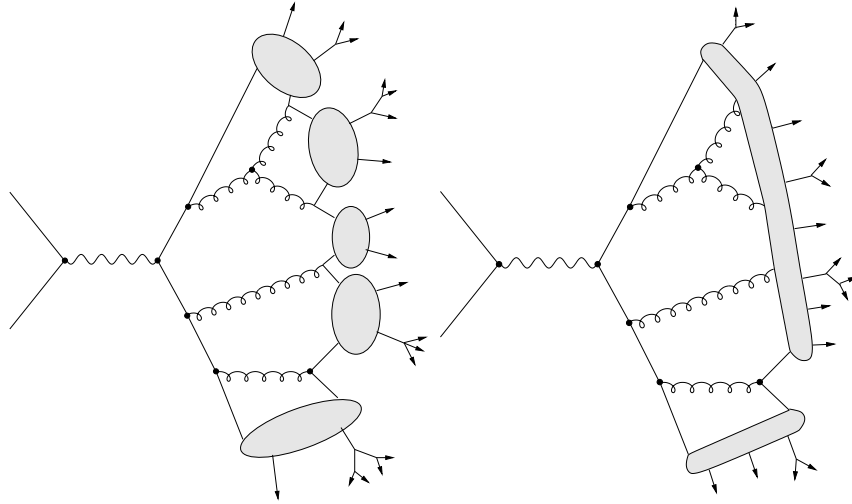


Figure 5.6: Illustrations of the cluster (left) and string (right) hadronization models [10]

5.4 MONTE CARLO ALGORITHMS

There are several general purpose ME generators available. The relevant ME generators for the analysis presented in this thesis are POWHEG-BOX and MG₅_AMC@NLO .

POWHEG-BOX is a parton-level ME generator that computes amplitudes to NLO precision (up to one loop) [89]. It uses the POWHEG method, in which the hardest emission in the parton shower is replaced with its own NLO accurate emission, allowing the POWHEG-BOX output to be easily interfaced into p_T -ordered parton shower algorithms [90, 91]. POWHEG generators have the advantage of producing events with very low rates of negative event weights (few percent for POWHEG-BOX , but can be as large as 30% in generators such as SHERPA).

MG₅_AMC@NLO is another NLO ME generator that uses the MADLOOP module of MADGRAPH to automatically compute diagrams up to 1 loop accuracy [92]. It relies on the MC@NLO method to perform NLO+PS matching [93]. This has recently been extended to allow ME+PS multi-leg merging for events with one real emission at NLO (FxFx merging) [94]. The FxFx multi-leg merging has been recently made possible for $t\bar{t}W$ production [95]. Spin correlations among heavy resonances (e.g. $t\bar{t}$) are handled by MADSPIN [96].

Events generated by POWHEG-BOX and MG₅_AMC@NLO can subsequently be showered by PYTHIA and HERWIG , which are themselves more general purpose ME and PS algorithms [97, 98]. PYTHIA features momentum-ordered parton showers and uses the string hadronization model, while HERWIG features angular-ordered parton showers including color-coherence effects and uses the cluster hadronization model. Both algorithms can be interfaced with the EVTGEN generator that simulates the decays of heavy flavor hadrons, which can undergo $\mathcal{CP}$ violating decays, taking

into account angular and time-dependent correlations through the full decay chain [99].

Last but not least is the SHERPA generator, capable of LO/NLO ME+PS matching and merging [100]. It relies on interfaces with one-loop providers such as OPENLOOPS for NLO ME calculations [101]. Parton showering is performed using the Catani-Seymour dipole factorization scheme [102]. Matching for NLO QCD matrix elements uses the MC@NLO method.

5.5 SIMULATING THE ATLAS DETECTOR

After a set of Monte Carlo events has been generated, showered, and hadronized, stable particles must be passed into a simulation of the ATLAS detector. The ATLAS experiment is simulated in detail using GEANT₄ (GEometry And Tracking), a software framework written in C++ capable of simulating material interactions of particles with simulated volumes [103]. The interactions that are supported within GEANT₄ are specified by a set of physics lists that can be provided by the user. Standard material interactions like ionization and showering are included by default.

The most accurate simulation of the ATLAS detector using GEANT₄ is referred to as FullSim. Its major drawback is its computational cost. ATLAS has developed a fast simulation algorithm (AFII) that achieves an order of magnitude reduction in computing time, as shown in Figure 5.7 [104]. This is achieved in part by replacing the calorimeter showering step (involving $\mathcal{O}(100)$ material interactions per shower) with pre-defined shower shape templates. This simplification is reliable for most purposes except for the study of jet substructure variables, but FullSim samples are preferred for most processes except those that contribute least to a particular measurement's phase space. After particles are propagated through the simulated ATLAS detector, the simulated detector hits are digitized and passed into ATLAS reconstruction.

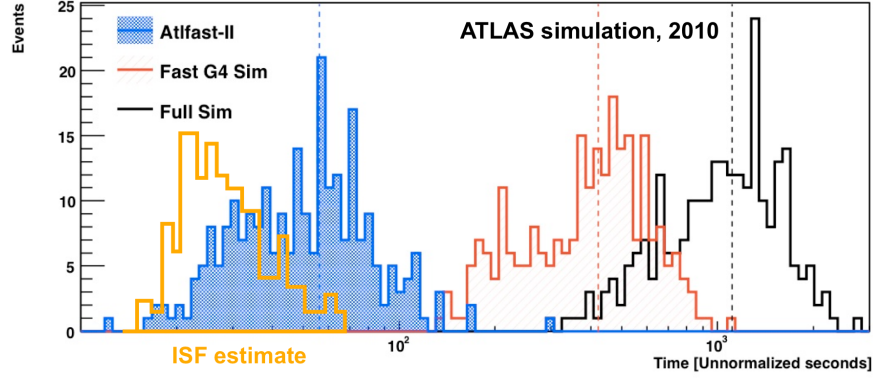


Figure 5.7: Comparison of CPU time for a set of $t\bar{t}$ events using FullSim and AFII

The ATLAS model within GEANT4 is limited in its detail and must be corrected to more faithfully reproduce reconstruction and tagging efficiencies of various physics objects. This is typically achieved through the derivation of scale factors (SF) applied to reconstructed MC events, defined by the double ratio:

$$SF = \frac{N_{data}^X / N_{data}^{total}}{N_{MC}^X / N_{MC}^{total}} = \frac{\epsilon_{data}}{\epsilon_{MC}} \quad (5.8)$$

Where X refers to any reconstruction algorithm (e.g. triggers, object reconstruction and identification, isolation, and tagging algorithms). Specific examples of this calibration procedure will be discussed in Chapter 6.

The last part of the pp interaction not yet mentioned is the remnants of the inelastically scattered protons that do not participate in the hard scattering interactions. These low-momentum beam remnants are referred to as the underlying event, which may be deposited in the detector volume and contribute to backgrounds in object reconstruction. The underlying event is accounted for by overlaying events similar to those collected with a very loose trigger. These constitute a sample of baseline inelastic scattering events that are minimally biased towards higher $\sqrt{s}$ by the trigger. Specific generator tunes are defined in order to produce events that agree with minimum bias data

[105]. It is also possible for multiple hard scattering interactions to occur between the partons of a single pair of colliding hadrons, called multiple-parton interactions. The effect of such events is relevant for predicting dijet production cross sections, for example [106].

6

ATLAS Reconstruction

The measurement of $t\bar{t}W$ production relies on the reconstruction of light leptons (electrons and muons) that define the measurement channels. It also relies on jet clustering and heavy flavor tagging to identify b -jets produced in top quark decays. Measurements from the tracker, calorimeters, and muon spectrometers must be combined to reconstruct these physics objects. This chapter will give an overview of the reconstruction and calibration of physics objects, focusing on aspects that are most relevant for the $t\bar{t}W$ measurement.

6.1 TRACKING AND VERTEXING

Tracking algorithms in ATLAS fit hits measured in the ID to reconstruct the trajectories of charged particles as they are deflected in a magnetic field. Trajectories are defined by a set of perigee parameters $(d_0, z_0, \phi, \theta, q/p_T)$ shown in Figure 6.1. Impact parameters d_0 and z_0 determine the distance of closest approach of the particle trajectory to a given vertex position, while ϕ and θ determine the direction of the trajectory at the position of closest approach. Note that these parameters depend on a specific reference point (the beamspot or reconstructed collision vertices are common choices). The charge and momentum of a particle can also be reconstructed if the magnetic field strength is known via the Lorentz force law.

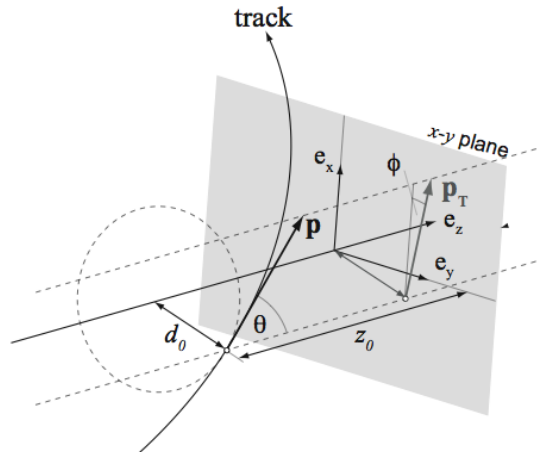


Figure 6.1: Illustration of a particle trajectory and its defining perigee parameters

A key feature of tracking algorithms is the ability to efficiently find the correct combination of $\mathcal{O}(1000)$ hits across multiple detector systems. ATLAS tracking involves two sequential algorithms: the primary inside-out track reconstruction followed by outside-in tracking (back-tracking) [107, 108]. While inside-out tracking can efficiently find track candidates, it is sensitive to ambiguities in

assigning hit clusters to track candidates. Outside-in tracking helps resolve these ambiguities and recover missed tracks. Outside-in tracking is also useful for reconstructing tracks from secondary vertices and photon conversions ($\gamma \rightarrow e^+ e^-$) that can occur within the tracking volume.

The inside-out sequence begins by forming track seeds from sets of 3 hit clusters within the silicon layers. Track seeds are extended outward layer-by-layer using a combinatorial Kalman filter [109]. Search roads are defined that extend from track candidates to reduce the number of hits that must be considered for track extension into the outer layers. Ambiguities between multiple possible hit extensions are resolved with fit quality requirements (e.g. χ^2). The tracks are extended into the TRT region if compatible hits are found and refitted. After the inside-out sequence has produced a set of candidate tracks, the back-tracking sequence is run. It is seeded by sets of 3 clusters in the TRT layers in regions of interest defined by hits in the electromagnetic calorimeter. The same iterative track extension procedure is used as in the inside-out approach. Performance measurements of track reconstruction in early Run II are given in References [110, 111].

Tracks are extrapolated towards the beamline to form vertices characterized by their position, the number of tracks associated to it, and the $\sum p_T^2$ of all associated tracks. The primary vertices (PV) are vertices found near the overlapping region between the incoming proton beams (the beamspot). PV are reconstructed as those that have at least two high-quality tracks associated to it [112]. The number of primary vertices increases with instantaneous luminosity of the LHC. The number of reconstructed PV per bunch crossing μ is shown in Figure 6.2 during the Run II data taking period. The hard scattering interaction is associated to the PV with the highest $\sum p_T^2$.

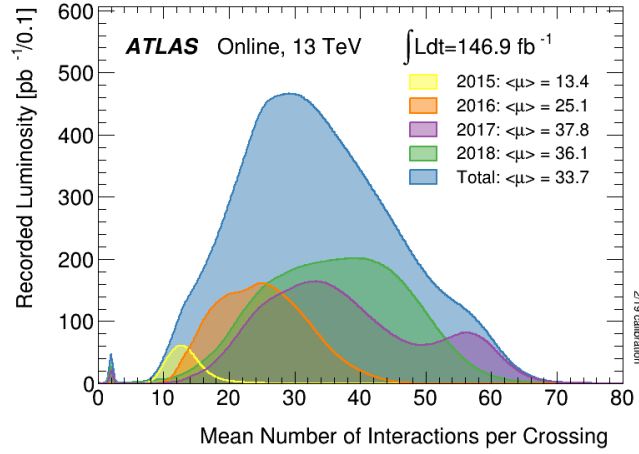


Figure 6.2: Average number of primary vertices per bunch crossing recorded by ATLAS during Run II

6.2 ELECTRONS AND PHOTONS

Electrons and photons are indistinguishable in the EM calorimeter and are therefore reconstructed using similar strategies. The identification of an EM shower as an electron or photon is determined by the presence of a track pointing to it with similar momentum. Since photon reconstruction techniques are also used for electrons and the $t\bar{t}W$ measurement does not consider photons, this section will focus on electron reconstruction and calibration.

The combination of tracking and calorimetry for electron reconstruction is depicted in Figure 6.3. Electrons are well reconstructed in the region $|\eta| < 2.47$, ensuring its narrow shower is fully contained within the LAr calorimeter, excluding the $1.37 < |\eta| < 1.52$ where coverage transitions from the barrel to the end-cap calorimeter (the so-called LAr crack region). Hits in the silicon and SCT layers are used for momentum calibration, while TRT hits can be used to identify electrons by the x-ray transition radiation that is characteristic of low mass particles. These are combined with TopoClusters [113] of calorimeter cells into a likelihood-based identification algorithm

that is defined at Loose and Tight working points with different levels of electron identification efficiency and misidentification rates [114]. Electrons are required to have tracks reconstructed with $|z_0 \sin \theta| < 0.5 \text{ mm}$ and $|d_0|/\sigma_{d_0} < 5$ to improve rejection of electrons from photon conversions and secondary decays (collectively referred to as non-prompt production).

Electrons are required to be isolated from other activity in the detector to further increase rejection of non-prompt electrons. The quantities of interest are the sum of p_T (E_T) of tracks (calorimeter cells) observed within an isolation cone of width ΔR centered on the identified electron. Track-based isolation can support very narrow isolation cones, while calorimeter cones can be only as narrow as $\Delta R = 0.2$ due to the granularity of the LAr calorimeter. Multiple working points are provided that offer a trade-off between electron efficiency and background rejection, including a Loose selection with fixed cuts on the isolation criteria (FCLoose) [11].

Electron charge is determined by the track curvature direction in the ID. Charge can be misidentified if an electron undergoes material interactions and produce secondary electrons and photons that are mis-reconstructed as the original electron. In the high- p_T regime, charge misidentification can also occur as the track sagitta (and curvature direction) is poorly resolved by the intrinsic tracking resolution. Electron charge misidentification is suppressed using a boosted decision tree (BDT) trained on electron kinematics, impact parameters, and SCT hits from the electron and neighboring tracks. [11].

Software-based photon, single-lepton, and di-lepton high level triggers (HLT) are available within the ATLAS trigger menu. Electron p_T thresholds are set depending on the run conditions of the data-taking period (typically . Both photon and electron triggers are seeded by hits in the LAr calorimeter that define regions of interest (ROI) to perform approximate but fast cluster recon-

struction and isolation [115]. If the HLT is fired, an offline precision step is performed to refine the HLT trigger decision.

All identification, isolation, and trigger efficiency calibrations are performed using the tag-and-probe method [116], in which an unbiased sample of electrons is obtained using the characteristic ee decays of the Z and J/ψ resonances. A strict selection criteria is applied to a well-reconstructed electron (the tag electron) and a second electron (the probe) is used for calibration in events consistent with one of the aforementioned resonant decays. If the electrons are well-separated within the detector volume, the probe electron identification, isolation, and trigger efficiencies are unbiased by the requirements placed on the tag electron.

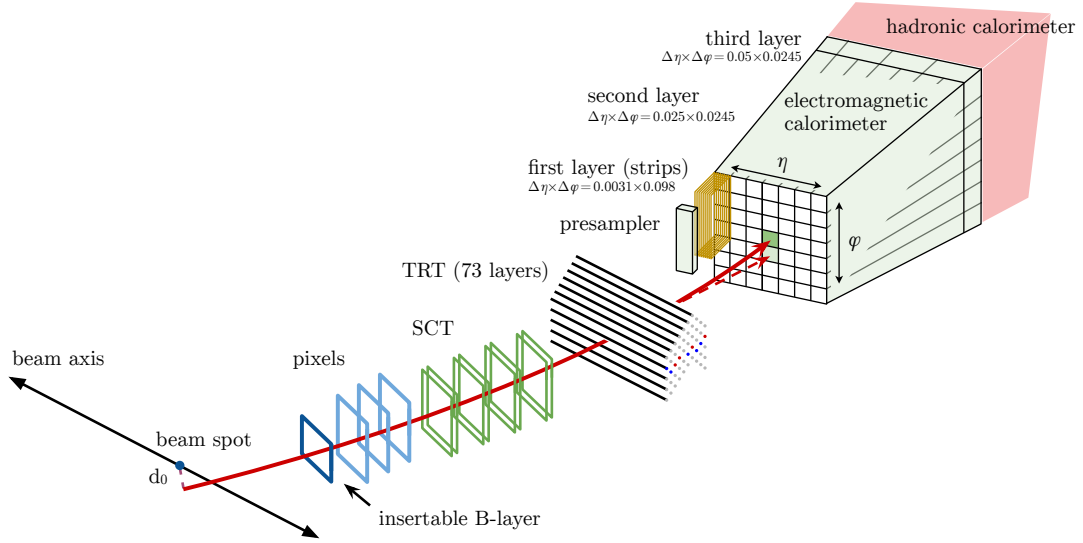


Figure 6.3: Overview of detection techniques involved in electron identification and reconstruction [11]

6.3 MUONS

Muons penetrate the calorimeters with minimal energy loss and can be reconstructed in the ID and MS independently. Track information in these subsystems (with additional information from the calorimeters to correct for multiple scattering and energy loss) are used to fully reconstruct muons. Muons in the MS are reconstructed by building up local track segments in each of its three station layers into full track candidates [117]. Muons can be further reconstructed in several types (summarized in Figure 6.4):

- Combined (CB) muons are obtained with a global refit of ID and MS track candidates accounting for deflection and energy loss in the calorimeters. These are the highest quality muons.
- Segment-tagged (ST) muons are those with complete ID tracks but and matched to at least one track segment in the MS.
- Calo-tagged (CT) muons consist of a complete ID track matched to a calorimeter deposit consistent with a minimum ionizing particle.
- Extrapolated (ME) muons consist of a sole MS track fit loosely constrained by the beamspot position. These are typical of muons in $2.5 < |\eta| < 2.7$ where the MS extends beyond the ID coverage.

Different muon types are used to define muon reconstruction working points with varying degrees of efficiency and background rejection. Medium quality muons used in the $t\bar{t}W$ measurement only use CB and ME muons. Additional quality requirements are imposed on the compatibility between the q/p and p_T reconstructed in the ID and MS for CB muons. Isolation for muons is performed in a similar way to electrons, where an FCLoose isolation requirement is defined.

Single-lepton and di-lepton HLT can also be defined for muons that are seeded by L_1 triggers on deposits in the MS. These triggers are insensitive to identification and isolation working points

and so need not be calibrated separately for each. The tag-and-probe method is used to calibrate identification, isolation, and trigger efficiencies. Muons (and electrons) are affected by weak mode alignment imperfections in the ID and MS, resulting in a charge-dependent sagitta bias that must be corrected and calibrated [118].

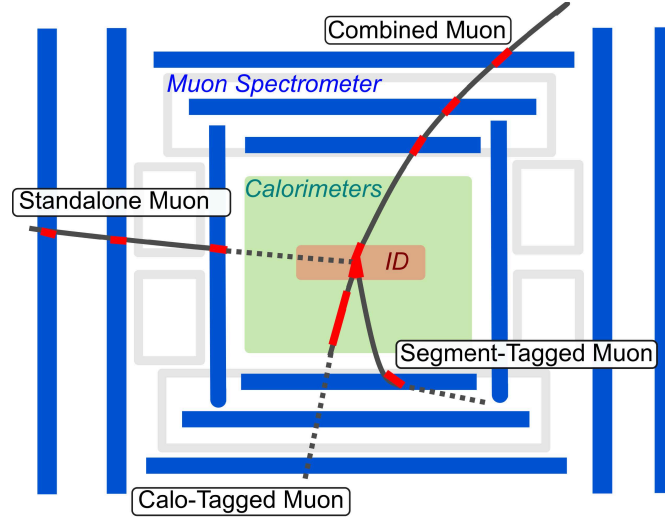


Figure 6.4: Overview of detection techniques involved in muon identification and reconstruction [12]

6.4 JETS

Energetic quarks and gluons fragment and hadronize to form highly collimated particle ejections called jets. They are reconstructed by their energy deposition in the electronic and hadronic calorimeters in $|\eta| < 4.9$ into topological clusters (TopoClusters). The reconstruction of jets in the calorimeters into topological clusters is similar in principle to the reconstruction of electromagnetic showers in the LAr calorimeter, but is complicated by large and irregular shower shapes of hadronic showers and higher levels of detector noise. TopoClusters can be combined with tracking information of charged hadrons in the region $|\eta| < 2.5$ using the particle flow algorithm [119].

The particle flow reconstruction algorithm attempts to match tracks to individual TopoClusters based on pointing direction and compatibility of track momentum and cluster energy. Steps to merge split calorimeter clusters, TopoClusters matched to a track are removed, and remnant cell deposits consistent with upward energy fluctuations of the shower are also removed and associated to the track. After the associations between the collection of TopoClusters and tracks are made, they are passed into the anti- k_T clustering algorithm with radius parameter 0.4 [120] implemented in FastJet [121].

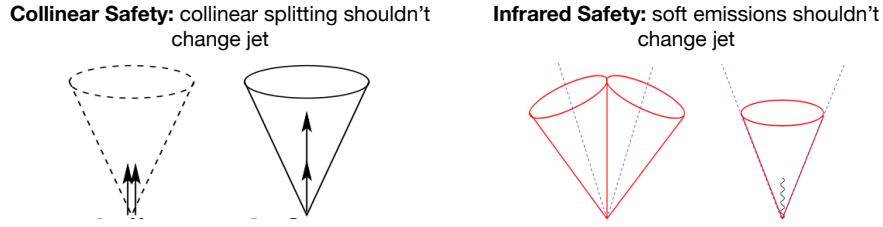


Figure 6.5: Sketch of IR and collinear unsafe effects

The anti- k_T algorithm is one of a family of three sequential clustering algorithms of a collection of objects (e.g. particles, tracks, TopoClusters). These have the important features of collinear and infrared (IR) safety, meaning that the clustering output should be insensitive to radiation. These effects are sketched in Figure 6.5. The Clustering relies on the definition of a distance measure between objects d_{ij} and between objects and the beam d_{iB} . The algorithm proceeds in the following steps:

1. Calculate $\{d_{ij}\}$ for all objects in the event
2. Beginning with the smallest d_{ij} :
 if $d_{ij} < d_{iB}$: replace objects i, j with $i + j$ (where the sum is addition of 4-momentum)
 else: i is a clustered jet, remove it from the collection.
3. Repeat from step 2 until all clustered objects are removed

The distance measure can be defined with the choice of R and p :

$$d_{ij} = \min \left(k_{T,i}^{2p}, k_{T,j}^{2p} \right) \frac{\Delta R_{ij}^2}{R^2} \quad (6.1)$$

$$d_{iB} = k_{T,i}^{2p}, \quad \Delta R_{ij} = (y_i - y_j)^2 + (\phi^2 - \phi_j)^2 \quad (6.2)$$

There are three main choices for p : $p = 1$ (k_T), $p = 0$ (Cambridge/Aachen), and $k = -1$ (anti- k_T).

These three choices progressively yield more conically shaped clusters and increased robustness to soft QCD features due to the increased importance of hard radiation. The typical choice for R is 0.4, which in the anti- k_T algorithm can be considered as the jet width parameter. Figure 6.6 shows a comparison of jets clustered with the different algorithms.

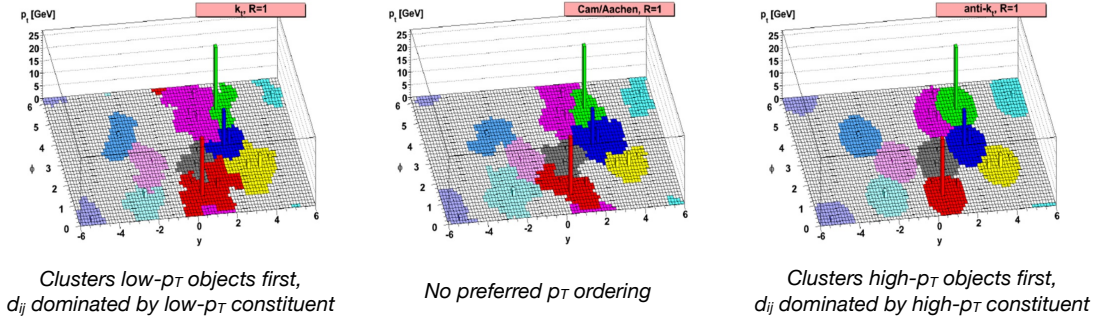


Figure 6.6: Examples of sequentially clustered jets among three commonly used algorithms

Particle flow jets are calibrated in the momentum range $20 < p_T < 1500$ GeV, where the primary attributes of interest are the absolute jet energy scale (JES) and the jet energy resolution (JER). In the first step, jets are corrected for pile-up contamination using the jet ghost-area subtraction method [122, 123]. A numerical inversion based on Monte Carlo simulation of di-jet events corrects the JES to match the jet response at particle level [124]. Remaining fluctuations in the JES and JER are corrected using the global sequential correction process [125]. In it, a sequence

of multiplicative corrections are applied to jets that are each a function of the jet p_T and another jet structure variable (e.g. amount of energy deposited into the hadronic/electromagnetic calorimeter layers) binned in η of the jet. Finally, an in-situ calibration step is performed to correct for residual mis-matches in the JES to data using Z +jet, γ +jet, and multi-jet events [126].

A total of 65 systematic uncertainties are defined for the reconstruction and calibration procedure, each of which is handled in a likelihood fit by a nuisance parameter (NP). These set of NP are reduced to a set of 24 based on a reduction scheme that carefully treats the correlations of the largest eigencomponents while simplifying subdominant eigencomponents with approximate correlation schemes [124]. Uncertainties are derived separately for light jet and heavy flavor jets and uncertainties are derived based on the differences in response for quark and gluon-initiated jets.

Jets originating from b -quarks or c -quarks (i.e. heavy flavor jets) are identified by the presence of a secondary vertex in a jet that is characteristic of heavy B and D hadrons' time of flight. Track-based information of jets reconstructed within the ID coverage of $|\eta| < 2.5$ are tagged using b/c -tagging algorithms [127]. Multiple approaches are used: the IP3D algorithm [128] identify tracks with large impact parameters relative to the PV using a 3D likelihood estimation, the SV1 algorithm [129] attempts to reconstruct all secondary vertices of a jet, and the JetFitter algorithm [130] attempts to reconstruct the full decay chain of the b - to c -hadron decay chain.

These low-level inputs are fed into a deep feed-forward neural network called DL1 [128]. The DL1 algorithm is augmented with additional input from the RNNIP algorithm [131], an impact parameter-based *Recurrent Neural Network* (RNN) that accounts for inter-track correlations where the IP3D algorithm does not. The augmented algorithm is referred to as DL1r and is the latest and most powerful b -tagging algorithm used by ATLAS. Figure 6.7 shows the typical signature of a b -jet.

Heavy flavor tagging efficiencies are calibrated to data using the characteristic $t \rightarrow Wb$ topology of fully-leptonic $t\bar{t}$ events in which the leptonic decays are opposite flavor (one electron and one muon) [127]. Multiple working points with fixed b -jet efficiencies (60%, 70%, 77%, and 85%) with decreasing c -jet and light jet rejection factors are available. A pseudo-continuous calibration of these working points is performed to allow a mixture of these working points to be used while taking into account the pattern of correlations between the exclusive fixed efficiency working points.

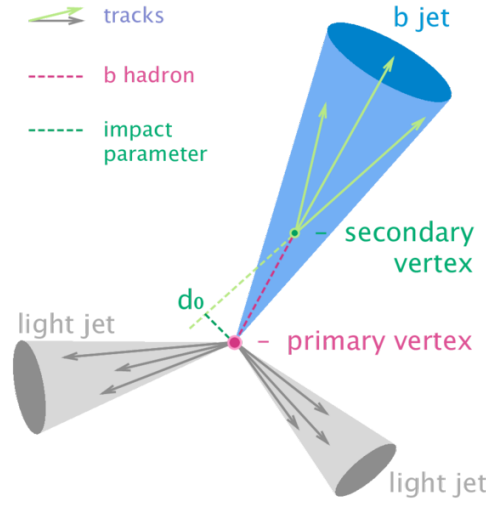


Figure 6.7: Diagram showing the characteristic secondary vertex associated to a b -hadron decay within a jet

A *Jet Vertex Tagger* (JVT) algorithm [132] has been developed by ATLAS to help reject jets originating from pile-up vertices in the same bunch crossing. It is based on the fraction of a jets track p_T that are associated with each PV and similar variables that additionally take into account the total jet p_T with pileup subtraction and the dependence on total number of tracks in the event. Signal jet efficiencies of 90% are achieved with a pileup fake rate of 2.2%. Separate calibrations are performed for b -jets, as the presence of a secondary vertex requires special treatment when assigning jet vertex fractions and the like.

6.5 E_T^{miss}

Neutrinos are produced in leptonic decays of the top quark and W boson. They carry away some fraction of the events total energy as they exit the ATLAS detector without interaction. While the total momentum of the hard scattering interaction along the beam axis is unknown due to the proton PDF, the total transverse momentum is constrained to zero. The missing transverse energy can be reconstructed as the negative sum of all visible p_T :

$$\vec{E}_T^{\text{miss}} \equiv - \sum_{j \in \text{objects}} \vec{p}_{T,j} - \sum_{j \in \text{soft}} \vec{p}_{T,j} \quad (6.3)$$

where hard objects are fully calibrated reconstructed objects (jets, leptons, photons) and the soft term captures low-momentum tracks associated to the hard-scatter PV that are not reconstructed as part of an object [133]. An overlap removal procedure is defined to remove double-counted tracks in the hard term. The vector quantity $\vec{E}_T^{\text{miss}}$ can also be written like $(E_T^{\text{miss}}, \phi)$ since it is constrained in the transverse direction. The E_T^{miss} scale is calibrated in $Z \rightarrow \mu\mu$ decays, where value of E_T^{miss} projected along the precisely reconstructed $\vec{p}_T^Z$ axis has a zero expectation value for unbiased E_T^{miss} reconstruction. A systematic underestimate of the soft term is expected (and corrected for) since neutral particles, charged particles with $|\eta| > 2.5$, and charged particles with $p_T < 500$ MeV or poor quality are not reconstructed. The E_T^{miss} resolution is measured in $W \rightarrow e\nu$ or $t\bar{t}$ events (where true $E_T^{\text{miss}} > 0$) and in $Z \rightarrow \mu\mu$ events (where true $E_T^{\text{miss}} = 0$) [133]. Resolution decreases gradually as a function of $\langle\mu\rangle$ but is driven primarily by jet resolution, leading to the general dependence of E_T^{miss} on $H_T \equiv \sum E_T$ of $\sigma(E_T^{\text{miss}}) \propto \sqrt{H_T}$.

For production processes like semi-leptonic and fully-leptonic $t\bar{t}$ production, E_T^{miss} can be as-

signed unambiguously to up to 2 neutrinos using M_t and M_W mass constraints in a kinematic likelihood (KL) fit [134]. The measurement of $t\bar{t}W$ cannot utilize a KL fit because the decay kinematics under-constrain the assignment of E_T^{miss} to 2 or 3 neutrinos in the final state.

Part IV

Measurements

7

Phenomenology of $t\bar{t}W$ Production

The only Feynman diagram that enters into $t\bar{t}W$ production in pp collisions at leading order (LO) in QCD corresponding to $\mathcal{O}(\alpha_s^2\alpha)$ is shown in Figure 7.1. Since the only available initial state for $t\bar{t}W^+$ ($t\bar{t}W^-$) at LO is $u\bar{d}$ ($d\bar{u}$) and the valence quark content of the proton is uud , the ratio of W^+ to W^- production is roughly 2:1. In light of the multi-lepton excesses that have been discussed in Chapter 2, many studies of $t\bar{t}W$ phenomenology and modeling have been published over the last few years. This chapter will give an overview of NLO effects [135, 136, 137, 15, 138, 139], off-shell effects [140, 141], calculations at NLO+NNLL QCD [17], EFT interpretations [16], and

charge asymmetries [13] and will present the modeling of $t\bar{t}W$ with MC samples used within the differential measurement in view of these theoretical studies. Proceedings that summarize some aspects of this body of work can be found in [142, 143, 14].

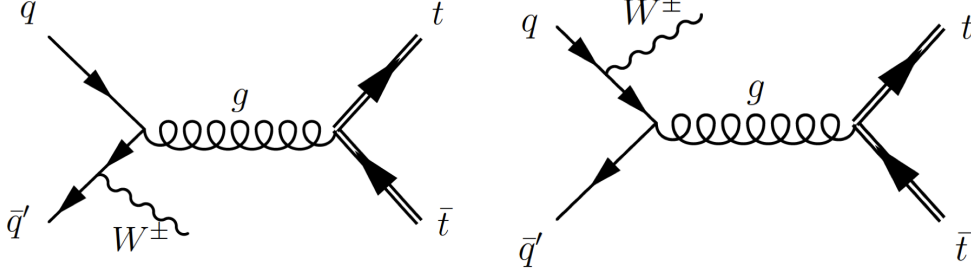


Figure 7.1: Leading order Feynman diagrams for $t\bar{t}W^\pm$ production at the LHC [13]

7.1 BEYOND LEADING ORDER

Contributions beyond LO in QCD can be summarized as follows:

$$\sigma_{\text{QCD+EW}}^{\text{NLO}} = \underbrace{\sigma_{\text{QCD}}^{\text{LO}}}_{\mathcal{O}(\alpha_s^2\alpha)} + \underbrace{\delta\sigma_{\text{QCD}}^{\text{NLO}}}_{\mathcal{O}(\alpha_s^3\alpha)} + \underbrace{\delta\sigma_{\text{EW}}}_{\mathcal{O}(\alpha^3), \mathcal{O}(\alpha_s\alpha^3)} \quad (7.1)$$

These contributions to $t\bar{t}W$ production entering in at various orders in α_s and α are summarized in Figure 7.2. Working through these terms systematically, we begin by noting the LO QCD term described above. The mixed LO term $\mathcal{O}(\alpha_s\alpha^2)$ does not contribute since no diagrams can be drawn for it. A representative LO EW diagram at $\mathcal{O}(\alpha^3)$ is shown in Figure 7.3, where the gluon is replaced by γ/Z . There is no interference between the non-vanishing LO diagrams since the $t\bar{t}$ is a color octet (singlet) in the LO QCD (EW) production.

The most dominant NLO contribution comes at $\mathcal{O}(\alpha_s^3\alpha)$, depicted in Figure 7.3. Terms at $\mathcal{O}(\alpha_s^2\alpha^2)$ affect $t\bar{t}W$ production only through the production of an additional heavy boson [137],

which is not only a very small effect but is a separable physical process. It is therefore generally neglected. Terms at $\mathcal{O}(\alpha_s \alpha^3)$ had initially been thought to be negligibly small [136], but later work indicated that this may not be the case due to internal $tW \rightarrow tW$ scattering [15]; this subject is elaborated below. Finally, terms at $\mathcal{O}(\alpha^4)$ have been shown to be small, as expected by the $1/\alpha$ suppression relative to $\mathcal{O}(\alpha^3)$, primarily coming from $q\bar{q}' \rightarrow t\bar{t}W\gamma$ [15]. The $\mathcal{O}(\alpha^4)$ terms are therefore generally neglected.

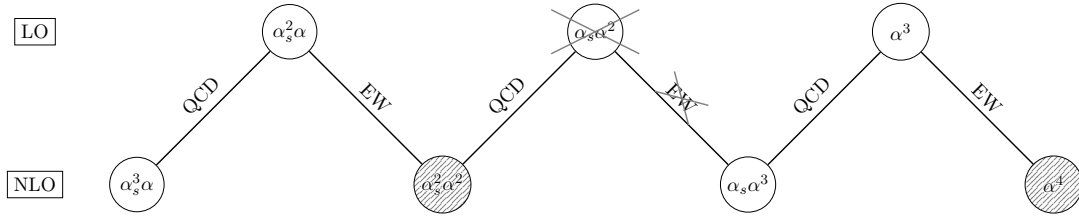


Figure 7.2: Summary of contributions considered for calculations of $t\bar{t}W^\pm$ inclusive cross section [14]

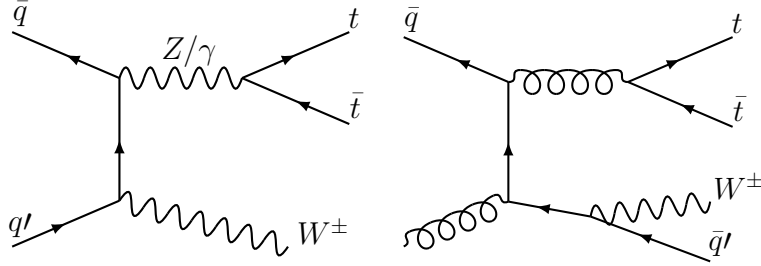


Figure 7.3: Representative Feynman diagrams for $t\bar{t}W$ production at $\mathcal{O}(\alpha^3)$ (left) and $\mathcal{O}(\alpha_s^3\alpha)$ (right) [15]. NLO terms are connected to LO terms from which they receive a factor of α_s (QCD line) or α (EW line).

Table 7.1: Inclusive cross sections for $t\bar{t}W^\pm$ at $\sqrt{s} = 13$ TeV [136]

Process	$\sqrt{s}$	$\sigma_{\text{QCD}}^{\text{NLO}}$	$\sigma_{\text{QCD+EW}}^{\text{NLO}}$	K_{QCD}	$\delta_{\text{EW}}[\%]$	Scale[%]	PDF[%]	$\alpha_s[\%]$
$t\bar{t}Z$	13	841.3(1.6)	839.3(1.6)	1.39	-0.2	+9.6% - 11.3%	+2.8% - 2.8%	+2.8% - 2.8%
$t\bar{t}W^+$	13	412.0(0.32)	397.6(0.32)	1.49	-3.5	+12.7% - 11.4%	+2.0% - 2.0%	+2.6% - 2.6%
$t\bar{t}W^-$	13	208.6(0.16)	203.2(0.16)	1.51	-2.6	+13.3% - 11.7%	+2.1% - 2.1%	+2.9% - 2.9%
$t\bar{t}W^- + t\bar{t}W^+$	13	620.6(0.36)	600.8(0.36)	1.50	-3.2	+12.9% - 11.5%	+2.0% - 2.0%	+2.7% - 2.7%

The $t\bar{t}W$ inclusive cross sections reported in the LHC Higgs Cross Section Working Group’s Yellow Report 4 (YR4) are given in Table 7.1. Their calculations indicate that NLO QCD corrections increase the inclusive cross section by 50% over the LO QCD calculation, while the EW corrections lead to more subtle effect of a 3.2% reduction. However, the calculation performed here only includes $\mathcal{O}(\alpha^3)$ terms in the EW correction term. It has been shown more recently [15] that $\mathcal{O}(\alpha_s\alpha^3)$ terms can increase the $t\bar{t}W$ cross section up to 10% inclusively and 20% differentially, for instance as in the N_{jet} distribution. Both effects are shown in Figures 7.4-7.5, driven primarily by internal tW scattering. This calculation is performed within MG5_AMC@NLO computed to NLO QCD + EW corrections and with a variable scale choice of $\mu_R = \mu_F = H_T/2$ using the NLO PDF4LHC PDF set. The top quarks are decayed to bW with branching fraction 100% and all W bosons are decayed inclusively to all possible leptonic and hadronic final states using the MADSPIN framework matched to PS. The authors select events where the top quark decays leptonically to muons and the W bosons decays leptonically to electrons. This is simply to keep track of the decay products of the $t\bar{t}$ system and the associated W boson. Finally, they consider events in which no selection is applied and in events with 2 leptons of the same charge ($2\ell SS$) or 3 leptons (3ℓ). Additional selections are imposed to mirror event selections of typical multi-lepton measurements.

Besides inducing large inclusive and differential effects, $\mathcal{O}(\alpha_s\alpha^3)$ terms can make $t\bar{t}W$ sensitive probe for some EFT operators affecting the $t\bar{t}Z$ coupling [16]. A more complete illustration of the tW scattering diagrams is shown in Figure 7.6 to clarify this fact. A dedicated effort within ATLAS to measure this contribution in the $t\bar{t}W + 1\text{jet}$ final state is ongoing and is not specifically targeted by the full differential measurement that is the subject of this thesis.

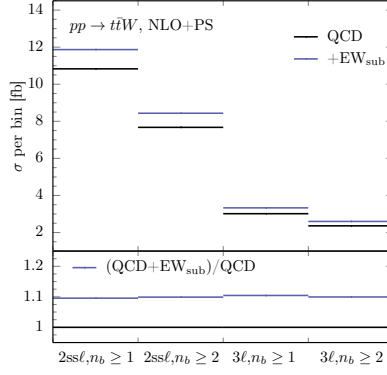


Figure 7.4: Effect of $tW \rightarrow tW$ scattering diagrams inclusively in lepton channels with varying thresholds on $N_{b\text{-jets}}$ [15]

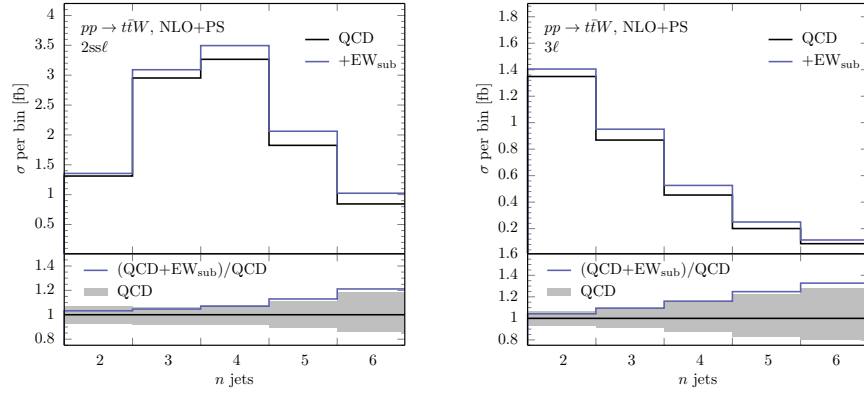


Figure 7.5: Effect of $tW \rightarrow tW$ scattering diagrams in N_{jets} [15]. The uncertainty band in the lower panels correspond to scale uncertainties.

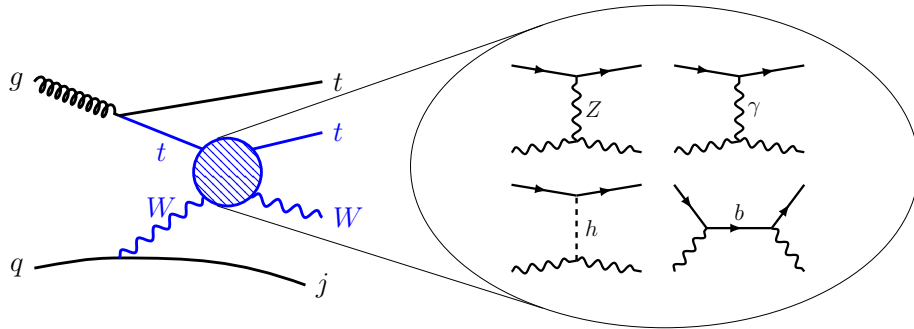


Figure 7.6: Feynman diagram involving tW scattering entering in EW corrections [16]

While the addition of NLO QCD and large NLO EW effects helps address the apparent theoretical underestimation of the inclusive $t\bar{t}W$ cross section, a NNLO QCD calculation is sorely needed. To demonstrate this fact, the NLO QCD calculation with soft resummation at NNLL was performed in [17]. In it, the authors calculate the inclusive cross section for $t\bar{t} + X$, with $X = W^\pm, Z, H$ at NLO QCD, +NLL, and NNLL in both the soft-collinear effective theory (SCET) and explicitly in QCD. Multiple nominal scale choices (μ_R and μ_F) are considered as a function of $Q = (p_t + p_{\bar{t}} + p_X)^2$ in and varied in $[\mu_0/2, 2\mu_0]$ to evaluate the theoretical uncertainty associated to neglecting higher order terms.

The comparison for the three processes is shown in Figure 7.7. In both $t\bar{t}H$ and $t\bar{t}Z$, the nominal cross section predicted among the different scale choices converges when including effects up to NLO+NNLL and the envelope of scale variations decreases. This indicates that additional terms at NNLO can safely be neglected for a precision theory prediction on the inclusive cross section. On the other hand, $t\bar{t}W$ shows persistent sensitivity to nominal scale choice as well as scale variation up to NLO+NNLL. This indicates that contributions at NNLO in QCD can be large. This can be understood as the effects of gg -initiated diagrams being pushed to NNLO, while gg -initiated production of $t\bar{t}Z$ and $t\bar{t}H$ occurs at tree level. In the present absence of a full calculation at this precision, the inclusive cross section must be obtained through experimental measurement.

The NWA simplifies calculations and allows production cross sections and branching fractions to factorize, in this case after the production of an on-shell W boson and top quarks. The first off-shell calculation was performed in [140] and most recently calculated by the same authors in [141]. Their calculation includes non-resonant W production in the full $pp \rightarrow \ell^+ \nu \ell^- \ell^\pm \nu b \bar{b}$ phase space using the HELAC-NLO framework at NLO QCD accuracy at $\mathcal{O}(\alpha_s^3 \alpha^6)$ and $\mathcal{O}(\alpha_s \alpha^8)$. Example diagrams are shown in Figure 7.8.

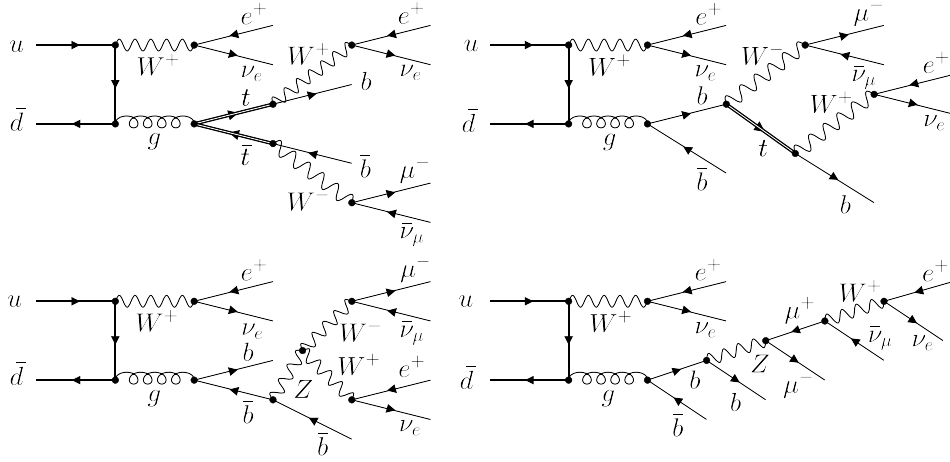


Figure 7.8: Representative Feynman diagrams for non-resonant $pp \rightarrow \ell^+ \nu \ell^- \ell^\pm \nu b \bar{b}$ production

The authors compare their calculation to a fixed-order NLO QCD+PS calculation and derive a simple correction term to approximate non-resonant and interference effects included in the off-shell calculation. The magnitude of these effects at the inclusive level are small but become relevant at the differential level, as can be seen in Figure 7.9. It is clear that these effects are subdominant to the EW corrections and spin polarization effects discussed in the following section.

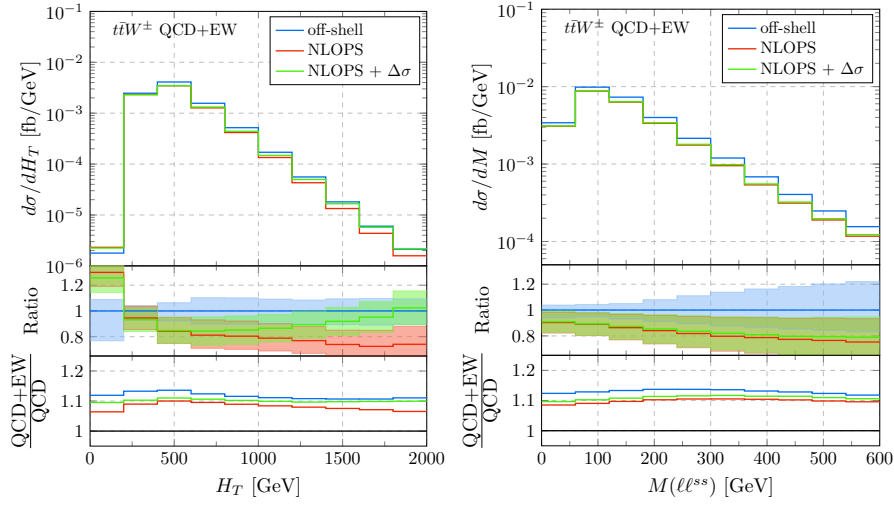


Figure 7.9: Comparison of $H_T = \sum_i p_{T,i}$ and $M_{\ell\ell}$ of the same-sign lepton pair in $2\ell SS$ events

7.3 CHARGE ASYMMETRIES

An interesting feature of $t\bar{t}W$ worth mentioning is its utility for studying the $t\bar{t}$ lepton charge asymmetry, which were studied in measurements of forward-backward asymmetry (A_{FB}) in $t\bar{t}$ events produced at $p\bar{p}$ experiments at the Tevatron [144, 145]. The effect enters at NLO QCD in $q\bar{q}$ -initiated production but not in gluon fusion, which is completely symmetric. The lepton charge asymmetry is defined by the quantity:

$$A_c^t = \frac{N(\Delta_\eta^t > 0) - N(\Delta_\eta^t < 0)}{N(\Delta_\eta^t > 0) + N(\Delta_\eta^t < 0)} \quad (7.3)$$

where $\Delta_\eta^t = |\eta_t| - |\eta_{\bar{t}}|$ [13]. However, a nonzero A_c^t arises only in $q\bar{q} \rightarrow t\bar{t}$, which constitutes 85% of $t\bar{t}$ events at the Tevatron and only 15% at the LHC. BSM physics that affects A_c^t are therefore challenging to see over the dominant s -channel $gg \rightarrow t\bar{t}$ production.

The characteristics of $t\bar{t}W$ discussed above make it a useful platform for measuring A_c^t at the

LHC. The first key benefit is that gg -initiated production is eliminated through NNLO in QCD.

A second benefit is that the emission of a W boson polarizes the initial state quark line, leading to polarized production of $t\bar{t}$ that are carried to their leptonic decay products. The measurement of A_c^t in $t\bar{t}W$ has a dedicated measurement effort within ATLAS and so is also excluded from the scope of this thesis.

While A_c^t will be neglected in the present measurement, a similar charge asymmetry variable dubbed the relative charge asymmetry A_C^R can be defined by

$$A_C^R = \frac{N(t\bar{t}W^+) - N(t\bar{t}W^-)}{N(t\bar{t}W^+) + N(t\bar{t}W^-)} \quad (7.4)$$

Since A_C^R is only sensitive to the relative rates of $t\bar{t}W^\pm$, it is insensitive to some systematic uncertainties that are correlated between $t\bar{t}W^+$ and $t\bar{t}W^-$. A_C^R can be measured inclusively and also differentially in any observable. The results of a recently published measurement [18] of $\sigma(t\bar{t}W^+)$, $\sigma(t\bar{t}W^-)$, and their ratio by the CMS collaboration are summarized in Figure 7.10. The persistent $t\bar{t}W$ -like excess with the full Run II dataset and experimental indication that the excess is more charge-symmetric further motivates the differential measurement of A_C^R , a key result of the the work of this thesis.

$$\begin{array}{ll} \sigma_{t\bar{t}W} = 868 \pm 40 \text{ (stat)}_{-50}^{+52} \text{ (syst) fb} & \sigma_{t\bar{t}W}^{\text{theo.}} = 592_{-96}^{+155} \text{ (scale)}_{-12}^{+12} \text{ (PDF) fb} \\ \sigma_{t\bar{t}W^+} = 553_{-29}^{+30} \text{ (stat)}_{-30}^{+31} \text{ (syst) fb} & \sigma_{t\bar{t}W^+}^{\text{theo.}} = 384_{-32}^{+52} \text{ (scale)}_{-8}^{+8} \text{ (PDF) fb} \\ \sigma_{t\bar{t}W^-} = 343 \pm 26 \text{ (stat)} \pm 25 \text{ (syst) fb} & \sigma_{t\bar{t}W^-}^{\text{theo.}} = 198_{-16}^{+26} \text{ (scale)}_{-5}^{+5} \text{ (PDF) fb} \\ R_{t\bar{t}W^+/t\bar{t}W^-} = 1.61_{-0.14}^{+0.15} \text{ (stat)}_{-0.05}^{+0.07} \text{ (syst)} & R_{t\bar{t}W^+/t\bar{t}W^-}^{\text{theo.}} = 1.94_{-0.24}^{+0.37} \end{array}$$

Figure 7.10: Summary of CMS measurements and corresponding theoretical predictions [18].

7.4 $t\bar{t}$ SPIN CORRELATIONS

The theorists who performed the calculation detailed in Section 7.1 also studied multiple spin-correlation effects in $t\bar{t}W$ production, considering effects of higher Björken x values probed by $t\bar{t}W^+$ than $t\bar{t}W^-$ (PDF effect), forward-backward asymmetry in the top pairs, the $V - A$ structure of the W boson couplings, and the polarization of the $t\bar{t}$ polarization that results from the W coupling, as described in Section 7.3. Figure 7.11 shows that the effect of $t\bar{t}$ polarization is dominant in terms of the η of the leptons from the top quarks. The impact on inclusive production event rates as a function of η_ℓ is shown in Figure 7.12, where the production of central (forward) leptons from t ($\bar{t}$) increases by 15% relative to the prediction without spin effects. This results in an increase in the acceptance of $t\bar{t}W^+$ into the event selection (via $|\eta| < 2.5$) and manifests in the differential cross section of N_{jets} in Figure 7.13. While the differential measurement does not intend to measure $\eta(\ell)$, the opposing effects of $t\bar{t}W^+$ and $t\bar{t}W^-$ acceptance will be discernible in the A_C^R measurements.

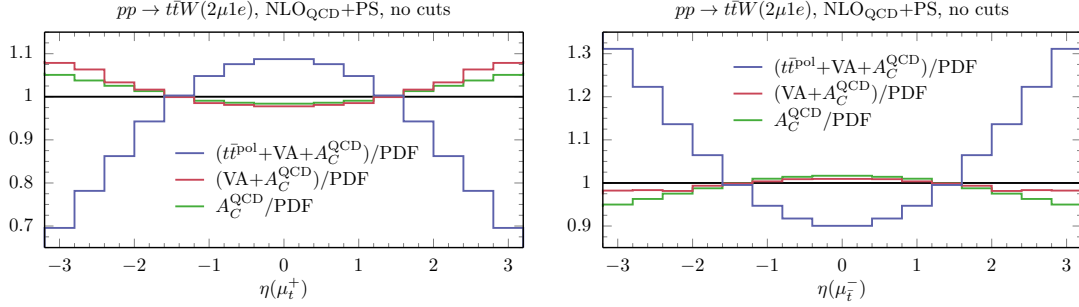


Figure 7.11: Comparison of multiple spin correlation effects relative to the PDF effect [15].

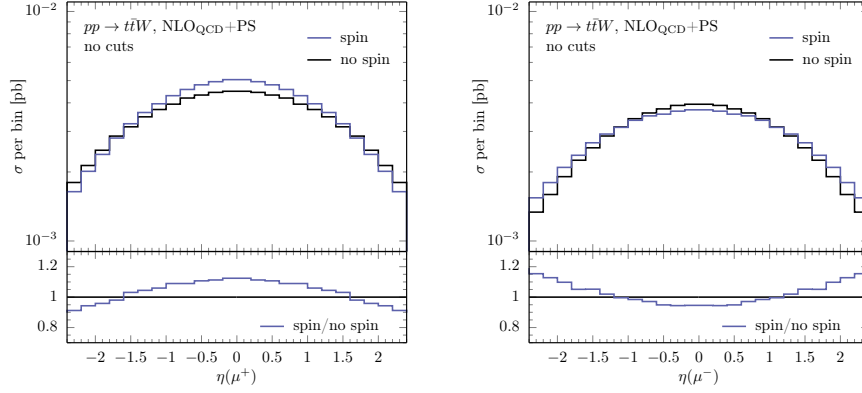


Figure 7.12: Effect of $t\bar{t}$ polarization with an inclusive event selection [15].

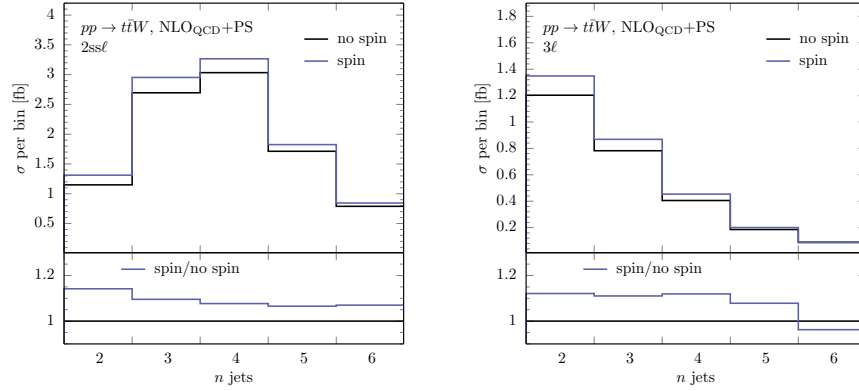


Figure 7.13: Effect of $t\bar{t}$ polarization on N_{jets} after event selection [15].

7.5 MONTE CARLO MODELING

It has been observed that calculations of $t\bar{t}W + 1j@NLO + 2j@LO$ using multi-jet merging can increase the inclusive cross section by up to 10% [139], where the FxFx scheme implemented in MG5_AMC@NLO was compared to fixed-order NLO QCD+PS. At the time of this writing, an FxFx sample centrally produced in ATLAS is not available but may ultimately be used within the analysis strategy. However, our nominal signal sample is generated at the same precision in the matrix element calculation implemented in SHERPA 2.2.10 with multi-jet merging performed using

the MEPS@NLO algorithm and a CKKW merging scale of 30 GeV [100]. This sample uses the NNPDF 3.0 NNLO PDF set. There are dedicated samples for the NLO QCD component and the EW corrections described in Section 7.1.

In addition to the SHERPA sample, we generate $t\bar{t}W$ at fixed-order NLO QCD sample using MG5_AMC@NLO with a separate sample for the EW corrections, both showered with PYTHIA 8. Finally, we also study events generated with POWHEG-BOX at NLO in QCD and showered using either PYTHIA 8 or HERWIG 7. The MG5_AMC@NLO sample is used as an alternate MC sample to define the primary theoretical uncertainty of both the matrix element and parton shower. It will be used until the FxFx sample becomes available. A list of signal MC samples considered within the analysis is given in Table 7.2. There is similar agreement of the NLO QCD cross section among the alternate samples, while that of the nominal SHERPA sample is higher by about 50 [fb]. This is due to the higher precision of its matrix element calculation using multi-jet merging.

Generator	Parton Shower	σ_{QCD}	σ_{EW}	σ_{QCD+EW} [fb]	$\frac{\sigma_{QCD+EW}}{\sigma_{QCD}}$
SHERPA 2.2.10	SHERPA 2.2.10	597	42	639	1.07
MG5_AMC@NLO	PYTHIA 8	548	57	605	1.10
POWHEG-BOX	PYTHIA 8	558	49	607	1.09
POWHEG-BOX	HERWIG 7	558	49	607	1.09

Table 7.2: Summary of various $t\bar{t}W$ samples considered and inclusive cross section prediction.

The modeling of differential $t\bar{t}W$ production is compared among all available samples in Figures 7.14-7.15. Observables are defined at the particle-level in an inclusive event selection (to be described in detail in Chapter 10). The observables shown are those that will be unfolded in the final measurement. The effects of EW corrections are consistent with what has been observed in the literature, where dimensionful variables and jet multiplicities see an increase in cross section predominantly in the tails up to 20%.

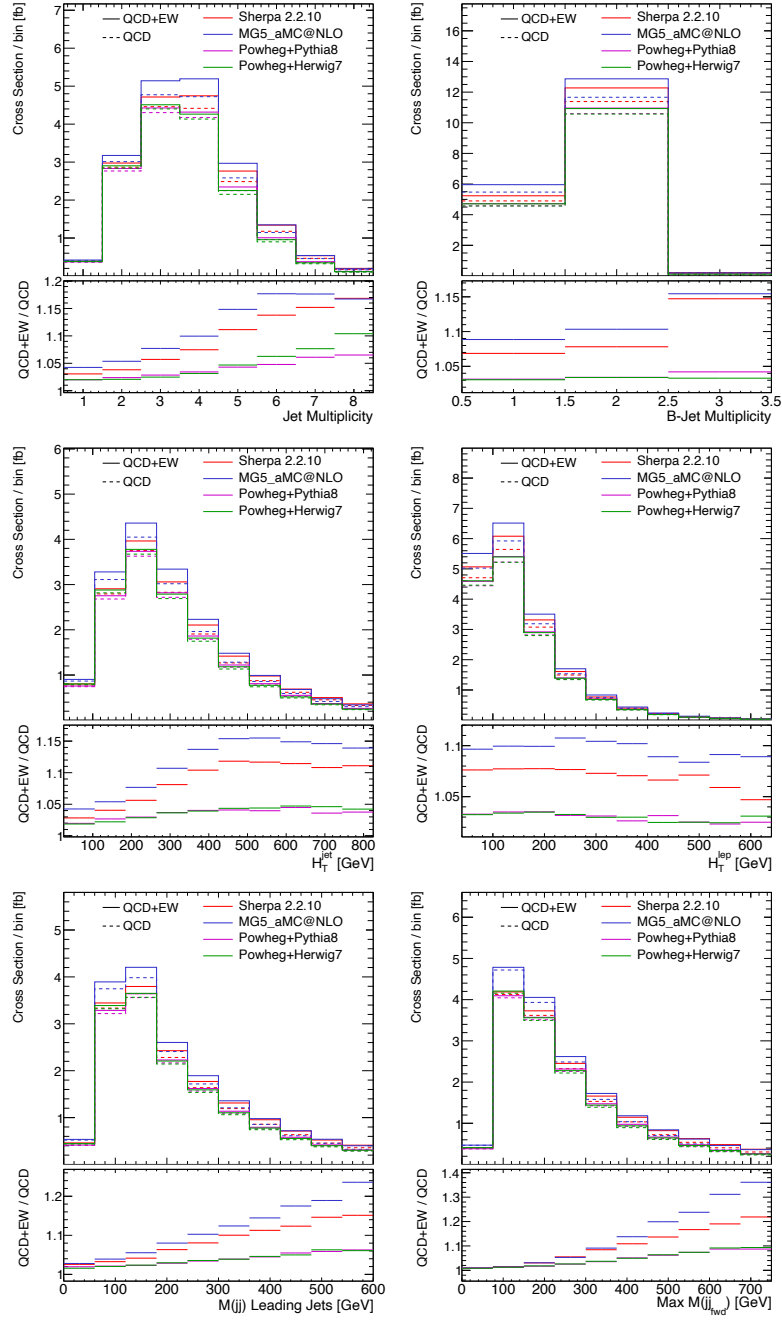


Figure 7.14: Modeling comparisons between available MC signal samples (1)

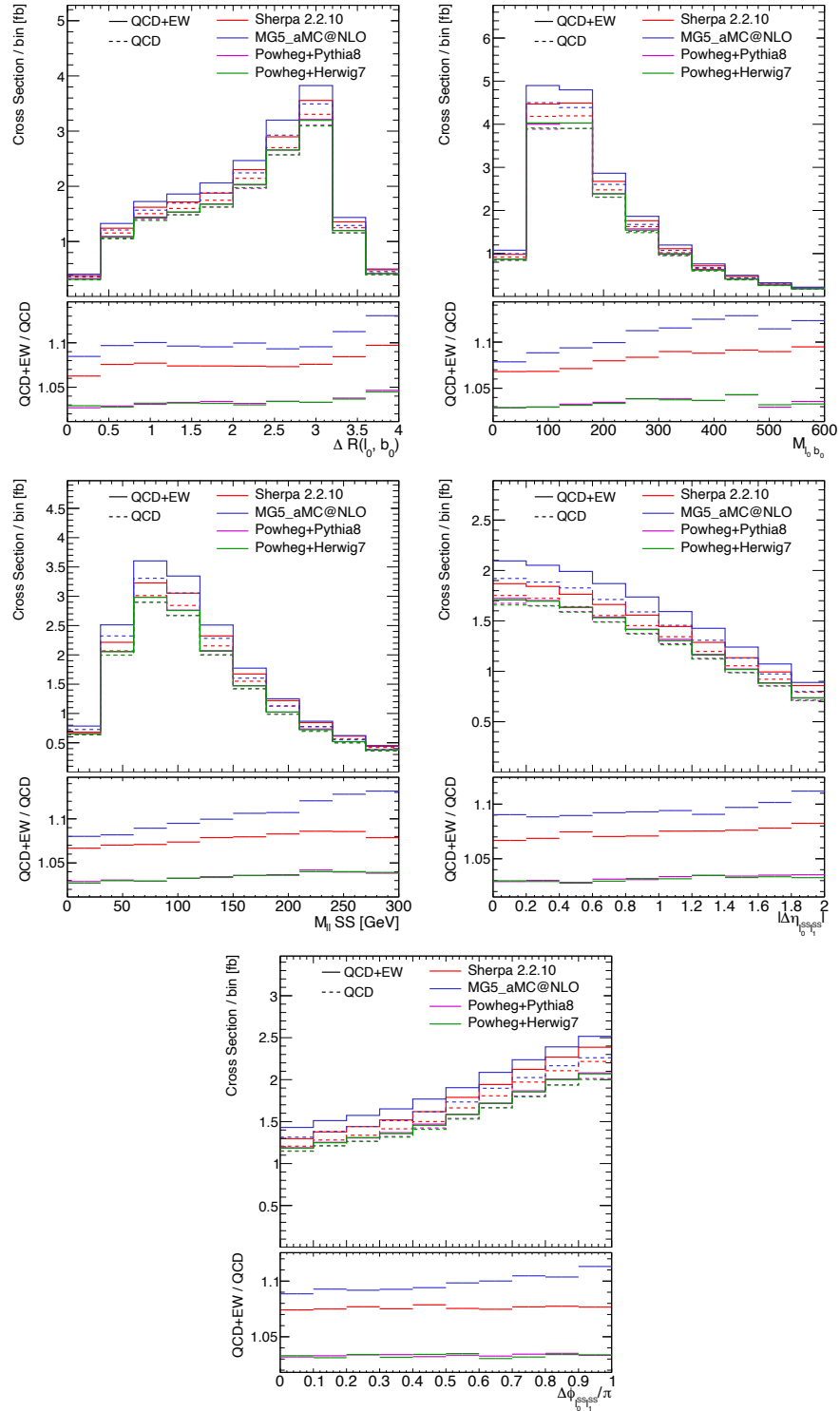


Figure 7.15: Modeling comparisons between available MC signal samples (2)

8

Background Modeling

The top quarks and W boson produced in $t\bar{t}W$ events are extremely short-lived and we can therefore only detect their decay products. Since $|V_{tb}| \gg |V_{td}|, |V_{ts}|$ the top quark decays essentially only to Wb , so $t\bar{t}W^\pm \rightarrow W^+W^-W^\pm b\bar{b}$. The signatures of $t\bar{t}W$ production are then driven primarily by the W boson branching fractions but also the τ branching fractions. Taking combinations of all possible decays of the three W bosons yields the channel composition as a function of the number of light leptons ℓ observed in the event (including leptonic τ decays). Branching fractions and channel composition are shown in Table 8.1. The zero and one-lepton channels are

completely drowned in backgrounds including multi-jet and $t\bar{t}$ production. The two lepton channel with opposite sign ($2\ell OS$) is similarly dominated by di-leptonic $t\bar{t}$ production. The only usable channels are two leptons with same sign $2\ell SS$ and three lepton 3ℓ channels, which constitute only 5.5% of $t\bar{t}W$ events. In addition to this basic selection, we require the detection of 1 or 2 jets, one of which must be b -tagged.

With the basic event selection defined, we turn to the subject of background contamination in these channels. Backgrounds are composed of both promptly produced leptons (e.g. $t\bar{t}H$ and $t\bar{t}Z$) and from non-prompt leptons produced primarily in heavy flavor decays from semi-leptonic $t\bar{t}$ production. This chapter will outline the dominant backgrounds and the methods by which they are modeled and estimated.

Table 8.1: Branching fraction of W boson (left) and resulting channel composition

W Decay Mode	Branching Fraction	Light Leptons	Composition
$W \rightarrow \ell\nu$	21.6%	Zero	44.8%
$W \rightarrow \tau\nu$ (hadronic)	7.39%	One	41.3 %
$W \rightarrow \tau\nu \rightarrow \ell\nu$	4.01 %	Two (Opposite sign)	8.4 %
$q\bar{q}$	67.4%	Two (Same sign)	4.2%
		Three	1.3%

8.1 PROMPT BACKGROUNDS

The most dominant backgrounds where leptons are produced through the decay of heavy resonances at the primary vertex (prompt production) are $t\bar{t}H$, $t\bar{t}Z/\gamma^*$, and VV ($V = W, Z$) production. Other prompt backgrounds have much lower rates and are less significant. These include $t\bar{t}WW$, tZ , tWZ , $tHqb$, $t\bar{t}(t/\bar{t})$, $t\bar{t}t\bar{t}$, VVV , VH , and others. Details of the MC samples used to model these processes are given in Table 8.2.

As per the discussion of previous $t\bar{t}H$ measurements in multi-lepton final states, it has an overlapping final state phase space with $t\bar{t}W$ in the multi-lepton final states. Backgrounds from $t\bar{t}H$ production occur mostly in the $H \rightarrow WW^*$ modes with small additional acceptance of $H \rightarrow ZZ^*$ and $H \rightarrow \tau^+\tau^-$ decays with one or both τ decaying to leptons. The $t\bar{t}H$ background process are modeled with POWHEG-BOX at NLO using the NNPDF2.0NLO PDF set and interfaced with PYTHIA 8 with h_{damp} parameter set to $3/4 \times (m_t + m_{\bar{t}} + m_H) = 325$ GeV. The h_{damp} parameter limits the p_T of the first additional emission of the PS, which in turn limits the recoil of the $t\bar{t}$ system. Theoretical uncertainties are derived by varying the μ_R/μ_F scale choice in from $[0.5\mu_0, 2\mu_0]$ in the ME and PS calculations. Additional uncertainties on the ME and PS calculations are obtained by a comparison to samples produced with MG5_AMC@NLO +PYTHIA 8 and POWHEG +HERWIG 7.

The $t\bar{t}Z/\gamma^*$ process leads to a $t\bar{t}\ell^+\ell^-$ final state with the characteristic falling production in $m_{\ell\ell}$ with large resonance at m_Z . The dominant contribution from $t\bar{t}Z/\gamma^*$ is in the 3ℓ region, where $Z/\gamma^* \rightarrow \ell^+\ell^-$ and one of the top quarks decays leptonically. It is also possible to accept such events into the $2\ell\text{SS}$ region if one lepton falls out of the 3ℓ selection acceptance. This can occur if the opposite-sign lepton is soft (low p_T) or is erroneously reconstructed as another physics object (e.g. jets). Similarly, the 3ℓ regions may accept fully leptonic $t\bar{t}Z/\gamma^*$ decays where one lepton fails to be reconstructed. With a cross section of 840 fb computed at NLO in QCD [50] and a phase space highly overlapping with that of $t\bar{t}W$, $t\bar{t}Z/\gamma^*$ is a significant background. This is why it has been measured simultaneously with $t\bar{t}W$ in previous measurements by ATLAS [54]. The $t\bar{t}Z/\gamma^*$ process is modeled using MG5_AMC@NLO interfaced with PYTHIA 8 for PS separately for $1 < m_{\ell\ell} < 5$ GeV and $m_{\ell\ell} > 5$ GeV. Uncertainties on the A14 shower tune affecting ISR/FSR

are derived using alternate samples with the VAR3cvariation [146]. An uncertainty on the $t\bar{t}Z/\gamma^*$ PS is obtained by comparison with a MG5_AMC@NLO +HERWIG 7 sample. Renormalization and factorization scale uncertainties are derived in the typical way, as is done for $t\bar{t}H$.

Similar to the $t\bar{t}Z/\gamma^*$ process are the rare top quark decays. The production of $t\bar{t}$ can involve virtual photons γ^* as either ISR or FSR which decay into $\ell^+\ell^-$. Such photon (or equivalently the $\ell^+\ell^-$ photon decay products) are characterized by $m(\gamma^*)$ and $p_T(\gamma^*)$. The rare top decays are modeled by three different samples and a dedicated phase space overlap removal procedure is used to maximize the kinematic modeling precision. The first sample is described above in the $t\bar{t}Z/\gamma^*$ NLO sample, which covers $1 < m(\gamma^*) < 5$ GeV in which the photon is produced as ISR but not radiation from the top quark decay products (FSR). A second 8-body decay sample of $pp \rightarrow f\bar{f}b\bar{f}f\bar{b}\ell^+\ell^-$ is produced at LO accuracy in MG5_AMC@NLO through s -channel top quark propagators. It covers both ISR and FSR virtual photon production but also has a mass cutoff at $m(\gamma^*) > 1$ GeV. The last sample is of lower quality and is used to cover remaining regions of phase space. It is a POWHEG +PYTHIA 8 NLO $t\bar{t}$ sample including FSR photons simulated at leading log accuracy with the PYTHIA QED parton shower algorithm, populating the region $p_T(\gamma^*) > 0$ and $2m_{e/\mu} < m(\gamma^*) < 10$ GeV.

The production of two massive vector bosons $W^\pm Z$ and ZZ (collectively referred to by VV) also contributes significantly to the $t\bar{t}W$ phase space in unsurprising ways due to the possible combinations of leptonic and hadronic decays of the W and Z bosons. It is modeled using SHERPA 2.2.2 +1j@NLO. Theoretical uncertainties are also evaluated by varying μ_R and μ_F . It is known that VV modeling is poor at high N_{jets} , so a data-driven correction is derived in a VV -enriched validation region. It proceeds by fitting non-closure factors to a 3-parameter analytical function as-

suming no strong dependence on the flavor of additional jets. Systematic uncertainties are derived by varying the best-fit parameters within their fit uncertainties. Since these uncertainties are subdominant, they are multiplied by a factor 3 to be conservative with no negative effect to the final analysis sensitivity.

8.2 NON-PROMPT AND FAKE BACKGROUNDS

The primary source of non-prompt lepton production for the $t\bar{t}W$ measurement is semi-leptonic $t\bar{t}$ with a single lepton produced from the secondary decay of b -hadron from the $t \rightarrow Wb$ decay, with additional contributions from single-top, V +jets, and $V\gamma$ production. An illustration of HF fake lepton production is shown in Figure 8.1. Heavy flavor fakes are split into electron and muon channels (HFe and HF μ) based on the flavor of the same-sign lepton of lower p_T (subleading), as this is more likely to have come from the non-prompt production. An additional type of fake lepton backgrounds from these processes are internal and material conversions, which are separated based on the position of the $\gamma^{(*)} \rightarrow \ell^+ \ell^-$ conversion vertex (CV) and the invariant mass of the two tracks used to reconstruct the leptons, M_{trtr} . Internal conversions are those with a presumed virtual photon with a CV position $R < 20$ mm and M_{trtr} calculated at the PV of less than 100 MeV. Material conversions occur when an electron undergoes material interaction to produce a photon that converts to a lepton pair. They are defined as events in which a CV occurs with $R > 20$ mm and M_{trtr} calculated at the CV of less than 100 MeV. Conversion events generally come from trident events ($e^\pm \rightarrow e^\pm \gamma^* \rightarrow e^\pm e^+ e^-$), as shown in Figure 8.2. Heavy flavor and conversion fakes are estimated using a semi data-driven background estimation technique, where shape information of differential production is taken from MC and the normalization is fitted to data in control regions.

Table 8.2: Overview of used MC samples for different processes, including ME and PS generators

Process	Generator (alternative)	Parton Shower (alternative)	PDF	Tune
$t\bar{t}W$	SHERPA -2.2.10 (MG5_AMC@NLO)	SHERPA -2.2.10 (PYTHIA -8)	NNPDF 3.0 NNLO	SHERPA default
$t\bar{t}H$	POWHEG-BOX	PYTHIA 8	NNPDF 3.0 NLO / NNPDF 2.3 LO	A14
$t\bar{t}Z$	MG5_AMC@NLO	PYTHIA 8	NNPDF 3.0 NNLO	A14
$t\bar{t}\gamma$	MG5_AMC@NLO	PYTHIA -8	NNPDF 2.3 LO	A14
Rare top	MG5_AMC@NLO	PYTHIA -8	NNPDF 2.3 LO	A14
$t\bar{t}$	POWHEG-Box (POWHEG-Box) (MG5_AMC@NLO) (aMC@NLO)	PYTHIA 8 (HERWIG) (PYTHIA -8) (HERWIG)	NNPDF 2.3 LO	A14
Single-top (s -/ t -channels)	POWHEG-BOX	PYTHIA 8	NNPDF 2.3 LO	A14
tW	POWHEG-BOX	PYTHIA 8	NNPDF 2.3 LO	A14
$t\bar{t}WW$	MG5_AMC@NLO	PYTHIA -8	NNPDF 2.3 LO	A14
tZ	MG5_AMC@NLO	PYTHIA -8	CTEQ6L1	Perugia2012
tWZ	MG5_AMC@NLO	PYTHIA -8	NNPDF 2.3 LO	A14
tWH	MG5_AMC@NLO	PYTHIA -8	NNPDF 2.3 LO	A14
$tHqb$	MG5_AMC@NLO	PYTHIA -8	NNPDF 2.3 LO	A14
$t\bar{t}(t/\bar{t})$	MG5_AMC@NLO	PYTHIA -8	NNPDF 2.3 LO	A14
$t\bar{t}t\bar{t}$	MG5_AMC@NLO	PYTHIA -8	NNPDF 2.3 LO	A14
VV	SHERPA -2.2.2	SHERPA -2.2.2	NNPDF 3.0 NNLO	SHERPA default
VVV	SHERPA -2.2.2	SHERPA -2.2.2	NNPDF 3.0 NNLO	SHERPA default
$ggVV$	SHERPA -2.2.2	SHERPA -2.2.2	NNPDF 3.0 NNLO	SHERPA default
$V + \text{jets}$	SHERPA -2.2.1	SHERPA -2.2.1	NNPDF 3.0 NNLO	SHERPA default
VH	PYTHIA -8	PYTHIA -8	NNPDF 2.3 LO	A14
$V\gamma$	SHERPA -2.2.8	SHERPA -2.2.8	NNPDF 3.0 NNLO	SHERPA default

The choice of performing a semi-data-driven non-prompt background estimation rather than a fully data-driven estimation will be discussed in Chapter 9.

The $t\bar{t}$ events are generated using POWHEG-BOX at NLO in QCD interfaced with PYTHIA 8 for PS with $\mu_{R/F} = \sqrt{m_{\text{top}}^2 + p_{T, \text{top}}^2}$ calculated before radiation. The h_{damp} parameter is set to $1.5 \times m_{\text{top}}$. Alternative $t\bar{t}$ samples showered in HERWIG 7.1.3 are used to estimate PS uncertainties. Single top-quark production in s - and t - channels and tW production are simulated using POWHEG-BOX and PYTHIA 8 with the same MC settings as the $t\bar{t}$ samples. Since these single-top contributions are small, no alternate PS algorithm is used to derive uncertainties. These MC settings are chosen based on recommendations provided centrally within the ATLAS Collaboration [147]. A correction factor of 1.3 is applied to the $t\bar{t} + \geq 1b$ component that is underestimated in MC. This mis-modeling of $t\bar{t}$ is consistently demonstrated in the $t\bar{t}H(bb)$ [148] and $t\bar{t}t\bar{t}$ [149] measurements performed by ATLAS.

Additional fake lepton backgrounds come from electron charge misidentification, as described in Section 6.2, where electron material conversions produce conversion electrons that are misreconstructed (QMisID) as an electron with the incorrect charge. This may occur in trident events (see Figure 8.2) in which TopoClusters from conversion electrons are associated to the prompt electron instead of being reconstructed as separate electrons. The constraint from the TopoClusters may lead to a track fit with incorrect curvature. While the $t\bar{t}W$ analysis uses the ECIDS MVA tool to reject most of the QMisID contamination, what remains is estimated using a data-driven procedure that uses $Z \rightarrow e^+e^-$ events to determine QMisID rates as a function of electron p_T and η , since the hard bremsstrahlung depends on the electron p_T and the η -dependent detector material profile. Excess events with same-sign electron pairs within the m_Z window are assumed to originate

from $Z \rightarrow e^+e^-$ QMisID events, where the rate of electron QMisID is determined by a maximum-likelihood estimate of a Poisson likelihood function dependent on the QMisID rate, which range from 10^{-5} to 10^{-2} in the $t\bar{t}W$ phase space. See Appendix H of the $t\bar{t}W$ internal note [20] for additional information.

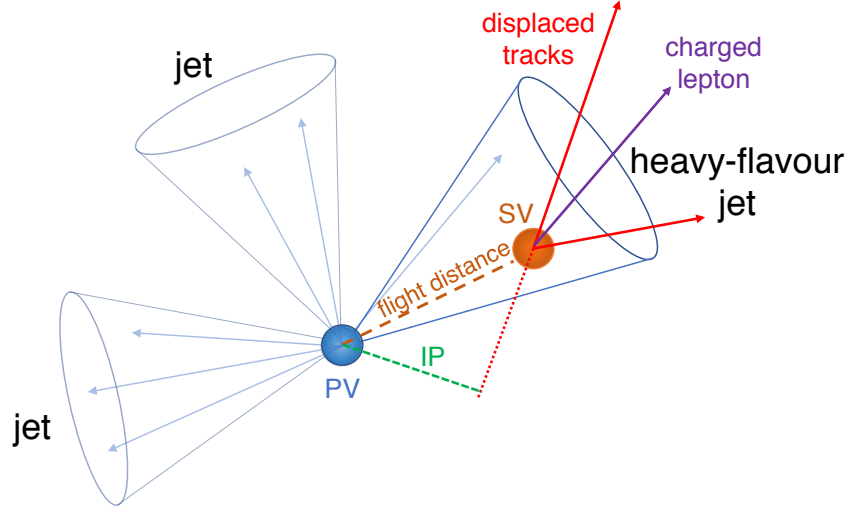


Figure 8.1: A cartoon depicting heavy flavor fake lepton production through the decay of a b -meson reconstructed as a secondary vertex [19]

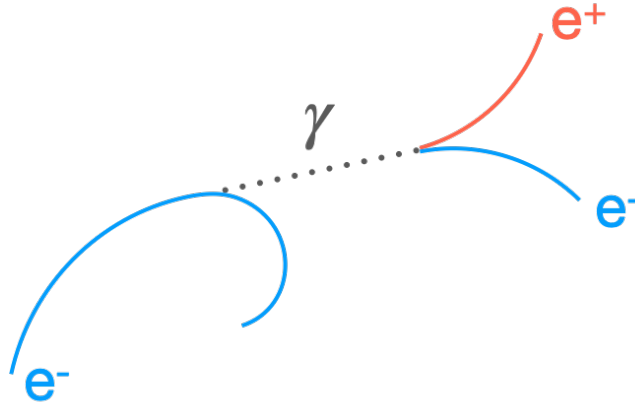


Figure 8.2: A depiction of a trident event

In the end, the classification of these production modes into specific background components

relies on a truth classification scheme used specifically for the ATLAS $t\bar{t}H$ and $t\bar{t}W$ multi-lepton analyses:

1. **Prompt.** This definition is used to define the non-prompt backgrounds including conversions, HF fakes. The category contains isolated muon or electron, muons with no truth origin defined, and electrons produced from photon conversion but the type of their parent particle is an isolated electron of the same charge.
2. **QMisID.** This definition includes electrons with reconstructed charge opposite of to that of its truth-matched electron charge
3. **Material Conversions.** Leptons with an assigned origin of a photon conversion but whose parent particle is not an isolated lepton.
4. **Internal Conversions.** Leptons whose parent type is a generating particle with non-defined origin
5. **Heavy flavor.** Leptons failing the above criteria.

9

Analysis Strategy

The greatest sensitivity to the $t\bar{t}W$ process comes in multi-lepton channels $2\ell SS$ and 3ℓ , in which the largest backgrounds come from prompt lepton production in $t\bar{t}H$, $t\bar{t}Z/\gamma^*$, and VV and from non-prompt and fake lepton production from HF decays and charge misidentification. The $t\bar{t}W$ measurement strategy is required to robustly estimate various background processes over a range of possible values for $\sigma(t\bar{t}W)$, since it is expected that the inclusive $t\bar{t}W$ signal strength will be 20%-70% higher than the NLO QCD prediction. The key choice for the measurement is how to handle the fake lepton backgrounds.

A fully data-driven method typically used within ATLAS for measuring non-prompt lepton backgrounds is called the *Matrix Method* (MM) [150], and was attempted in the $80 \text{ fb}^{-1} t\bar{t}H$ multilepton measurement [53]. The principle of the MM technique relies on defining *Control Regions* (CRs) orthogonal to the SR in which the total rate of non-prompt lepton production is measured. The SR and CR need to be similar enough that the composition of non-prompt lepton sources (e.g. HF fakes, conversions) is similar and an inclusive non-prompt lepton rate measurement in the CR can be reliably applied to the SR. On the other hand, the CR must be different enough from the SR that the contamination of the signal process is low in the CR and the non-prompt lepton measurement has low correlation with the signal strength.

A Tight and Loose lepton isolation criterion must be defined in each region. The *Prompt Lepton Improved Veto* (PLIV) algorithm is a powerful machine learning based tool for identifying non-prompt leptons and supports VeryTight, Tight, and Loose working points. For the purpose of the MM, the working points used are T (VeryTight) and L (Loose). The number of events with one tight (loose) lepton N^T (N^L) can then be written as

$$\begin{aligned} N^L &= N_R^L + N_F^L \\ N^T &= N_R^T + N_F^T = \epsilon_R N_R^L + \epsilon_F N_F^L \end{aligned} \tag{9.1}$$

where $\epsilon_{R/F} = N_{R/F}^T / N_{R/F}^L$ are the fraction of events with real/fake leptons passing the loose selection that also pass the tight selection. Equation 9.1 can be rearranged into a matrix equation and inverted, such that N_F^T can be calculated after $\epsilon_{R/F}$ are measured in the CR. The full implementation of the MM in the $t\bar{t}W$ measurement is given in Appendix F of the $t\bar{t}W$ internal note [20].

The MM is considered for $t\bar{t}W$ but was ultimately not used due to the difficulty in constructing

quality CR with low $t\bar{t}W$ contamination without explicitly using the PLIV tool for the CR definition. The background estimation strategy adopted for the $t\bar{t}W$ measurement is the semi data-driven *Template Fit* (TF) method, which relies on MC for modeling the shape of background distributions while fitting normalizations to data. In exchange, the TF method can use the PLIV tool in the definition of signal and control regions, allowing much better separation of the background and signal processes. Prompt and non-prompt backgrounds can be estimated simultaneously with the $t\bar{t}W$ signal strength measurement using the TF method as well, a desirable feature under the expectation that $\mu_{t\bar{t}W}$ will be pulled from unity.

This chapter will describe the definition of signal regions and control regions beyond the basic 2ℓ SS and 3ℓ lepton definitions, the description and implementation of the PLIV algorithm, systematic uncertainties, and the statistical formalism used to perform the measurement.

9.1 PROMPT LEPTON IMPROVED VETO

The PLIV is a multivariate tagger designed by the Isolation and Fake Forum of the ATLAS Collaboration to identify non-prompt leptons. It is a *Boosted Decision Tree* (BDT) that is trained on variables constructed from lepton and jet tracks. It is a powerful tool for rejecting fake leptons beyond the isolation cone method in situations where high- p_T secondary leptons are produced within a track jet but outside of a narrow isolation cone, as illustrated in Figure 9.1. If instead all tracks within the larger jet radius are considered, more information can be used to determine the nature of candidate leptons. The PLIV is trained for muons, barrel electrons ($|\eta_e| < 1.37$), and endcap electrons ($|\eta_e| > 1.52$) to maximize the performances in each case.

Three variables are defined that characterize the lepton and the track jet that is matched to the

lepton:

- The ratio of the lepton track p_T to the track jet p_T
- The ΔR between the lepton and the track jet central axis
- The lepton's momentum in the plane transverse to the track jet central axis (electrons only)
- Number of tracks within the track jet matched to the lepton (electrons only)

Four additional variables are defined that evaluate the isolation of the lepton to calorimeter clusters:

- The sum of electron cluster E_T divided by the electron track p_T (electrons only)
- Calorimeter cluster E_T associated to the muon divided by the E_T expected by a *Minimum Ionizing Particle* (MIP) (muons only)
- Sum of track p_T in a cone of $\Delta R < 0.3$ around the lepton track divided by lepton track p_T
- Sum of calorimeter cluster E_T in a cone of $\Delta R < 0.3$ around the lepton track divided by lepton track p_T

Finally, two variables sensitive to the *Secondary Vertex* (SV) are used:

- The score of a RNN trained to identify secondary vertices (the same used in the DL1r b -tagging algorithm)
- The longitudinal distance between *Primary Vertex* (PV) and SV reconstructed using tracks with $p_T > 500$ MeV divided by its uncertainty

The lepton p_T is also passed into the MVA with these variables during training and evaluation.

The PLIV output score evaluated for leptons in the $t\bar{t}W$ phase space are shown in Figure 9.2.

The VeryTight, Tight, and Loose working points are defined based on p_T -dependent cuts on the PLIV score to achieve a smooth efficiency as a function of lepton p_T [151]. These three working points are inclusive, in the sense that events passing the Loose WP will also pass Tight and Very-Tight. The innovation of the $t\bar{t}W$ TF measurement strategy is to define exclusive working points akin to pseudo-continuous b -tagging available within ATLAS. These exclusive working points can

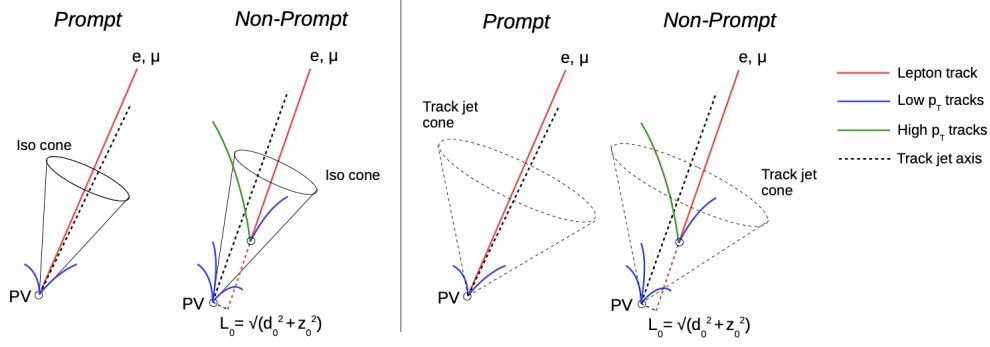


Figure 9.1: Example of non-prompt leptons that would not be identified using the isolation cone method (left) but could be identified if track jets are considered, as in PLIV (right)

then be used to define orthogonal signal and control regions enriched in the $t\bar{t}W$ signal and non-prompt backgrounds, respectively. The $t\bar{t}W$ analysis defines the Tight (T) exclusive working point as leptons passing the VeryTight PLIV WP and Medium (M) exclusive WP as leptons passing Tight but failing VeryTight (i.e. TightNotVeryTight). The definition of the exclusive working points as a function of p_T and PLIV is shown in Figure 9.3. The calibration of these analysis-specific working points will be discussed in Section 9.3.

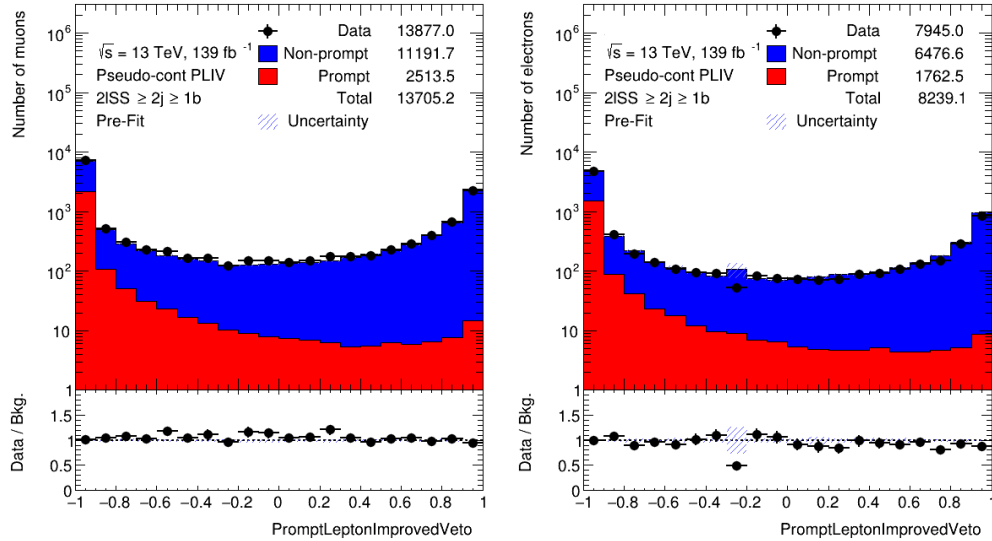


Figure 9.2: PLIV output score for electrons (left) and muons (right) in the $t\bar{t}W$ phase space [20]

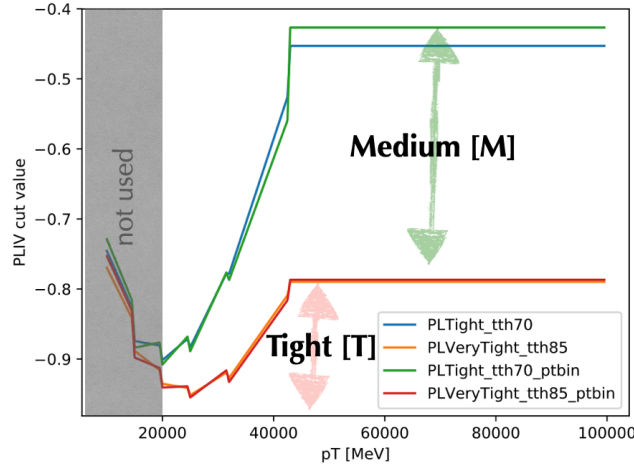


Figure 9.3: Exclusive PLIV working point definitions [20]. The p_T -dependent PLIV cuts are shown derived calibrated and uncalibrated lepton p_T , such that the `_ptbin` suffix is ultimately used with properly calibrated lepton p_T .

9.2 SIGNAL AND CONTROL REGION DEFINITIONS

Events in data recorded during the years 2015-2018 while detector subsystems were in good conditions are considered for this analysis. Events are required to have been selected by the lowest p_T -threshold un-prescaled dilepton *High Level Trigger* (HLT) given in Table 9.1. Electrons used to fire the HLT are required to pass the very loose or loose likelihood identification requirement without a requirement on d_0 . The addition of single lepton triggers does not increase the expected $t\bar{t}W$ significance against the background-only hypothesis because of the similar acceptance of $t\bar{t}W$ and non-prompt leptons. Single lepton triggers are therefore not considered.

A loose inclusive (Linc) preselection is used to define an initial set of leptons and jets which are used to define the 2ℓ SS and 3ℓ analysis channels. Electrons passing $p_T > 10$ GeV with $|\eta| < 2.47$ and $1.37 < |\eta| < 1.52$ are considered. Electron candidates are further required to pass the LooseLH electron identification working point and the FCLoose isolation working point. Elec-

Table 9.1: List of lowest p_T -threshold, un-prescaled dilepton triggers used for the Run 2 data taking periods. The strings lh(v)loose refer to electron identification requirements, nod0 refers to the absence of d_0 requirement, and L12EM10VH refers to the number of EM and hadronic calorimeter cells with energy above threshold in the L1 trigger algorithm that seeds the HLT.

Dilepton triggers (2015)		
$\mu\mu$	HLT_mu18_mu8noL1	$p_{T,HLT} \geq 18$ and 8 GeV
ee	HLT_2e12_lhloose_L12EM10VH	$p_{T,HLT} \geq 12$ GeV (both)
$e\mu, \mu e$	HLT_e17_lhloose_mu14	$p_{T,HLT} \geq 17$ (e) and 14 (μ) GeV
Dilepton triggers (2016)		
$\mu\mu$	HLT_mu22_mu8noL1	$p_{T,HLT} \geq 22$ and 8 GeV
ee	HLT_2e17_lhvloose_nod0	$p_{T,HLT} \geq 17$ GeV (both)
$e\mu, \mu e$	HLT_e17_lhloose_nod0_mu14	$p_{T,HLT} \geq 17$ (e) and 14 (μ) GeV
Dilepton triggers (2017 and 2018)		
$\mu\mu$	HLT_mu22_mu8noL1	$p_{T,HLT} \geq 22$ and 8 GeV
ee	HLT_2e24_lhvloose_nod0	$p_{T,HLT} \geq 24$ GeV (both)
$e\mu, \mu e$	HLT_e17_lhloose_nod0_mu14	$p_{T,HLT} \geq 17$ (e) and 14 (μ) GeV

tron tracks are required to have $|d_0|/\sigma_{d_0} < 5$ and $|z_0 \sin \theta| < 0.5$ mm with respect to the PV to be consistent with being produced by the hard scattering interaction. Muons with $p_T > 10$ GeV and $|\eta| < 2.5$ are considered. Candidate muons are required to pass the Loose identification working point, FCLoose isolation, and have $|d_0|/\sigma_{d_0} < 3$ and $z_0 \sin \theta < 0.5$ mm with respect to the PV. Preselection jets are reconstructed with the Particle Flow algorithm from jet tracks and TopoClusters clustered with the anti- k_T algorithm with $R = 0.4$. Jets are required to have $p_T > 25$ GeV and $|\eta| < 2.5$ while also passing the Tight working point of the JVT. Jets are considered in the overlap removal procedure before the JVT requirement is imposed. Finally, jets are b -tagged with the DL1r algorithm using pseudo-continuous b -tagging information.

An overlap removal (OR) procedure is performed to remove physics objects that are erroneously reconstructed from the same detector signatures. The OR procedure is chosen to maximize the reconstruction efficiency of leptons and b -tagged jets. A b -jet aware sequential OR procedure com-

monly used by ATLAS Supersymmetry searches is chosen [152], and proceeds as follows (using the 70% b -tagging working point)¹:

1. e/μ : if a muon and electron overlap with $\Delta R < 0.01$, the muon is removed if it is Calo-tagged (i.e. does not use any information from the MS) and the electron is removed otherwise
2. **Jet**/ e : if an electron and jet overlap with $\Delta R < 0.02$, the jet is removed if it is not b -tagged or if $p_T > 200$ GeV. The electron is not removed in any case.
3. **Jet**/ μ : if the muon is ghost-matched² to a jet within $\Delta R < 0.4$, the jet is removed if it is not b -tagged and has less than 3 tracks with $p_T > 500$ MeV. This condition is not frequently triggered.
4. **Jet**/ ℓ : if a jet overlaps with a lepton within $\Delta R = 0.04 + 10 \text{ GeV}/p_{T,\text{lep}}$ up to a maximum of 0.4, the lepton is removed. This variable OR cone removes low- p_T leptons more often as these are more likely to be reconstructed from jet tracks.

After the OR procedure is complete, the remaining leptons and jets are used to classify the event into the $2\ell\text{SS}$ and 3ℓ channels and are subject to the tighter M and T requirements. For electrons, the TightLH identification WP is imposed along with additional cuts to reject internal and external conversions. The electron ambiguity resolver is applied to reduce the mis-reconstruction of photons as electrons by approximately 11% [153]. Electrons are also required not to fall into the following categories:

- External conversion candidate: a *Conversion Vertex* (CV) is found with $R > 20$ mm and $M_{trtr} < 100$ MeV calculated at the CV
- Internal conversion candidate: not an external conversion candidate and $R < 20$ mm and $M_{trtr} < 100$ MeV calculated at the PV

¹Checks of the OR dependence on the b -tagging WP found the dependence to be ineffectual for the overall analysis sensitivity

²The ghost-association method matches tracks to calorimeter clusters by setting the track momentum to zero (a ghost) and clustered with calorimeter clusters [122]. In doing so, the p_T of calorimeter clusters that form jets are unaffected and the resulting clustering determine's the track's association to clustered jets.

Table 9.2: Loose inclusive (Linc), Loose exclusive (L), Medium inclusive (Minc), Medium exclusive (M), and Tight (T) light lepton definitions.

	e					μ				
	Linc	L	Minc	M	T	Linc	L	Minc	M	T
FCLoose isolation	Yes					Yes				
PLIV	No	PLIV < 0 and <i>not-Tight</i>	<i>Tight</i>	<i>Tight-not- VeryTight</i>	<i>VeryTight</i>	No	PLIV < 0 and <i>not-Tight</i>	<i>Tight</i>	<i>Tight-not- VeryTight</i>	<i>VeryTight</i>
Identification	Loose	Tight				Loose	Medium			
ECIDS	No	Yes				N/A				
Conversion rejection	No	Yes				N/A				
$ d_0 /\sigma_{d_0}$	< 5					< 3				
$ z_0 \sin \theta $	< 0.5 mm									

Electrons are additionally required to pass rejection by the *Electron Charge Identification Selector* (ECIDS) to reduce *Charge Misidentification* (QMisID) backgrounds. Medium and Tight muons are only required to additionally pass the Medium identification working point. Finally, leptons classified as M, Minc, and T are required to pass the Tight, TightNotVeryTight, and VeryTight PLIV WP. The various definitions of leptons are summarized in Table 9.2.

In both the 2ℓ SS and 3ℓ channels, SS leptons are required to have $p_T > 20$ GeV and pass the Tight lepton definition. Events in the 2ℓ SS (3ℓ) channel are required to have $N_{\text{jets}} \geq 2(1)$ and $N_{b\text{-jets}} \geq 1$. Finally, cuts on the invariant mass of the leptons are imposed to remove backgrounds coming from conversions and $t\bar{t}Z/\gamma^*$ production. In 2ℓ SS events, $m_{\ell\ell} > 12$ GeV for same flavor lepton pairs. In 3ℓ events, $m_{\ell\ell} > 12$ GeV for *Same-flavor opposite-sign* (SFOS) lepton pairs, $|m_{\ell\ell} - m_Z| > 10$ GeV for SFOS lepton pairs, and $|m_{3\ell} - m_Z| > 10$ GeV. The *Signal Region* (SR) definitions are summarized in Table 9.3. The 3ℓ channels are further split based on the number of SFOS pairs to further separate $t\bar{t}W$ from $t\bar{t}Z/\gamma^*$ and VV backgrounds. The expected yields in the SR are shown in Figure 9.4, where uncertainties are obtained after a fit to the Asimov dataset³

³The pseudodata obtained from the total yields of signal and background predictions is referred to as the Asimov dataset following ???. The name references Isaac Asimov’s “Franchise,” in which a single individual who best represents the population is chosen to cast political election ballots. By analogy, the Asimov dataset best represents the possible observed data given the SM hypothesis.

Table 9.3: Definition of the 2ℓ SS and 3ℓ SRs, which are both further split by their total charge (i.e. positive or negative). The leptons in the 3ℓ region are ordered such that lepton 0 has an opposite charge with respect to leptons 1 and 2 (i.e. the same-sign pair).

	2ℓ SS (+ + and - -)	3ℓ (+ and -)
N_{leptons}	= 2 (both passing Tight)	= 3 (passing Loose, Tight and Tight)
$\sum Q_{\ell,i}$	± 2	± 1
Lepton p_T	$p_T > 20 \text{ GeV}$	$p_{T,\text{OS}} > 10 \text{ GeV}$ $p_{T,\text{SS}} > 20 \text{ GeV}$
N_{jets}	≥ 2	≥ 1
$N_{b\text{-jets}}$	1@60% or at least 2@77%	1@60% or at least 2@77%
Inv. mass cuts	$m_{\ell\ell} > 12 \text{ GeV}$ for SF pairs	$m_{\ell\ell} > 12 \text{ GeV}$ for SFOS pairs $ m_{\ell\ell} - m_Z > 10 \text{ GeV}$ for SFOS pairs $ m_{3\ell} - m_Z > 10 \text{ GeV}$

without systematic uncertainties.

The CR used in the $t\bar{t}W$ measurement are summarized in Figure 9.5. In total, 10 CR are defined as follows and illustrated in Figure 9.5:

- *Heavy Flavor* (HF) CR: Six CR are defined in the 2ℓ SS channel where at least one of the leptons fails the VeryTight PLIV selection (e.i. TM, MT, MM). These regions are split by the flavor of the subleading lepton and binned in the subleading lepton's p_T . The transverse mass M_T of the dilepton- E_T^{miss} system is required to be less than 250 GeV⁴, which helps isolate $t\bar{t}$ events in which the only source of E_T^{miss} is a single $W \rightarrow \ell\nu$ decay, which has an upper bound of $M_T(\ell, \nu) \leq M_W$. They otherwise use the same object selections as the SR, including veto of conversion candidates.
- VV and $t\bar{t}Z$ CR: Two CR are defined in the 3ℓ channel where there is at least one SFOS lepton pair with $|m_{\ell\ell} - m_Z| < 10 \text{ GeV}$ (ensuring orthogonality with the 3ℓ SR). Leptons of the same charge are accepted passing the Minc definition. The VV CR includes events with 2 or 3 jets and exactly 1 b -jet (using the hybrid b -jet definition) and is primarily enriched in the $W^\pm Z$ background. A second CR targeting $t\bar{t}Z$ includes events with ≥ 4 jets and $\geq 1b$ -tagged jet. These regions are binned in $N_{b\text{-jets}}$.

⁴The transverse mass is defined as $M_T = \sqrt{2E_{T,1}E_{T,2}(1 - \cos \Delta\phi)}$ for massless particles with momenta $p_{1,2}$

- Conversion CR: Two CR are defined in the 3ℓ channel where the conversion veto criteria of the SR are inverted. Events are required to have no b -tagged jets to reduce the contribution of HF fakes. Events are not binned in any particular variable i.e. are counted in a single bin.

Normalization factors are applied to the $t\bar{t}Z$ +light, VV +HF, external conversion, internal conversion, $\text{HF}\mu$, and $\text{HF}e$ backgrounds and are freely floated in a fit to data. In this way, these semi-data-driven backgrounds estimations can be performed in the CR and extrapolated to the SR. Additional *Validation Region* (VR) are defined using a LooseNotTight selection on leptons for deriving corrections to VV backgrounds and non-closure uncertainties, which are summarized in Figure 9.6.

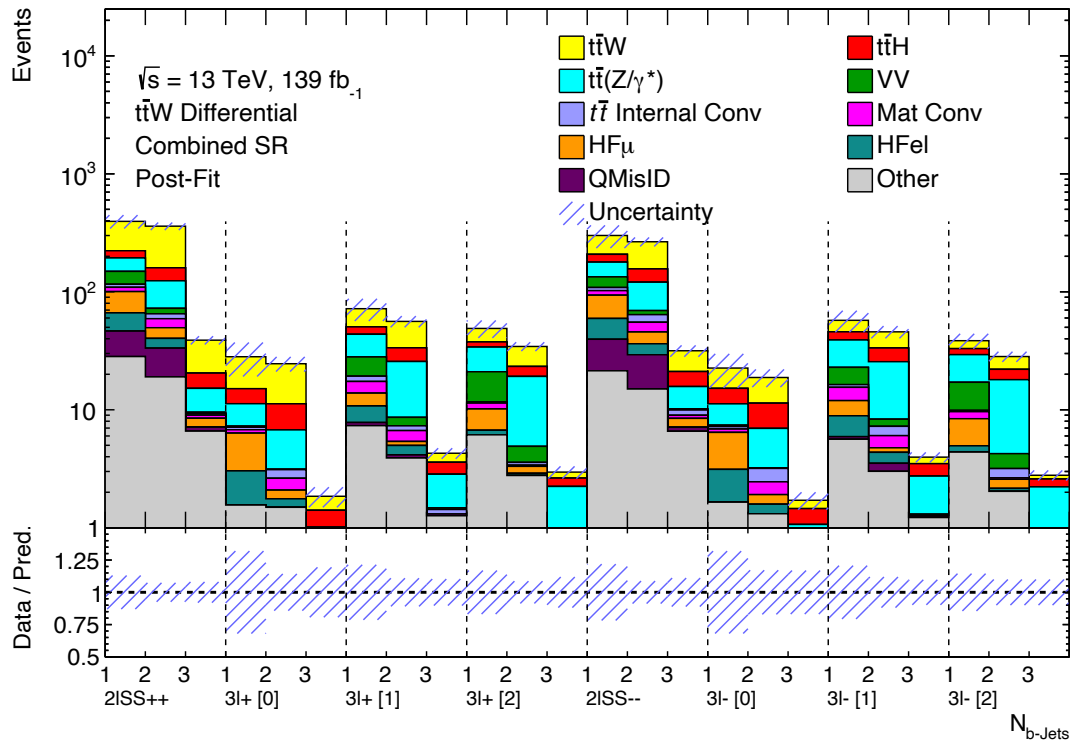
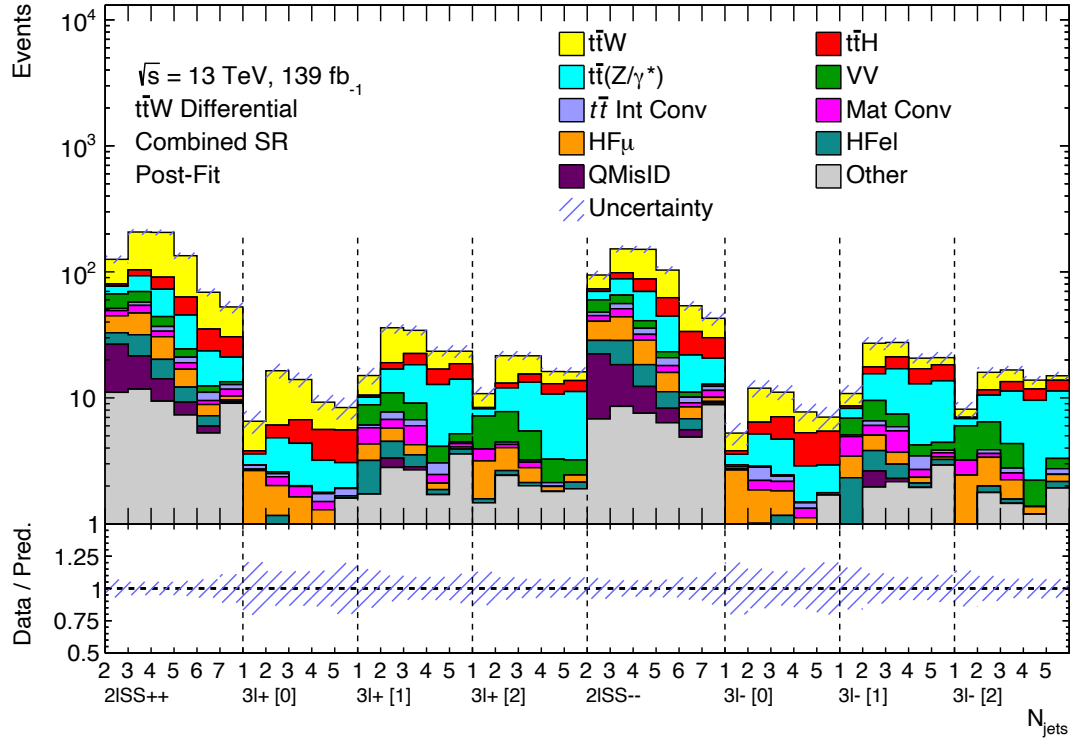


Figure 9.4: Expected yields in the $t\bar{t}W$ SR

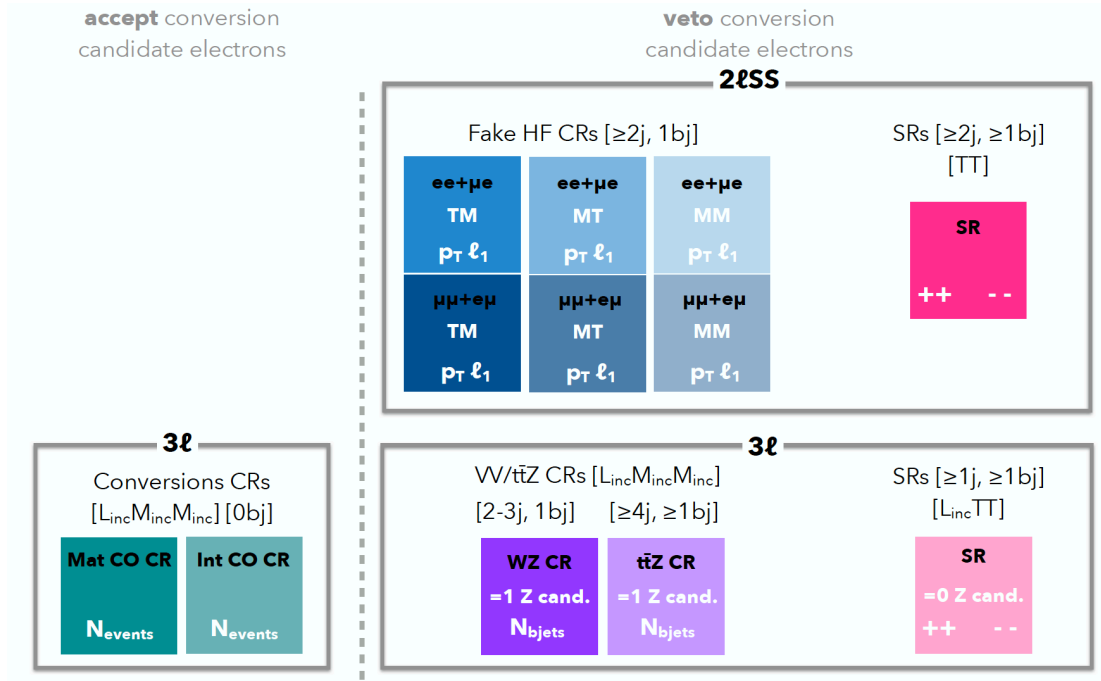


Figure 9.5: Illustration of SR and CR definitions [20]

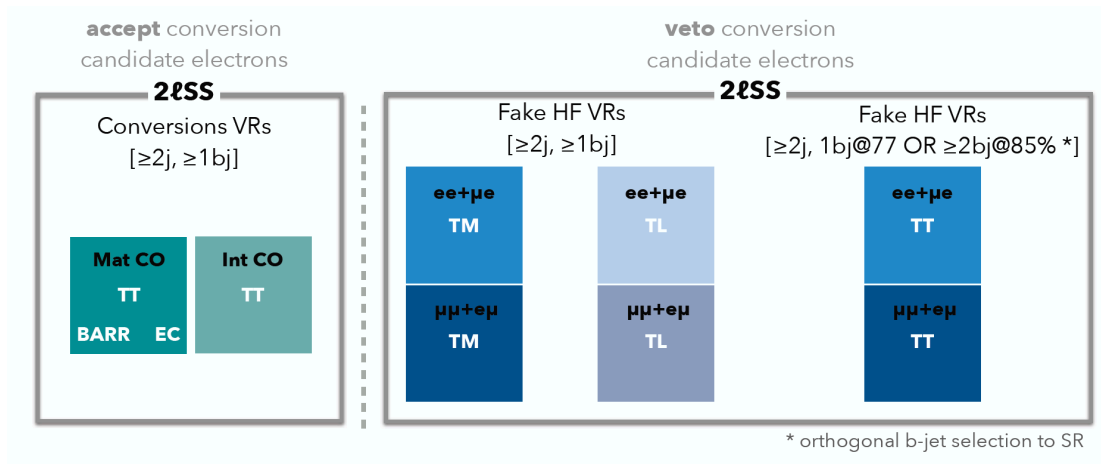


Figure 9.6: Illustration of VR definitions [20]

9.3 PROMPT LEPTON IMPROVED VETO CALIBRATION

The exclusive PLIV working point is used uniquely by the $t\bar{t}W$ analysis within ATLAS and special care is taken for the separate calibration for electrons and muons. In fact, Tight and Medium leptons used in the SR and CR use a cut on the ECIDS discriminant that is optimized for the $t\bar{t}W$ measurement [20], so both Tight and Medium electrons must be calibrated especially. The calibration is performed using the standard *Tag and Probe* (TaP) method with $Z \rightarrow ee/\mu\mu$ decays, where the tag lepton fires a single lepton trigger and passes a tight identification requirement. The probe lepton forms a dilepton invariant mass consistent with a Z decay and the PLIV(+ECIDS) efficiency is measured with respect to a baseline Loose (LooseLH) identification and FCLoose isolation for $\mu\mu$ (ee) events. Calibration *Scale Factor* (SF) are derived and applied to *Monte Carlo* (MC) events binned in lepton p_T and η :

$$SF = \frac{N_{\text{data}}^{\text{PLIV(+ECIDS)}}/N_{\text{data}}^{\text{Loose}}}{N_{\text{MC}}^{\text{PLIV(+ECIDS)}}/N_{\text{MC}}^{\text{Loose}}} = \frac{\epsilon_{\text{data}}^{\text{PLIV(+ECIDS)}}}{\epsilon_{\text{MC}}^{\text{PLIV(+ECIDS)}}} \quad (9.2)$$

Systematic uncertainties associated to these calibrations are derived for electrons and muons separately. In both cases, the leading systematic uncertainty is the so-called “Jet Modeling” uncertainty which is obtained by using the SHERPA 2.2.1 $Z \rightarrow \ell\ell$ MC sample instead of the nominal POWHEG +PYTHIA 8 sample. This captures the possible differences in the modeling of jet shapes between MC setups, but it is conservative as it also captures possible differences in *Matrix Element* (ME) precision and other aspects of the simulation. Another leading systematic uncertainty for electrons is the effect of differing pileup conditions across run years, since electron E_T measurement is sensitive to differences in calorimeter activity. The variances in $\langle\mu\rangle$ can be seen in Figure 6.2. The pileup uncer-

tainty is evaluated for electrons by taking the difference in calibration SF for $0 \leq \langle \mu \rangle < 23$ and $23 \leq \langle \mu \rangle < 80$ for 2015-2016 data and $0 \leq \langle \mu \rangle < 30$, $30 \leq \langle \mu \rangle < 40$, and $40 \leq \langle \mu \rangle < 80$ for 2017-2018 data. This uncertainty is most dominant in the forward regions of the detector.

Uncertainties on PLIV(+ECIDS) calibrations for the VeryTight and TightNotVeryTight working points are shown in Figure 9.7 for muons and Figures 9.8 for electrons. Total uncertainties for muons are large in the region $|\eta_\mu| < 0.1$ and $2.5 < |\eta_\mu| < 2.7$ driven by the probe ID uncertainty due to missing MS coverage at $\eta \sim 0$ where the two halves of the MS meet and ID coverage extending only to $|\eta| < 2.5$. In all other η bins the Jet Modeling uncertainty is largest. The Jet Modeling uncertainty as the largest impact for low-(high-) p_T muons in the VeryTight (TightNotVeryTight) WP. Statistical uncertainties from data are more significant in TightNotVeryTight muons because real $Z \rightarrow \mu\mu$ events have well-isolated muons. Electron uncertainties are primarily driven by the Jet Modeling and Pileup uncertainties, with additional subdominant contribution from statistical uncertainties in data for TightNotVeryTight electrons. There is a distinct valley shape to the Jet Modeling uncertainty is likely due to different p_T dependence of PLIV and ECIDS differences between the considered MC samples.

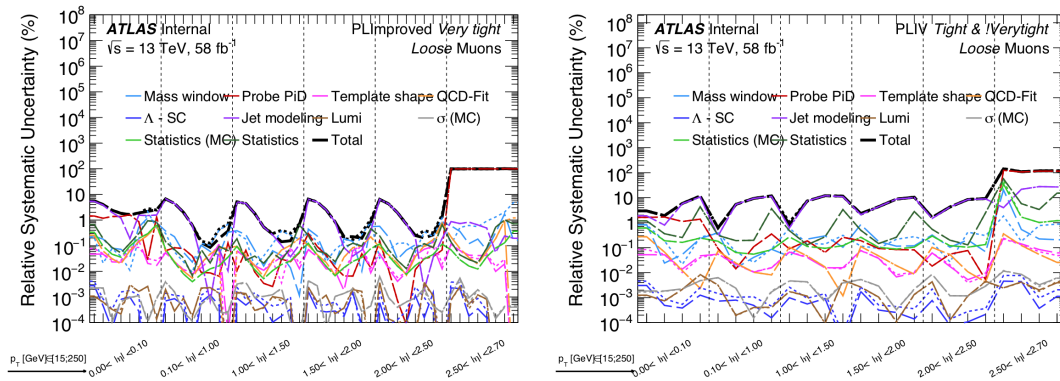


Figure 9.7: Systematic uncertainties for VeryTight (left) and TightNotVeryTight (right) muon PLIV working points as a function of p_T and η [20]

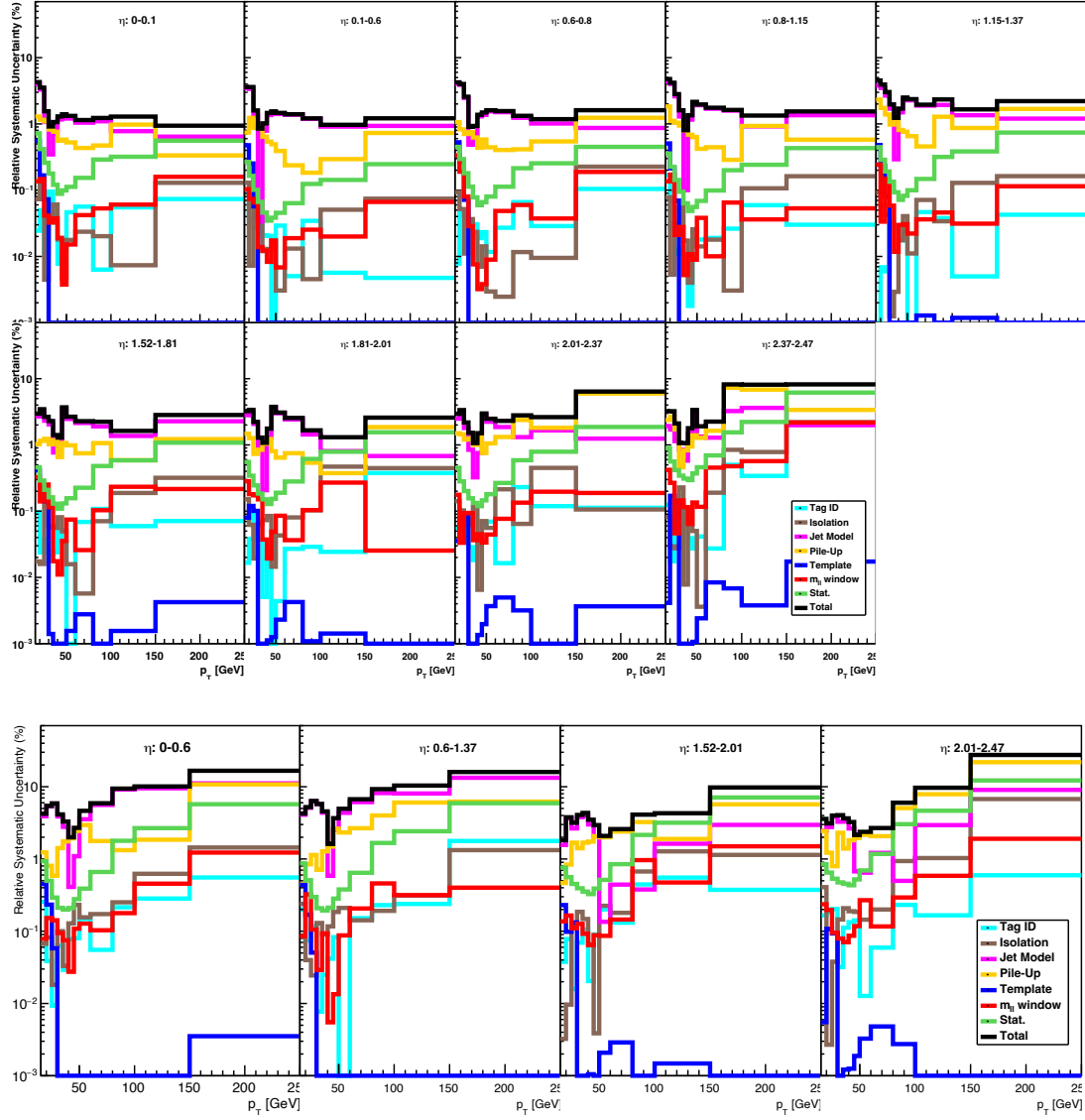


Figure 9.8: Systematic uncertainties for VeryTight (top) and TightNotVeryTight (bottom) electron PLIV working points as a function of p_T and η [20]

VALIDATION

Efficiency scale factors and their systematic uncertainties are derived for electrons and muons using $Z \rightarrow \ell\ell$ events inclusive in jet multiplicity. This topology is quite different from that of $t\bar{t}W$, where jet and b-jet multiplicities are higher. While it is common to apply isolation scale factors derived in $Z \rightarrow \ell\ell$ Tag and Probe procedures broadly among ATLAS analyses, dedicated validation studies are necessary due to the complexity of the PLIV algorithm, our novel use of pseudo-continuous isolation working points, and the central importance of this algorithm to the analysis strategy. To this end, a dedicated PLIV validation region is defined that is composed predominantly of dileptonic $t\bar{t}$ and a $\sim 10\%$ contribution from single top (tW) production. This region has a very similar topology to $t\bar{t}W$; validation of the PLIV calibrations for electrons and muons in this region supports the applicability of these calibrations to the $t\bar{t}W$ signal and control regions.

The $t\bar{t}$ validation region is defined as similarly as possible to the analysis channels, with the same selections used for trigger, lepton isolation, electron QMisID and photon conversion suppression. The selection also requires $N_{\text{jets}} \geq 2$ and $N_{b\text{-jets}} \geq 1$, where the hybrid b-jet definition is used and exactly 2 leptons of opposite charge and opposite flavor with $p_T > 20$ GeV. This selection will be referred to as the “baseline” selection. It removes sources of same-flavor leptons (i.e. Z +jets) and yields a region 90% enriched in di-leptonic $t\bar{t}$ with a 10% contribution of tW production [154].

The procedure for validating the PLIV scale factors proceeds as follows and an example procedure is shown for N_{jets} in Figure 9.9:

1. For each observable of interest (lepton p_T and η and those to be unfolded), produce data/MC comparisons with all selections and available calibrations in the baseline selection. This is done separately for events with a leading muon (μe) and events with a leading electron ($e\mu$). The pre-PLIV modeling is generally very good at this stage, shown for μe events in

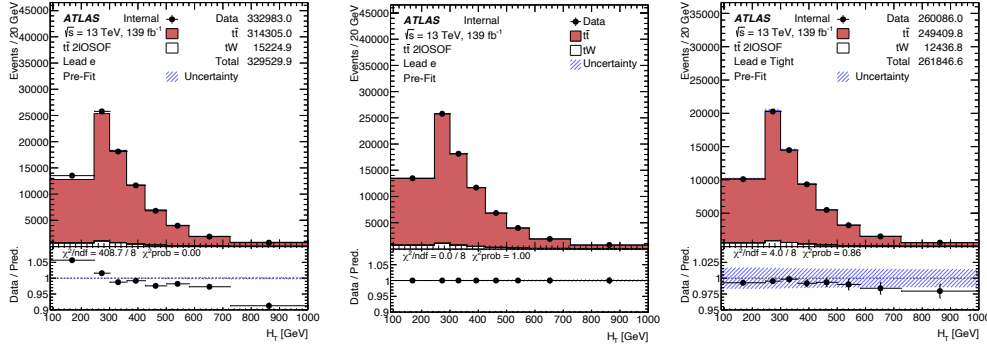


Figure 9.9: An example of PLIV reweighting procedure in H_T in the $e\mu$ channel. The baseline selection is shown on the left. The MC templates are scaled bin-by-bin to match data (center). The PLIV VeryTight selection and associated uncertainties are applied to the leading lepton.

Figure 9.10 and for $e\mu$ events in Figure 9.15.

2. Re-weight the MC yields bin-by-bin to exactly agree with data independently for each observable. In this way, all mis-modeling and associated systematic uncertainties not associated to PLIV are corrected.
3. Apply the PLIV(+ECIDS) selections with corresponding calibrations to the leading lepton. This is checked for the VeryTight and TightNotVeryTight working points. Any mismodeling of the data at this stage should be completely covered by the associated PLIV uncertainties.

This is a valid check for the PLIV calibrations only if there are no upstream selections that must be calibrated simultaneously with the PLIV tool, since the PLIV is explicitly factorized from others by the reweighting procedure. The most similar upstream selection to the PLIV is the FCLoose isolation, but has been shown to have very little correlation to the PLIV [20]. This is unsurprising since only isolation cones are used in both FCLoose isolation and PLIV, while several additional track-based variables are used to train the PLIV.

The final validation of the PLIV calibrations for electrons and muons in the VeryTight and TightNotVeryTight working points are shown for muons in Figures 9.11-9.12 and for electrons in Figures 9.16-9.17. The corrected MC is in good agreement with the data and residual mis-modeling

of the data is covered by systematic uncertainties in all cases. The dominant uncertainties applied to the $t\bar{t}$ component for muons are shown in Figures 9.13-9.14 and for electrons in Figures 9.18-9.19.

For muons, the relative scale and shape of each systematic is in good agreement with what is expected from the T+P framework⁵. In particular, the impact of the Jet Modeling systematic is largest with up to 0.6% (6.6%) impact on the overall normalization in the VeryTight (TightNotVeryTight) working point, with the greatest impact in the low-(high-) p_T region. The systematic uncertainty due to limited statistics reaches 4% in the TightNotVeryTight WP in the highest muon p_T bin, which is also consistent with what is seen in $Z(\mu\mu)$ T+P.

For electrons, The relative scale and shape of each systematic is in good agreement with what is expected from the T+P framework⁶. In particular, the impact of the Jet Modeling systematic is largest with up to 1.5% (4.7%) impact on the overall normalization in the VeryTight (TightNotVeryTight) working point, both exhibiting a minimum in uncertainty around p_T of 40 GeV. The impact of the pileup uncertainty is subleading and is largest at low-(high-) p_T for the VeryTight (TightNotVeryTight) WP; it is increasing (flat) in $|\eta|$ for the TightNotVeryTight (TightNotVeryTight) WP.

The conclusion of this validation study is that the calibrations derived using the $Z \rightarrow \ell\ell$ T+P methods can be reliably applied to the $t\bar{t}W$ phase space. The uncertainties of the exclusive PLIV working points are also validated and are demonstrated to cover differences between data and MC well. A consideration for the $t\bar{t}W$ fit is how to correlate these uncertainties. A systematic variation affecting the acceptance of events on the boundary between VeryTight and TightNotVeryTight

⁵Note that the uncertainties shown in the $t\bar{t}$ VR are relative uncertainties, whereas the muon T+P uncertainties are provided as absolute uncertainties, resulting in a smaller relative uncertainty when nominal scale factors are much greater than unity

⁶Note that the uncertainties shown in the $t\bar{t}$ VR are relative uncertainties, whereas the electron T+P uncertainties are provided as absolute uncertainties, resulting in a smaller relative uncertainty when nominal scale factors are much greater than unity

should drive an anti-correlation in this uncertainty. However, events on the boundary of the TightNotVeryTight and LooseNotTight region would only impact leptons in the TightNotVeryTight region. Due to the non-trivial correlation scheme of these uncertainties, the most conservative assumption that uncertainties are uncorrelated in TightNotVeryTight and VeryTight is taken. The correlation of uncertainties applied to the two regions can then be determined by fits to data, which will be discussed in Chapter [11](#).

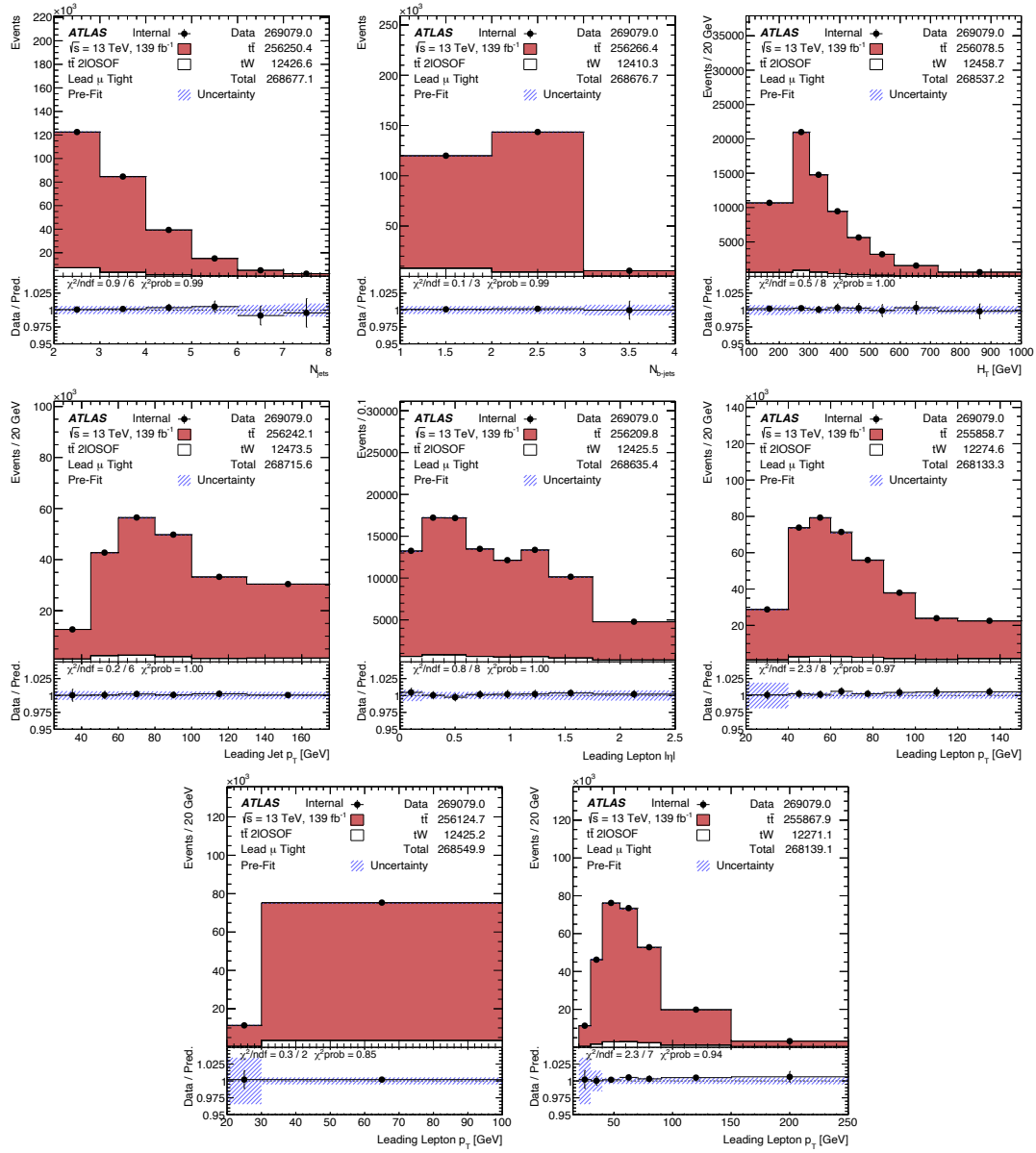


Figure 9.11: Data/MC comparisons in $\mu e t\bar{t}$ VR after baseline reweighting and application of TightNotVery-Tight PLIV selection and scale factors. The muon p_T distributions are shown in multiple binnings, which are the signal region binning, control region binning, muon VeryTight (Tight exclusive) working point calibration binning, and muon VeryTight (Tight exclusive) working point calibration binning.

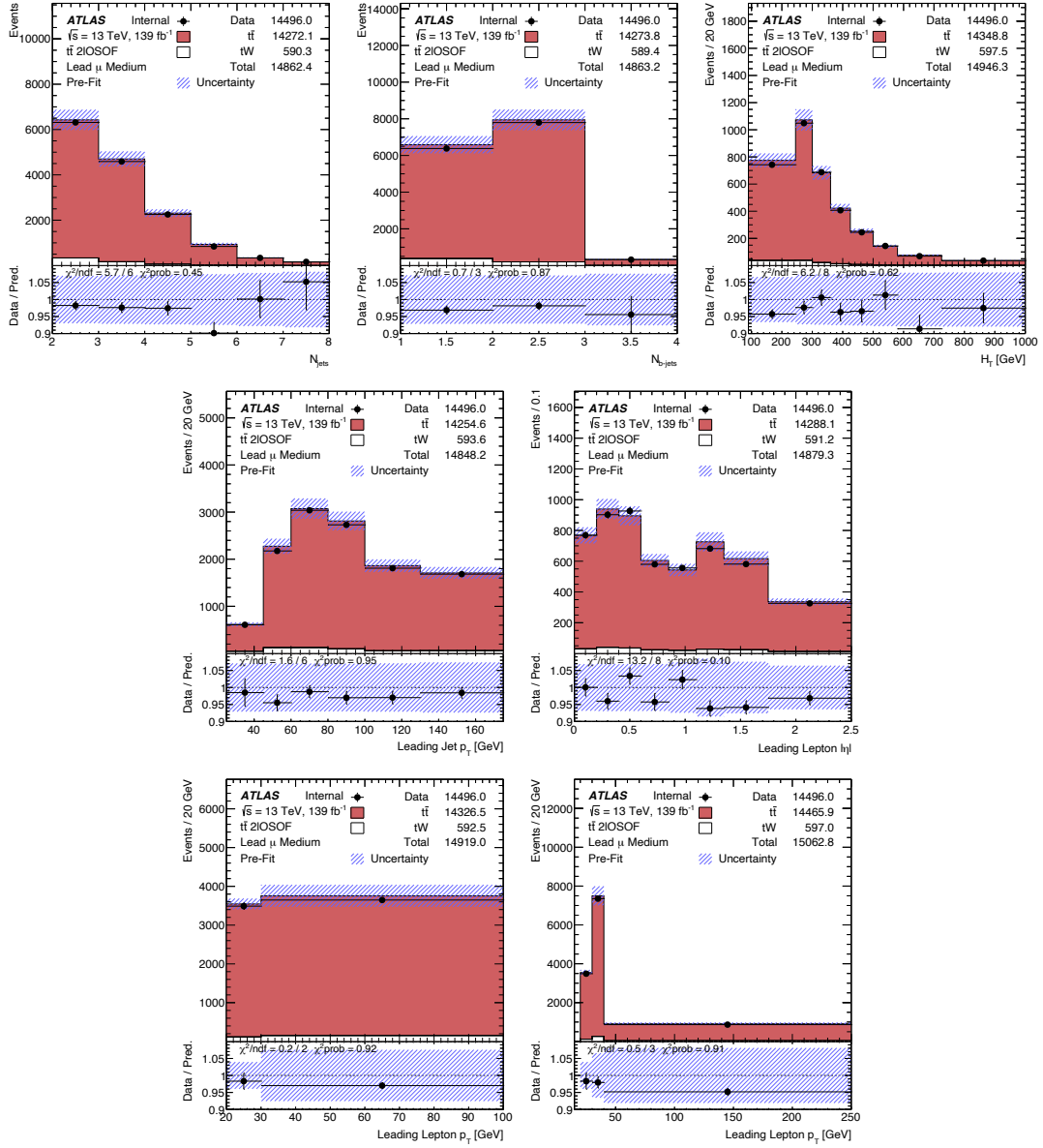


Figure 9.12: Data/MC comparisons in $\mu e t\bar{t}$ VR after baseline reweighting and application of TightNotVeryTight PLIV selection and scale factors. The muon p_T distributions are shown in multiple binnings, which are the signal region binning, control region binning, muon TightNotVeryTight (Tight exclusive) working point calibration binning, and muon TightNotVeryTight (Medium exclusive) working point calibration binning.

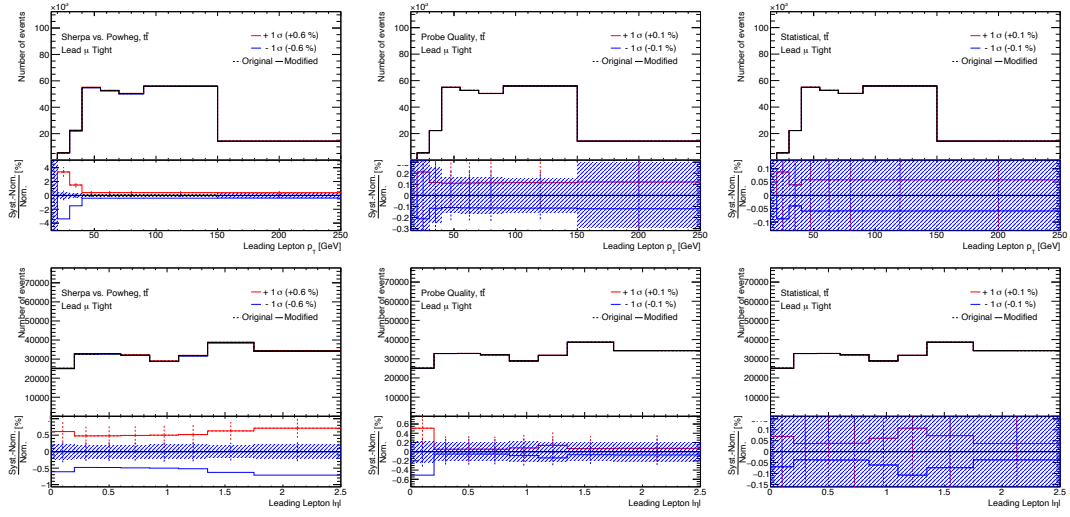


Figure 9.13: Jet modeling, probe ID, and statistical uncertainties in $\mu e t\bar{t}$ VR as a function of p_T (top) and η (bottom) for VeryTight PLIV calibration. Binning is the same as the calibration binning.

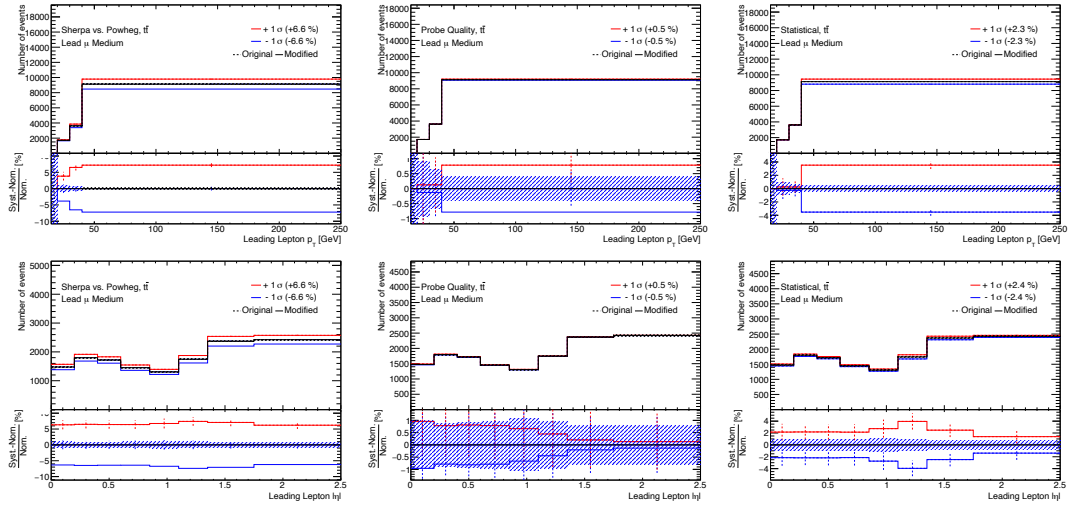


Figure 9.14: Jet modeling, probe ID, and statistical uncertainties in $\mu e t\bar{t}$ VR as a function of p_T (top) and η (bottom) for TightNotVeryTight PLIV calibration. Binning is the same as the calibration binning. Jet modeling systematic is labeled as "Sherpa vs. Powheg."

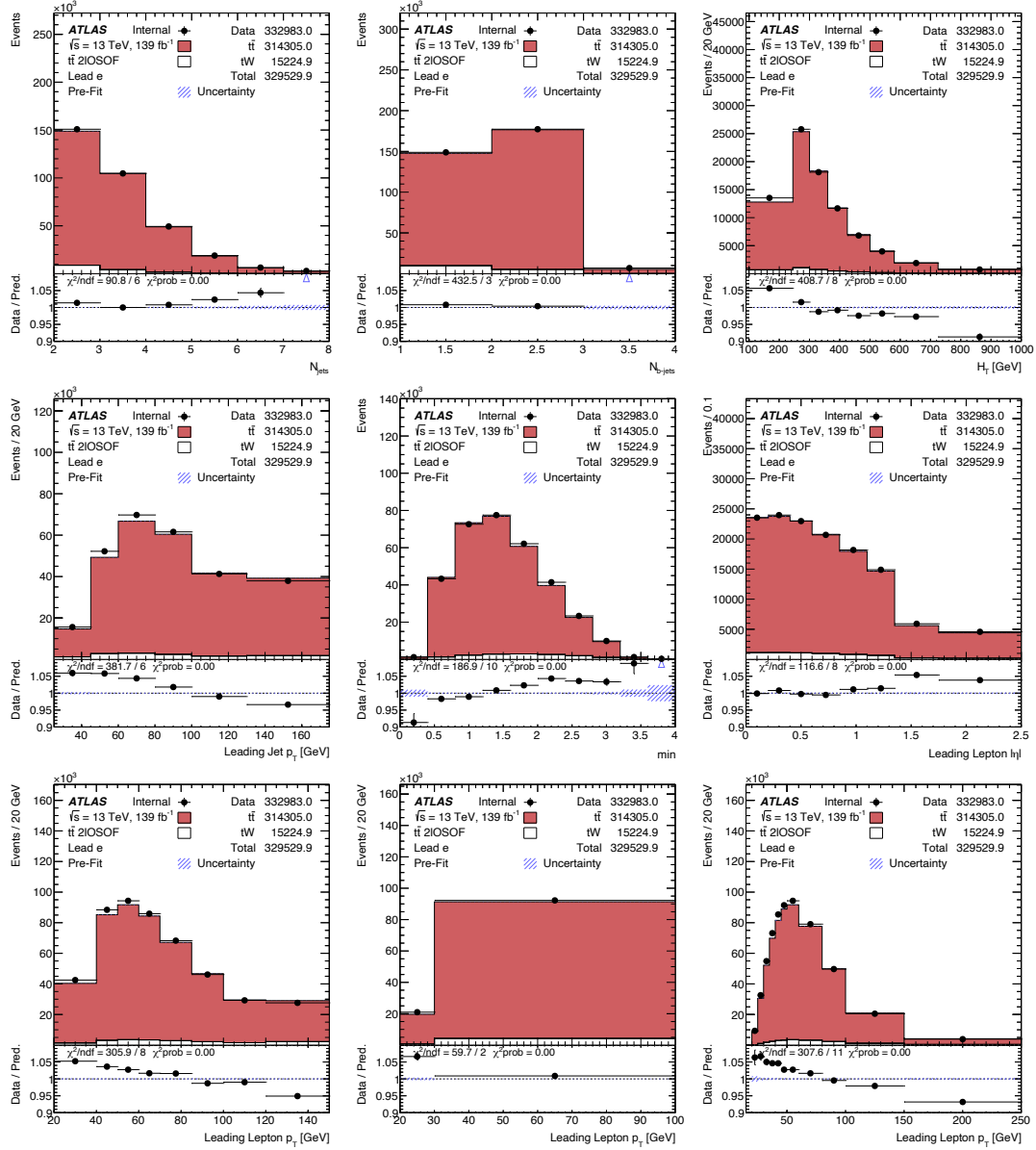


Figure 9.15: Data/MC comparisons in $\mu e \bar{t} t$ VR after baseline selection before reweighting. The electron p_T distributions are shown in multiple binnings, which are the signal region binning, control region binning, and electron calibration binning of both VeryTight and TightNotVeryTight + ECIDS.

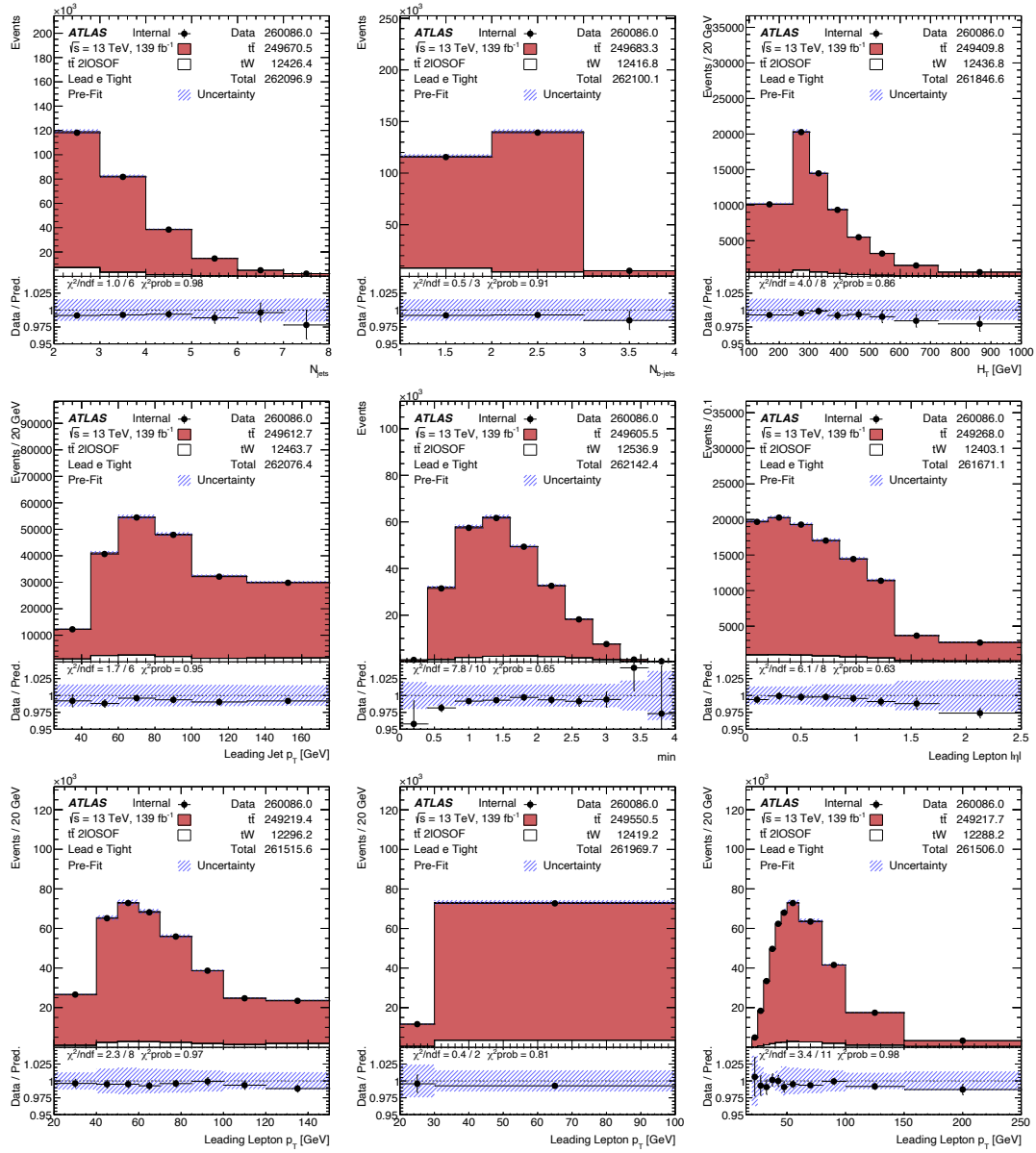


Figure 9.16: Data/MC comparisons in $\mu e t\bar{t}$ VR after baseline reweighting and application of PLIV Tight-NotVeryTight + ECIDS cuts and scale factors. The electron p_T distributions are shown in multiple binnings, which are the signal region binning, control region binning, and electron calibration binning of both VeryTight and TightNotVeryTight + ECIDS.

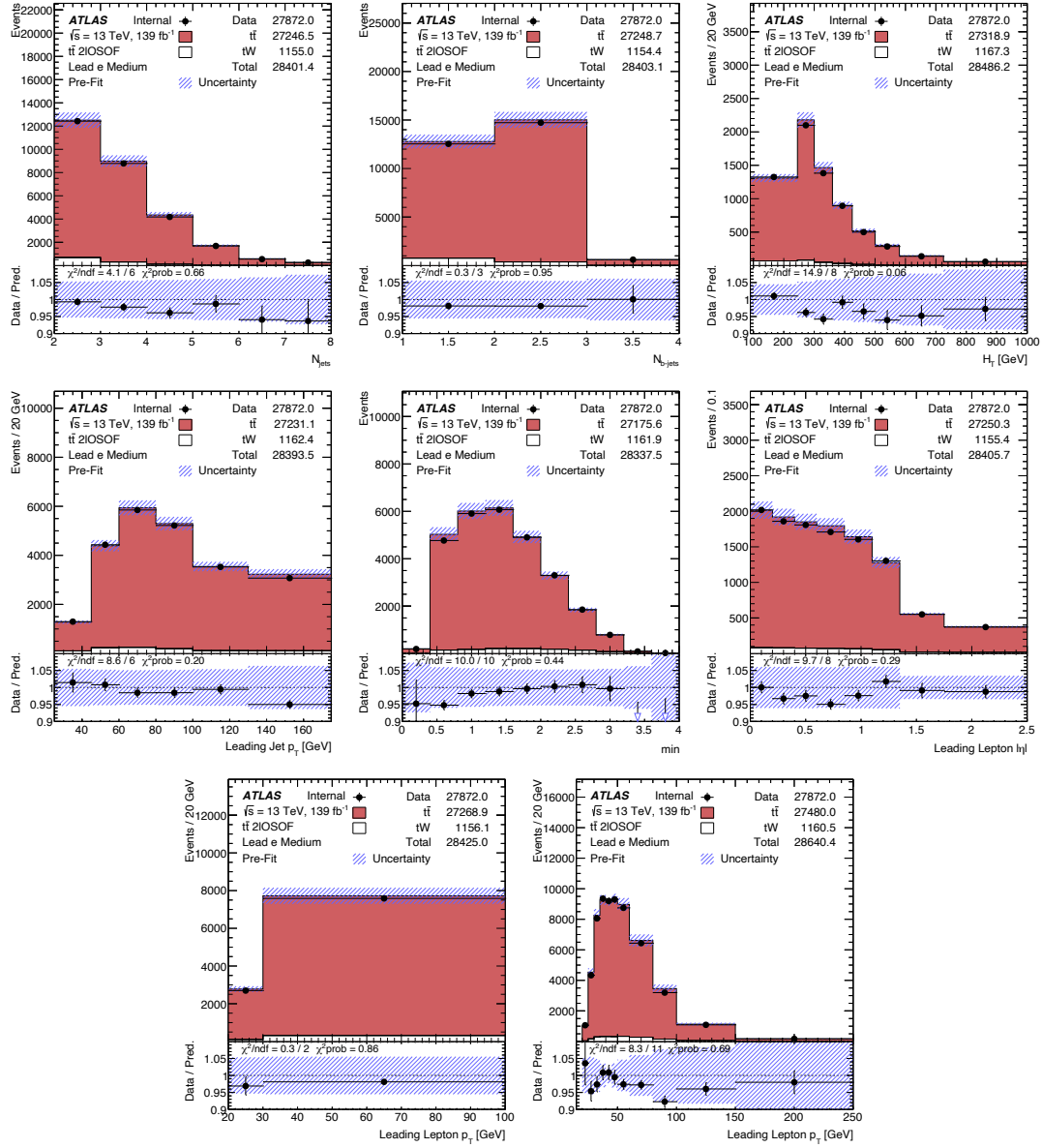


Figure 9.17: Data/MC comparisons in $\mu e t \bar{t}$ VR after baseline reweighting and application of PLIV Tight-NotVeryTight + ECIDS cuts and scale factors. The electron p_T distributions are shown in multiple binnings, which are the signal region binning, control region binning, and electron calibration binning of both Tight-NotVeryTight and VeryTight + ECIDS.

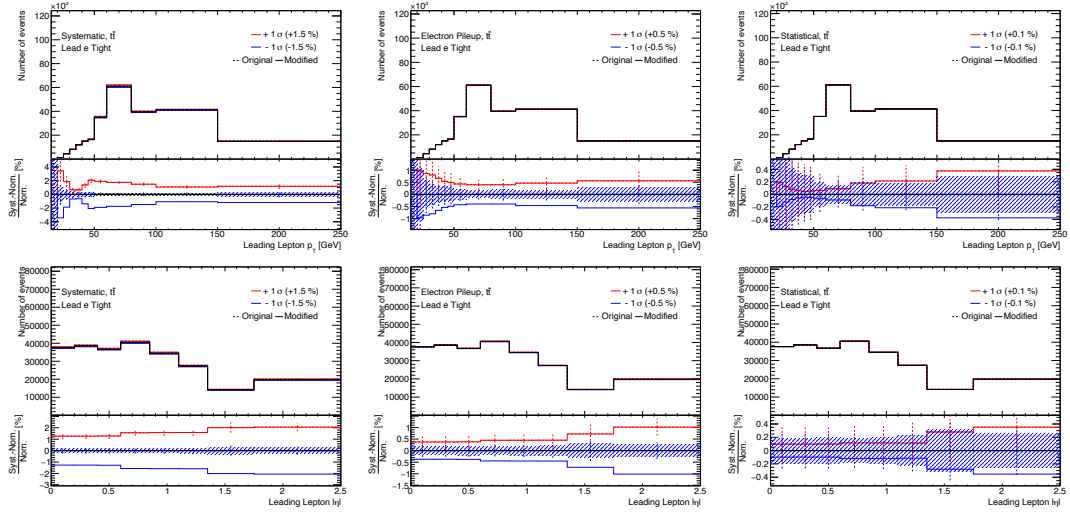


Figure 9.18: Jet modeling, pileup, and statistical uncertainties in $e\mu t\bar{t}$ VR as a function of p_T (top) and η (bottom) for VeryTight PLIV calibration. Binning is the same as the calibration binning. Jet modeling systematic is labeled as "Systematic."

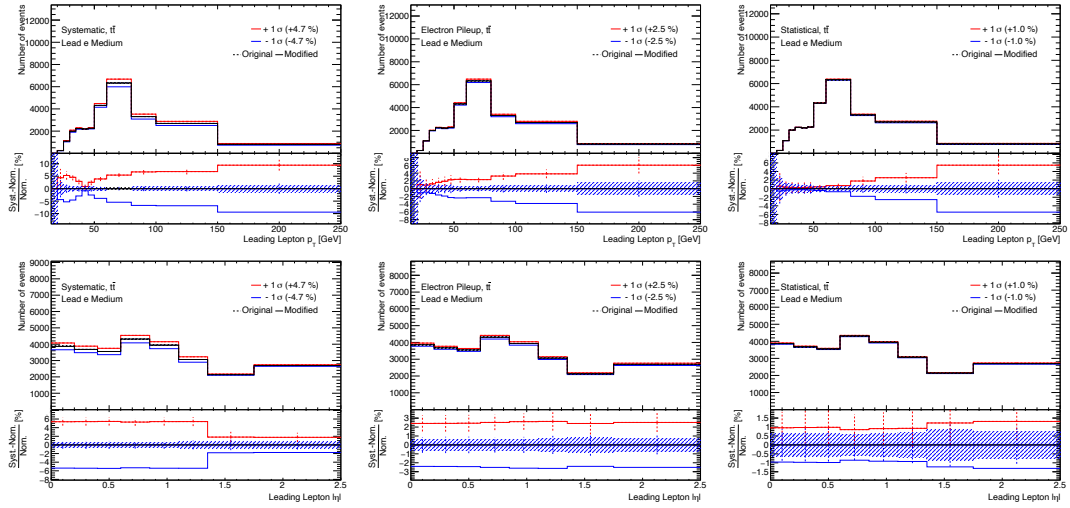


Figure 9.19: Jet modeling, pileup, and statistical uncertainties in $e\mu t\bar{t}$ VR as a function of p_T (top) and η (bottom) for TightNotVeryTight PLIV calibration. Binning is the same as the calibration binning. Jet modeling systematic is labeled as "Systematic."

9.4 SYSTEMATIC UNCERTAINTIES

The $t\bar{t}W$ measurement uses many physics objects and is therefore sensitive to many instrumental uncertainties. Such instrumental uncertainties are derived centrally within the ATLAS physics performance groups and provided for all physics analyses. There are also a set of theoretical uncertainties defined to capture the limited precision of MC generators and theoretical calculations on inclusive cross sections. Finally, an additional set of uncertainties are defined for analysis specific features relating to $t\bar{t}$ modeling and the use of pseudo-continuous PLIV.

INSTRUMENTAL UNCERTAINTIES

Experimental systematic uncertainties are related to the trigger efficiency; lepton reconstruction, identification, and isolation efficiency; the absolute scale and resolution of lepton momentum/energy; and many uncertainties related to the *Jet Energy Scale* (JES) and *Jet Energy Resolution* (JER) as well as *b*-tagging and JVT. Systematics are implemented either as alternate event weights (scale factors) or as copies of the MC dataset with smeared object energy and momentum, which are used for JES and JER.

Several uncertainties for leptons are considered. These relate to reconstruction, identification, and isolation efficiencies measured using the TaP method, track to vertex association (for muons), and p_T/E_T scale and resolution uncertainties. An uncertainty is also considered for the sagitta bias correction, which corrects for so-called weak alignment modes in ID and MS that induces a charge-dependent bias on the reconstructed muon p_T [118]. These uncertainties are derived centrally in the muon and electron performance groups [155, 156]. These uncertainties and the PLIV uncertainties derived specifically within the $t\bar{t}W$ measurement are shown in Table 9.4.

The “FullJER” reduction scheme is used for JES and JER uncertainties and reduces the complexity of the systematics model from roughly 100 (34) JES (JER) components to 30 (14) components with only small reduction in the precision of correlations across different regions of jet phase space [157]. This is the most complete of the reduction schemes and is robust if the nuisance parameters associated to these components are pulled in fits to data. The JER is corrected by smearing MC when it has better resolution than data, but in cases where data has better resolution than MC an uncertainty is applied to bridge the difference, which may be pulled in fits to data. There are also uncertainties applied to E_T^{miss} scale and resolution of soft activity in the detector that is not clustered into jets or reconstructed as leptons. These uncertainties are summarized in Table 9.5. An overall uncertainty of 1.7% is taken on the luminosity measurement during 2015-2018 data-taking periods using the van der Meer method [158].

Table 9.4: Summary of instrumental uncertainties related to electron and muon reconstruction.

Instrumental Systematic Uncertainties for Leptons			
Source	Description	# NPs	Application
Trigger			
Efficiencies	e Trigger Efficiency	2	Event Weight
	μ Trigger Efficiency	1	Event Weight
Muons			
Efficiencies	Reconstruction and ID	2	Event Weight
	Reconstruction and ID (low p_T)	2	Event Weight
	Track To Vertex Association	2	Event Weight
	FCLoose Isolation	2	Event weight
	PLIV VeryTight	10	Event weight
	PLIV TightNotVeryTight	10	Event weight
p_T Scale	Combined p_T Scale	1	p_T Corr.
p_T Resolution	ID Resolution	1	p_T Corr.
	MS Resolution	1	p_T Corr.
	MS Charge-dependent Sagitta Bias	1	p_T Corr.
Electrons			
Efficiencies	Reconstruction	1	Event Weight
	Identification	1	Event Weight
	FCLoose Isolation	1	Event Weight
	PLIV VeryTight	7	Event weight
	PLIV TightNotVeryTight	7	Event weight
E_T Scale	E_T Scale	1	Energy Corr.
E_T Resolution	E_T Resolution	1	Energy Corr.

Table 9.5: Summary of instrumental uncertainties related to jet and E_T^{miss} reconstruction.

Instrumental Systematic Uncertainties for Jets and E_T^{miss}			
Source	Description	# NPs	Application
Jets			
Efficiency	Jet Vertex Tagger	1	Event Weight
JES	Global Sequential Calibration	15	p_T Corr.
	η Inter-calibration	6	p_T Corr.
	High- p_T Jets	1	p_T Corr.
	Pileup Dependence	4	p_T Corr.
	Non-closure	1	p_T Corr.
JER	b -jet response	1	p_T Corr.
	q/g response and composition	2	p_T Corr.
	FullJER Reduction Scheme	12	p_T Corr.
	Data vs. Fullsim	1	p_T Corr.
	Data vs. AFII	1	p_T Corr.
E_T^{miss} (only used in Control Regions)			
Soft Track Terms	Resolution	2	p_T Corr.
	Scale	1	p_T Corr.

Table 9.6: Summary of instrumental uncertainties related to b -tagging and pileup.

Instrumental Systematic Uncertainties for b-tagging and Pileup			
Source	Description	# NPs	Application
Pseudo-continuous b-tagging			
Efficiency	DL1r b -tagger eff. of true b -jets	18	Event Weight
	DL1r b -tagger eff. of true c -jets	18	Event Weight
	DL1r b -tagger eff. of true light flavor jets	18	Event Weight
Pile-up reweighting			
Pileup	Pileup reweighting	1	Event Weight

AN ASIDE: JES FLAVOR UNCERTAINTIES

During the analysis development it was observed that the JES flavor response and composition uncertainties were among the most dominant at the differential level for N_{jets} . These uncertainties pertain to the difference in jet shapes and detector response for jets initiated by light quarks or by gluons⁷ due to differences in radiation patterns during shower evolution. The total flavor-related JES uncertainty is defined by

$$\Delta R_S = \underbrace{\Delta f_g \times (R_q - R_g)}_{\text{Flavor composition}} \oplus \underbrace{f_g \times \Delta R_g}_{\text{Flavor response}} \quad (9.3)$$

where $f_g \pm \Delta f_g$ is the fraction of jets that are produced by gluons (gluon composition), R_q and R_g are the responses for light quarks and gluons, and ΔR_g is an uncertainty in the gluon response defined by the difference between PYTHIA 8 and HERWIG 7 which is derived centrally by the Jet/ E_T^{miss} group.

Jet calibration tools that provide this uncertainty are agnostic to the gluon composition for a particular analysis by default and assume uniform $50\% \pm 50\%$ gluon composition. This maximally conservative assumption lead to large uncertainties. The magnitude of JES flavor composition and response uncertainties for the largest prompt backgrounds $t\bar{t}H$, $t\bar{t}Z$, and VV are shown in Figure 9.20. The normalization component of these uncertainties is small while the shape impact is significant at the level of up to 10% in the case of $t\bar{t}H$ and VV .

JES flavor uncertainties can be reduced by deriving precise gluon composition maps in $(p_T, |\eta|)$.

The binning is made fine enough to resolve the structure of gluon composition as a function of

⁷Referring to the difference between gluon- and light quark-initiated jets a “flavor” uncertainty is something of a misnomer, but is the standard naming scheme within ATLAS.

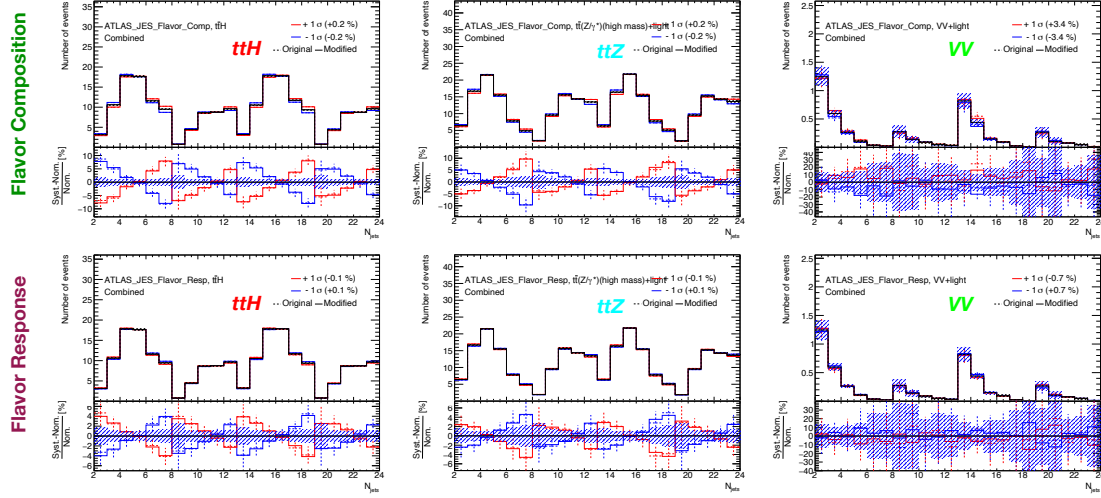


Figure 9.20: JES flavor uncertainties for $t\bar{t}H$, $t\bar{t}Z$, and VV backgrounds in SRs

jet kinematics, but not so fine as to increase sensitivity to MC statistics. The former assumption is confirmed after checking the bin-to-bin differences among all derived maps. The MC statistical uncertainties were also seen to be negligible. Two uncertainties are derived on these gluon composition: the simultaneous variation of μ_R and μ_F , and a generator uncertainty defined as the difference between the nominal MC sample and an alternate sample. The samples used to define the nominal and generator uncertainties are listed in Table 9.7. The total uncertainties used for the flavor composition uncertainty is defined as the bin-by-bin sum in quadrature of the two composition uncertainties.

	Nominal	Uncertainty
$t\bar{t}H$	POWHEG +PYTHIA 8	POWHEG +HERWIG $\oplus \mu_R/\mu_F$
$t\bar{t}W$	SHERPA 2.2.10	MG5_AMC@NLO +PYTHIA 8 $\oplus \mu_R/\mu_F$
$t\bar{t}Z$	SHERPA 2.2.11	MG5_AMC@NLO +PYTHIA 8 $\oplus \mu_R/\mu_F$
$t\bar{t}$	POWHEG +PYTHIA 8	POWHEG + HERWIG 7 $\oplus \mu_R/\mu_F$
VV	SHERPA 2.2.1	POWHEG +PYTHIA 8 $\oplus \mu_R/\mu_F$

Table 9.7: Samples used to define the nominal and generator uncertainties

Gluon fraction maps should be derived for specific analysis channels, using truth information to determine the originating parton of all jets in the event. Maps are derived for the $2\ell\text{SS}$ and 3ℓ channels separately, as they differ by a margin far larger than their combined uncertainties. The selections chosen for the derivation are a slightly relaxed version of the SR definition, where no conversion or PLIV(+ECIDS) cuts are made and the N_{jets} threshold is lowered to ≥ 1 and no b -jet cut is imposed for both $2\ell\text{SS}$ and 3ℓ channels. The final set of gluon composition maps and uncertainties that are used to derive the flavor uncertainties are given in Figures 9.21 - 9.25.

A check was performed to see if binning in jet multiplicity would reduce the difference between the two channels, since the 3ℓ channel is expected to have 2 fewer quark jets in the $t\bar{t}W$ final state and up to 2 fewer quark jets for background processes. It was found that the differences between channels persisted and was more significant than the differences in N_{jet} bins. The variation of the $N_{\text{b-jet}}$ threshold was shown to have a negligible effect on the gluon maps. The difference between MC campaigns corresponding to different years of data taking also showed a negligible differences among all samples.

The general features of the gluon compositions are similar across processes. In $t\bar{t}W$, VV , and $t\bar{t}$ production, the $2\ell\text{SS}$ channel involves a $V \rightarrow q\bar{q}^{(\prime)}$ which must alternative decay to $\ell\ell$ or $\ell\nu$ to be accepted by the 3ℓ selection. At leading order, jets in the 3ℓ channel can only come from gluon radiation in $t\bar{t}W$ and VV production. As a result, a greater fraction of jets in 3ℓ events are produced by soft QCD processes (ISR/FSR) in the PS algorithm, leading to an enhancement of the gluon fraction, particularly in the low- p_{T} central phase space where differences in $2\ell\text{SS}$ and 3ℓ reach 20%-30%. Due to the greater representation of PS jets in the 3ℓ channel, alternate showering algorithm uncertainties are larger by a factor of 2 or more. These features are not exhibited by $t\bar{t}Z$ and $t\bar{t}H$, which

have can have 2 or more q -initiated jets at tree level even if accepted into the 3ℓ channel.

To evaluate the effect of the derived gluon fraction maps, a simple fit implementation is used that contains a subset of systematic uncertainties. The fit is performed before and after the JES flavor uncertainties are revised with the new maps. Composition uncertainties decrease by an order of magnitude, while the response uncertainties have only minor reductions. This is as expected, because the absolute gluon fractions enter into the response uncertainty but do not differ extremely from 50/50, while the new maps uncertainties enter into the composition uncertainty and are significantly reduced from the agnostic 50% default uncertainty.

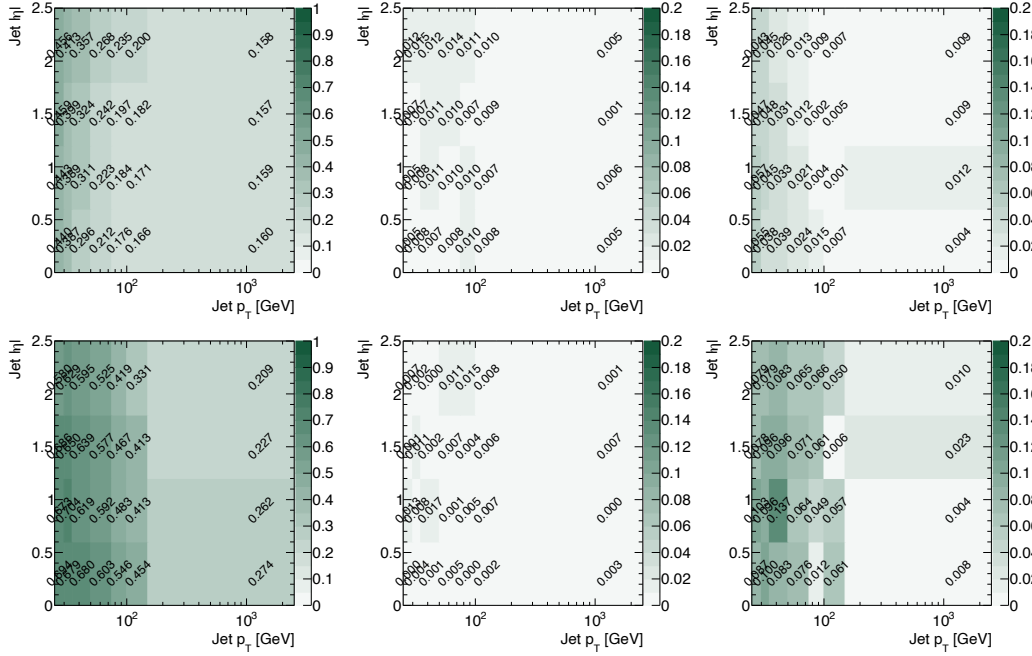


Figure 9.21: Gluon fraction maps for $t\bar{t}W$ production in $2\ell SS$ (top) and 3ℓ (bottom) channels, showing nominal fractions (left) with scale uncertainties (center) and generator uncertainties (right)

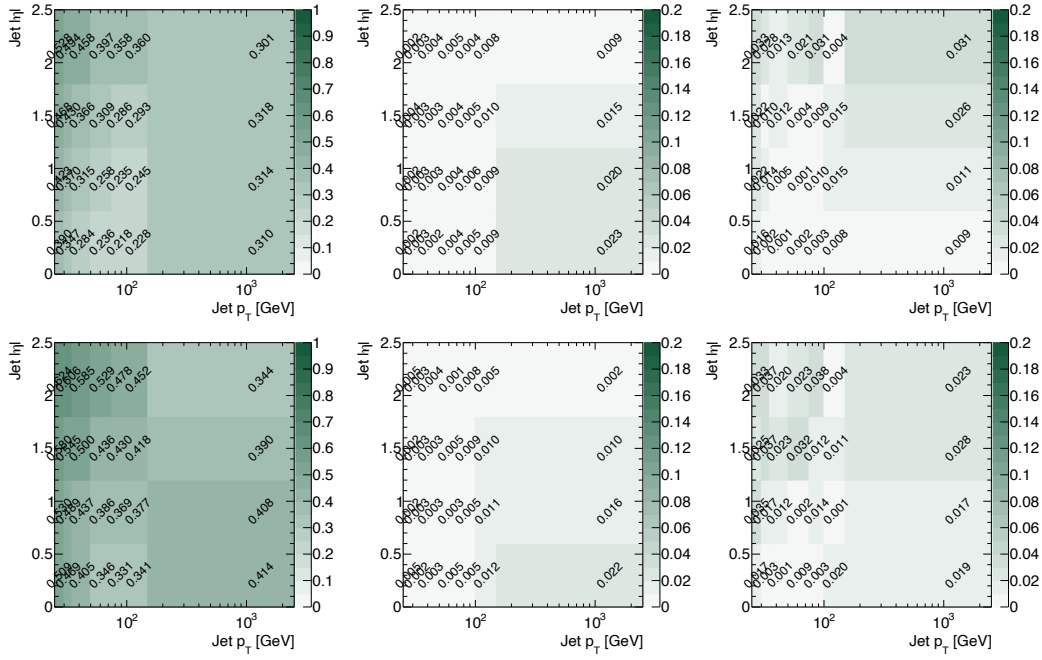


Figure 9.22: Gluon fraction maps for $t\bar{t}H$ production in $2\ell SS$ (top) and 3ℓ (bottom) channels, showing nominal fractions (left) with scale uncertainties (center) and generator uncertainties (right)

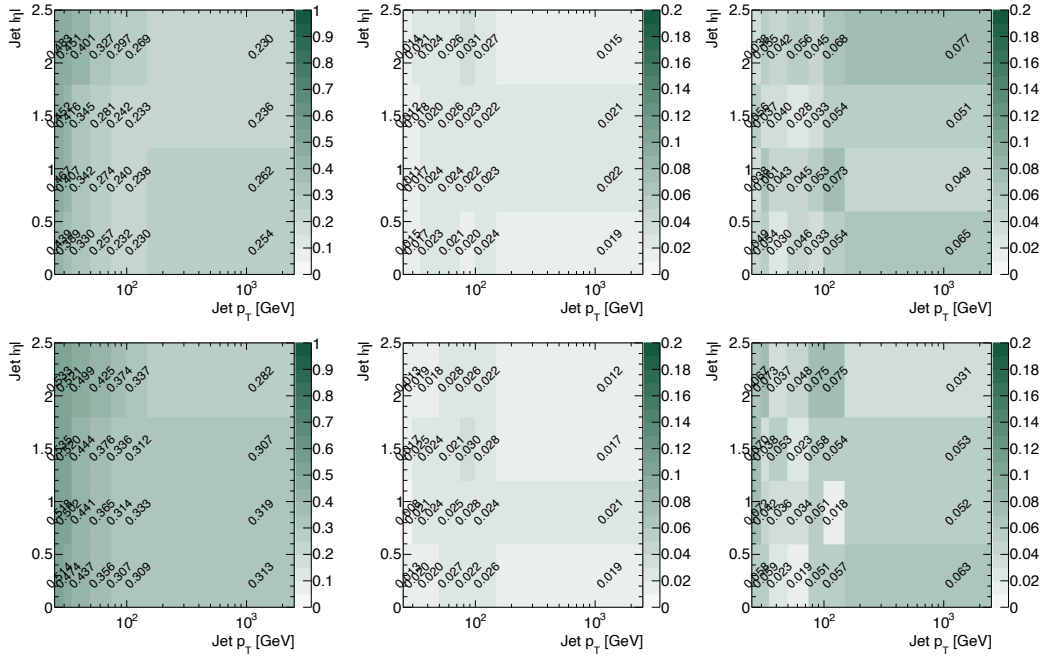


Figure 9.23: Gluon fraction maps for $t\bar{t}Z$ production in $2\ell SS$ (top) and 3ℓ (bottom) channels, showing nominal fractions (left) with scale uncertainties (center) and generator uncertainties (right)

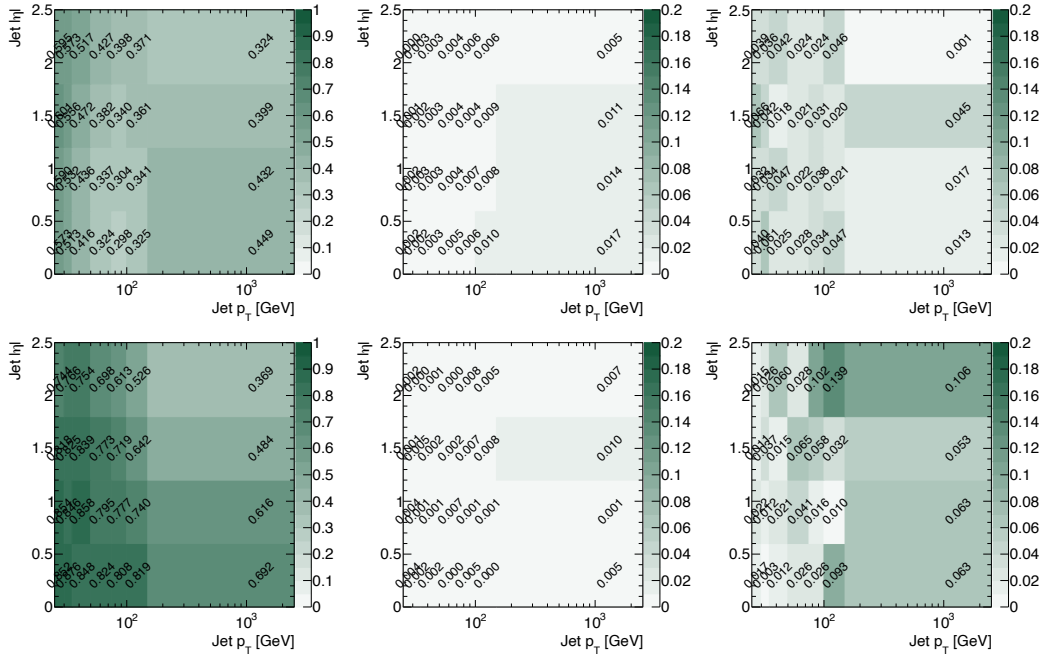


Figure 9.24: Gluon fraction maps for $t\bar{t}$ production in $2\ell SS$ (top) and 3ℓ (bottom) channels, showing nominal fractions (left) with scale uncertainties (center) and generator uncertainties (right)

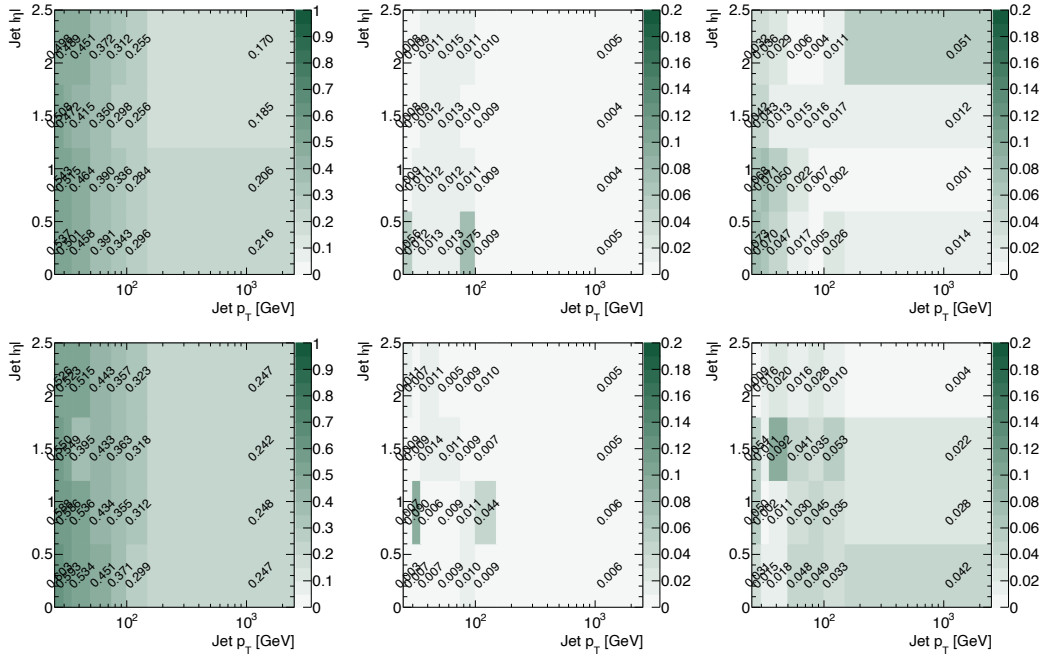


Figure 9.25: Gluon fraction maps for VV production in $2\ell SS$ (top) and 3ℓ (bottom) channels, showing nominal fractions (left) with scale uncertainties (center) and generator uncertainties (right)

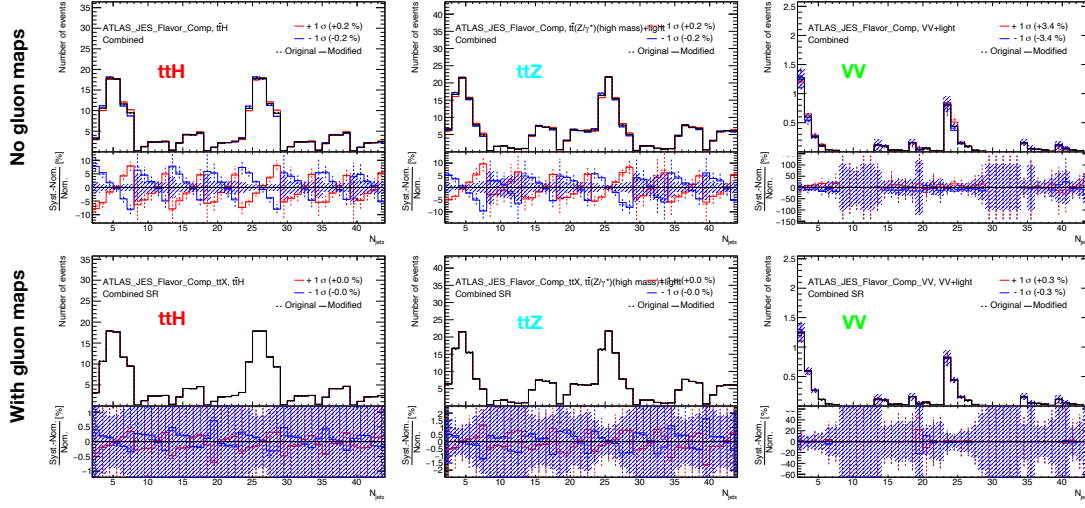


Figure 9.26: JES flavor composition uncertainties before and after derived maps are used

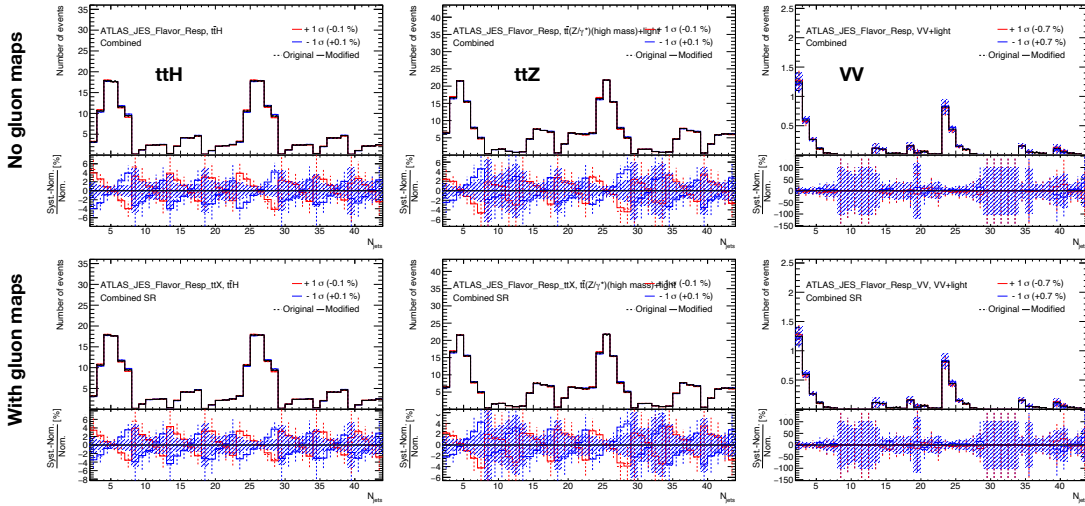


Figure 9.27: JES flavor response uncertainties before and after derived maps are used

THEORETICAL UNCERTAINTIES

Several theoretical uncertainties are applied to the MC predictions for the many processes considered in this analysis. Flat uncertainties are applied to several prompt processes that reflect the limited precision to which cross sections are known. Alternate generator and parton shower algorithms are used to define additional modeling uncertainties. Finally, scale uncertainties that simultaneously vary the μ_R and μ_F scales from $1/2\times$ to $2\times$ the nominal value are applied. These uncertainties are summarized in Table 9.8.

The $t\bar{t}H$ cross section uncertainty is set in line with the inclusive cross section of $\sigma(t\bar{t}H) = 445.7 \pm 51.3$ fb calculated at NLO QCD [50] while other cross section uncertainties are set to conservative values in line with other ATLAS measurements. Cross section uncertainties are not applied to VV +HF and $t\bar{t}Z$ +light because dedicated *Normalization Factors* (NF) for these components are floated in the fits to data. In addition to PS and scale uncertainties, an uncertainty varying the A14 tune of the $t\bar{t}Z$ sample is considered. Uncertainties on the PDF set used for $t\bar{t}W$ are considered as well. The value of the strong coupling constant used in the PDF is varied from $\alpha_s = 0.117$ to $\alpha = 0.119$ (nominally $\alpha_s = 0.118$) and the PDF set itself is changed to the CT14nnlo and MMHT2014nnlo68cl PDF sets defining 2 two-sided uncertainties. This procedure is consistent with the recommendations of the ATLAS Physics Modeling Group based on [159].

ANALYSIS-SPECIFIC UNCERTAINTIES

There are a handful of additional uncertainties specific to the $t\bar{t}W$ analysis strategy and pertain to the modeling of fake leptons:

Table 9.8: Summary of theoretical uncertainties for the MC predictions of different processes, including overall uncertainties to the inclusive cross section, alternative generator and/or parton shower algorithm, and scale variations.

Theoretical Uncertainties				
Process	σ [%]	Generator	Parton Shower	μ_R/μ_F
$t\bar{t}H$	$\pm 11\%$	MG5_AMC@NLO +PYTHIA 8	POWHEG +HERWIG 7	Event weight
$t\bar{t}Z$	$\pm 50\%$ (+ $\{c, b\}$ only)	— —	MG5_AMC@NLO + HERWIG 7	Event weight
$t\bar{t}W$ QCD	—	MG5_AMC@NLO + PYTHIA 8		Event weight
$t\bar{t}W$ EW	—	MG5_AMC@NLO + PYTHIA 8		Event weight
$t\bar{t}$	—	—	Powheg + Herwig 7.1.3	—
VV + light	$\pm 2\%$	—	—	Event weight
$VV + \{c, b\}$	—	—	—	Event weight
VH	$\pm 50\%$	—	—	—
VVV	$\pm 30\%$	—	—	—
ttt	$\pm 50\%$	—	—	—
$t\bar{t}t\bar{t}$	$\pm 30\%$	—	—	—
$t\bar{t}WW$	$\pm 50\%$	—	—	—
tZ	$\pm 5\%$	—	—	—
tWZ	$\pm 50\%$	—	—	—

- **T-to-M Extrapolation.** While the PLIV working points are calibrated, these calibrations only apply to promptly produced leptons. The efficiencies of non-prompt leptons in the VeryTight and TightNotVeryTight regions showed a difference of up to 20% for electrons while similar efficiencies are seen for muons. No shape dependence is observed as a function of lepton p_T . A conservative 20% extrapolation on the total normalization is applied between leptons in the two working points. This uncertainty is sub-dominant for inclusive and differential $t\bar{t}W$ measurements.
- **Conversion Extrapolation.** Validation regions are defined that are enriched in internal conversions, material conversions in the barrel region, and material conversions in the end-cap regions. After fits to data in the CR, a 50% (10%) non-closure is observed for internal (material) conversions. Flat uncertainties with these values are applied for extrapolation of conversion estimates in the CR to the SR.
- **PLIV Input Variables.** Two variables used in the PLIV training show a non-closure between best-fit MC estimate and data in validation regions. Uncertainties only affecting the shape of MC templates of non-prompt leptons are applied for the relative calorimeter cluster energy $E_{\text{cluster}}/E_{\text{exp}}$ for muons and the lepton track p_T fraction $p_{T, \text{lep}}/p_{T, \text{track-jet}}$ for electrons and are applied to all regions. All other variables show good agreement with data in validation regions.
- **$t\bar{t}$ +HF.** An uncertainty of 50% is applied to the prediction of $t\bar{t}$ in association with at least one additional c - or b -quark jet (identified using truth information).
- **VV N_{jets} Reweighting.** As mentioned in Section 8.1, a data-driven correction to the VV yields is derived as a function of N_{jets} by fitting non-closures in the N_{jets} distribution of a VV validation region to a 3-parameter analytical function. The best fit values for these parameters are varied in the parameters' eigenspace to derive uncorrelated uncertainties on the reweighting procedure. These uncertainties are subdominant, so a conservative factor 3 is applied without affecting the analysis sensitivity.

9.5 PROFILE LIKELIHOOD FORMALISM

Every 25 nanoseconds, the LHC samples probability distribution functions whose domain is a high-dimensional phase space over possible final state particle kinematics. Since collisions are independent⁸, the data is a sample of repeated identical measurements of a population distribution determined by the the Standard Model. A production cross section can be inferred through an event counting experiment. Principles of statistical inference in HEP experiments are covered in detail by Cowan [160] and practically by Cranmer [161].

The $t\bar{t}W$ measurement (and many others performed by ATLAS) relies on the profile likelihood formalism, in which a likelihood function is defined to represent the probability of having measured a given dataset as a function of parameters that modify the theoretical hypothesis. These parameters include those that the analyzer would like to measure, called *Parameter of Interest* (POI), and those that affect the prediction but are not of interest, called *Nuisance Parameter* (NP). For an inclusive measurement of a signal process with predicted yields S_i , background yields B_i , and observed data n_i (with i indexing bins), the *profile likelihood* is defined as

$$L(\mathbf{n}|\mu, \boldsymbol{\theta}) = \prod_{i \in \text{bins}} \mathcal{P}(n_i | [\mu S_i(\boldsymbol{\theta}) + B_i(\boldsymbol{\theta})] \gamma_i) \times \mathcal{G}(\gamma_i | 1, \delta_i) \times \prod_{j \in \text{syst}} \mathcal{G}(\theta_j | \theta_j^0, \Delta\theta_j) \quad (9.4)$$

where μ is the *signal strength* POI and δ_i is the total uncertainty on the MC estimate in bin i . There are several basic components of Equation 9.4, the first being the use of the Poisson and Gaussian

⁸Back-to-back bunch crossings can become correlated due to effects like out-of-time pileup, but most interesting processes are so rare that the time between events passing all analysis selections is large enough to remove any correlations due to detector conditions.

probability distributions:

$$\begin{aligned}\mathcal{P}(n|\lambda) &= \frac{\lambda^n e^{-\lambda}}{n!} \\ \mathcal{G}(x|\mu, \sigma) &= \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2} \frac{(x - \mu)^2}{\sigma^2}\right)\end{aligned}\tag{9.5}$$

The predictions S_i and B_i themselves depend on the NP θ and γ . Instrumental uncertainties typically take nominal value $\theta_j^0 = 0$ and $\Delta\theta_j = 1$ and the continuous dependence $S(\theta_j)$ ⁹ is determined by interpolating and extrapolating between $S(\theta_j^0)$ and $S(\theta_j^0 \pm \Delta\theta_j)$. The likelihood defined for the $t\bar{t}W$ measurement uses linear interpolation (see Figure 6 of [161] for examples). The NP can also take the form of freely floating normalization factors applied to background yields, which are not constrained in the likelihood. The S and B predictions are generated from MC samples with nonzero statistical uncertainty. The possible variation of the true yields within the total MC statistical uncertainty is handled by the γ_i parameters applied for each bin, a simplified implementation of the Barlow-Beeston method [162].

The best-fit values of μ , θ , and γ are obtained simultaneously using the *Maximum Likelihood Estimate* (MLE), where $\mathcal{L}$ is implemented in RooFIT [163] and maximized using MINUIT [164], all interfaced using the high-level wrapper TREXFITTER [165]. The deviations of the best fit values of NPs are referred to as *pulls*. The covariance of the likelihood parameters is estimated by the HESSE algorithm, which calculates the Hessian matrix:

$$\hat{\Sigma}_{\alpha_i \alpha_j}^{-1} = - \left. \frac{\partial^2 \log \mathcal{L}(\mathbf{n}|\boldsymbol{\alpha})}{\partial \alpha_i \partial \alpha_j} \right|_{\boldsymbol{\alpha}=\hat{\boldsymbol{\alpha}}}\tag{9.6}$$

⁹The same procedure is used to determine $B(\theta_j)$

There are two primary ways to quantify the contribution of individual systematic uncertainties to the total uncertainty on μ . The first is referred to as the *grouped impact* method, in which the full fit including all uncertainties is performed to obtain the total uncertainty on $\hat{\mu}$, σ_{total} . For each group of uncertainties (e.g. all JER systematics) the corresponding NP are fixed to the best fit value and the fit is performed again to obtain σ_{partial} . The uncertainty of that group of uncertainties is estimated by $\sigma_{\text{JER}} = \sqrt{\sigma_{\text{total}}^2 - \sigma_{\text{partial}}^2}$. This is an approximate method, as the uncertainties in the modified fit are from conditional maximum likelihood estimates rather than the fully unconditional estimate and in each fit, the common parameters may not converge to exactly the same value. If a particular group of systematics has a very small contribution to σ_{total} , the Gaussian approximation may fail as the quantity under the radical may be negative.

The second method by which uncertainties are evaluated is called *nuisance parameter ranking* and allows a more fine-grained splitting of uncertainties but perturbs the fit more severely than the grouped impact method. For each NP, a pre-fit (post-fit) mean and uncertainty are given by $\theta_i^{0+\Delta\theta+} (\hat{\theta}_i^{+\Delta\theta+})^{10}$. A conditional MLE $\hat{\mu}_{\pm}$ is obtained by fixing $\theta_i = \hat{\theta}_i \pm \Delta\theta_{\pm}$, and the pre-fit (post-fit) impact of NP θ_j are calculated as $\Delta\mu_{\pm} = \hat{\mu}_{\pm} - \hat{\mu}$. Nuisance parameters can then be ranked by their impact on μ . This method involves performing 2 or 4 likelihood minimizations for each nuisance parameter, which is very computationally expensive. For large uncertainties, fixing the corresponding NP to its variations may result in the fit converging to a different local minimum and so can be unreliable for fits with many POI. The $t\bar{t}W$ differential measurement will therefore only use the grouped impact method to evaluate systematic uncertainties.

¹⁰Since free-floating normalization factors are not constrained in the likelihood function, there is only a post-fit uncertainty estimate

10

Differential Cross Section Measurements

The goal of any measurement is to extract *truth-level* cross sections computed by theorists, while the analyzed data comes from the convolution of the physics of interest and detector effects. The data at the *detector-level* includes efficiency, acceptance, and resolution effects. An inclusive cross section can be extracted simply from the signal strength fit to data, as systematic uncertainties can account for signal efficiency and acceptance effects among analysis regions. Additional detector resolution effects of an observable $\mathcal{O}$ must be modeled when measuring the differential production cross section $d\sigma/d\mathcal{O}$. The procedure for deconvolving detector effects from data to obtain $d\sigma/d\mathcal{O}$

at the truth-level is called *unfolding*. Figure 10.1 gives a pictorial representation of the unfolding procedure for $t\bar{t}$. An unfolded $d\sigma/d\mathcal{O}$ can be directly compared with measurements obtained from other experiments (e.g. CMS) and with theoretical predictions.

Chapter 9 argued that the data-driven Matrix Method for fake lepton estimation is ill-suited for the $t\bar{t}W$ measurement because it is difficult to construct a CR depleted in $t\bar{t}W$ events (25% contamination is achieved in the analysis development). The MM is also a multi-step procedure in which 1) the fake rates are estimated in a CR with fixed $t\bar{t}W$ yield and 2) the rates are applied to the SR. If the $t\bar{t}W$ signal strength is pulled away from the nominal value, the fake rate must be recalculated. The template fit method therefore relieves two ailments: $t\bar{t}W$ contamination in the CRs are reduced by using the PLIV directly in their definition and the fake background and $t\bar{t}W$ normalizations can be fit to data *simultaneously*.

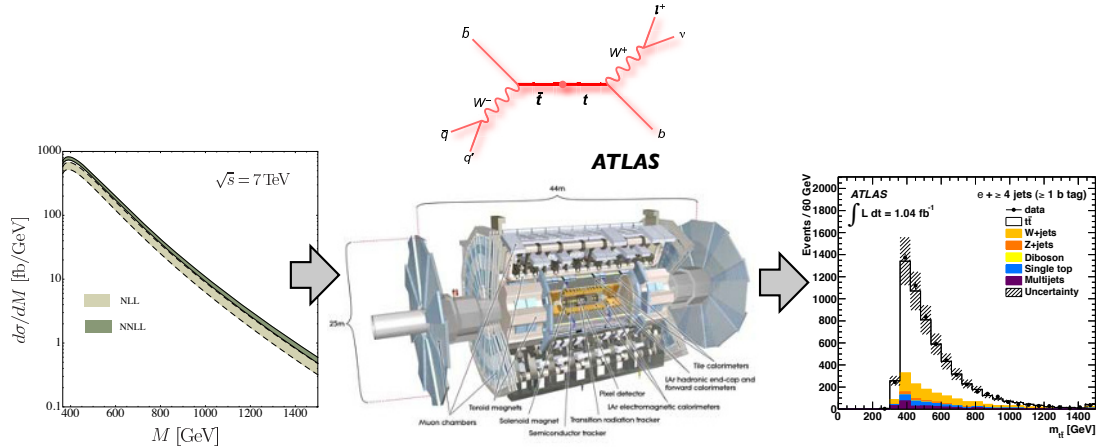


Figure 10.1: Example of the unfolding principle: $d\sigma/dM_{t\bar{t}}$ is known to NLO+NNLL, but its true form is convolved with detector effects to produce measureable data. The inversion of the gray arrows is called unfolding.

Unfolding falls into the class of inverse problems generally framed as solving a Fredholm equation

of the first kind [166],

$$\begin{aligned}
N_{\text{data}}(x_{\text{Det}}) &= \int R(x_{\text{True}}, x_{\text{Det}}) \frac{d\sigma}{d\mathcal{O}}(x_{\text{True}}) \cdot \mathcal{L}_{\text{int}} dx_{\text{True}} && \text{Continuous} \\
N_i^{\text{data}} &= \sum_{j=1}^{n_{\text{bins}}} R_{ij} \left\langle \frac{d\sigma}{d\mathcal{O}} \right\rangle_j \cdot \mathcal{L}_{\text{int}} && \text{Discrete/Binned}
\end{aligned} \tag{10.1}$$

where the *response kernel* $R(x_{\text{True}}, x_{\text{Det}})$ or *response matrix* R_{ij} models the efficiency, acceptance, and resolution effects of the detector and data selection. Reviews of unfolding methods used in HEP can be found in [166, 167, 168] and are mostly binned methods, but parametric unfolding methods have been used historically and new unfolding procedures based on machine learning techniques are an active area of development (e.g. OMNIFOLD [169]). Common binned unfolding methods include singular value decomposition [170], bin-by-bin correction (e.g. [171, 172, 173, 174]), a simple method ignoring bin migrations mostly used during Run I, and *Iterative Bayesian Unfolding* (IBU) due to D’Agostini [175], which is the most commonly used method by ATLAS in Run II (e.g. [176, 177, 178]). The IBU method will be discussed in Section 10.3.

Differential cross sections are typically unfolded to the *parton-level* of fundamental particles or the *particle-level* of quasi-stable colorless particles after parton showering and hadronization but typically before QED radiation. A *fiducial region* of the full phase space is defined in which the differential measurement is reported, which will be discussed in Section 10.1 for the $t\bar{t}W$ measurement. With the nomenclature defined, the response matrix in a binned unfolding procedure is defined in

terms of event counts N in truth-level bin j and detector-level bin i predicted by MC:

$$N_i^{\text{Det}} = \frac{1}{\alpha_i} \underbrace{\sum_j \epsilon_j M_{ij}}_{R_{ij}} N_j^{\text{Fid}}$$

$$M_{ij} = \frac{N_{ij}^{\text{Det} \cap \text{Fid}}}{N_j^{\text{Det} \cap \text{Fid}}}, \quad \alpha_i = \frac{N_i^{\text{Det} \cap \text{Fid}}}{N_i^{\text{Det}}}, \quad \epsilon_j = \frac{N_j^{\text{Det} \cap \text{Fid}}}{N_j^{\text{Fid}}}$$

where the α_i is the *acceptance*, ϵ_j is the *efficiency*, and M_{ij} is the *migration matrix*, which together constitute the full response matrix. The acceptance is defined as the fraction of events accepted in the detector-level selection that also pass the fiducial selection, which is typically larger than 80%. The efficiency is similarly defined as the fraction of events in the fiducial region that also pass the detector-level selection, which is typically poorer than acceptance since the forward folding of detector effects is lossy. The migration matrix determines how events migrate between bins which pass both levels of selection.

The response matrix R_{ij} can simply be inverted in Equation 10.1 to unfold bins to the truth level. However, this induces strong anti-correlations between neighboring bins, resulting in extremely large and unphysical oscillations in the unfolded distribution seeded by statistical fluctuations in the data. Put another way, matrix inversion erroneously interprets statistical fluctuations as physics in an attempt to extract high-frequency structure from the data. In reality, the high-frequency structure of the data is completely destroyed by the smearing effects of detection and reconstruction. To combat these effects, *regularization* constraints are imposed to prevent the unfolding procedure from capturing high-frequency structure to yield physically meaningful distributions at the particle-level based on medium- to high-frequency information that is at least partially preserved by the de-

tector smearing. Care must be taken when imposing regularization to optimize the tradeoff between bias and sensitivity to statistical fluctuations.

This chapter will describe the unfolding procedure used in the $t\bar{t}W$ differential measurement. Section 10.1 describes the fiducial volume definition while Section 10.2 covers the choice of unfolded observables and their binning. The remaining sections give a detailed description of the unfolding method used in the analysis.

10.1 FIDUCIAL VOLUME DEFINITION

As described in Chapter 5, there are many steps in the forward simulation chain from the hard scattering process to predictions of event rates. The choice of where to define the truth-level determines how many of these effects are unfolded. Two common choices are the particle-level and parton-level, which are sketched in Figure 10.2. Unfolding to the particle-level removes only detector effects (and sometimes QED radiation) to the level of stable hadrons clustered into jets, hard visible objects, and E_T^{miss} . Unfolding further to the parton-level removes the effects of hadronization, showering, QCD radiation, and sometimes also parton decays. The $t\bar{t}W$ differential measurement unfolds only to the particle-level due to the difficulty in correctly assigning charged leptons and E_T^{miss} to the W and t partons. The Recursive Jigsaw reconstruction method [179] was studied to help resolve association ambiguities but was not pursued after studies demonstrated poor association accuracy.

Inclusive fiducial cross sections are sometimes reported, but total inclusive cross sections extrapolated to the full phase space of a given process are more common. Extrapolation is done under the minimal assumption that branching fractions do not change and uncertainties of the acceptance of the given process into the analysis regions are taken into account. The picture is more complicated

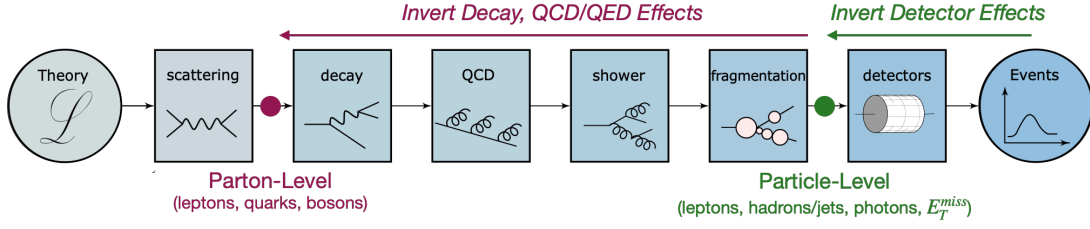


Figure 10.2: Diagram of parton- and particle-level events [21]

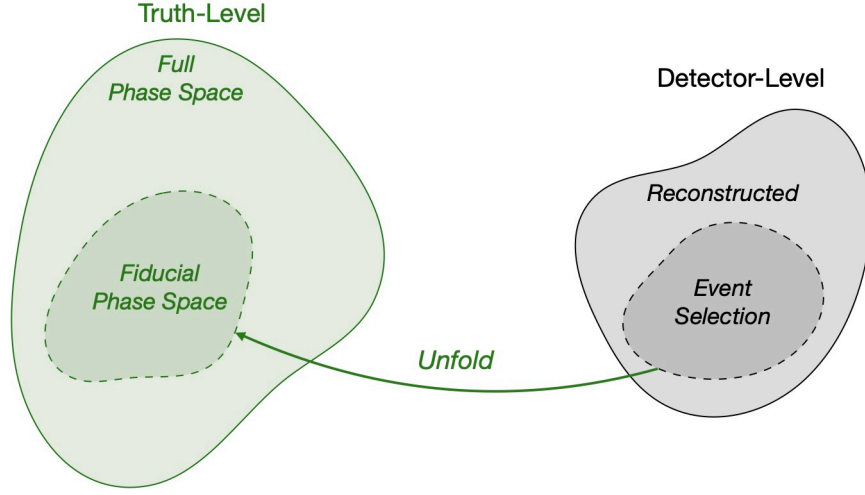


Figure 10.3: Sketch of fiducial truth-level region in relation to the detector-level

for differential measurements, where an observable $\mathcal{O}$ may have very different structure in different regions of the truth-level phase space. Concretely, ϵ_j decreases and M_{ij} becomes increasingly off-diagonal as the fiducial volume increases, enhancing unphysical anti-correlations in the unfolded data that must be smoothed with stronger regularization constraints. Unfolding to a fuller phase space necessarily incurs more bias. Phrased conceptually, the data can only constrain events in the truth-level phase space that are similar to those in the data. If the fiducial volume is too large, the unfolding extrapolation becomes less reliant on constraints from the data and more reliant on the intuition of the analyzer. A sketch of these definitions are shown in Figure 10.3.

The strategy for the fiducial volume definition therefore follows two principles:

1. Define the fiducial selection in alignment with the detector-level event selection
2. Make the fiducial selection as simple as possible for easy comparison to theoretical predictions and measurements by other experiments

There are four main analysis channels (in order of decreasing $t\bar{t}W$ yield): $2\ell\text{SS}^{++}$, $3\ell^+$, $2\ell\text{SS}^{--}$, and $3\ell^-$. Therefore, four fiducial phase spaces must be constructed into which these channels are unfolded. Selections in the fiducial phase space that do not significantly change the modeling of the response matrix and unfolding performance are removed for simplicity. Specific studies are performed on the particle-level overlap removal procedure and jet p_T threshold.

The fiducial phase space into which events are unfolded is defined by the particle-level selection:

- Object pre-selection
 - Select all anti- k_T jets with $p_T > 25$ GeV and $|\eta| < 4.5$
 - Select all muons with $p_T > 10$ GeV and $|\eta| < 2.5$
 - Select all electrons with $p_T > 10$ GeV and $|\eta| < 2.47$, veto electrons in the LAr calorimeter crack region $1.37 < |\eta| < 1.52$
- Overlap removal of objects passing pre-selection
 - Reject jet against electrons: when $dR(e, j) < 0.2$, keep jet if and only if it has a B -hadron and $p_T < 200$ GeV
 - Reject leptons against jets: when $dR(\ell, j) < \text{Min}[0.4, 0.04 + 10 \text{ GeV}/p_T(\ell)]$
- $2\ell\text{SS}$ selection:
 - Event contains at least 2 central jets with and at least 1 central jet containing a B -hadron
 - Event contains exactly 2 leptons of the same charge, leptons are required to have $p_T > 20$ GeV
 - Veto events if $M_{\ell\ell}^{\text{SF}} < 12$ GeV
- 3ℓ selection:
 - Event contains at least 1 central jet and at least 1 central jet containing a B -hadron
 - Event contains exactly 3 leptons with total charge $\pm 1e$, where the same-sign leptons are required to have $p_T > 20$ GeV

- Veto events if $M_{\ell\ell}^{\text{SF-OS}} < 12 \text{ GeV}$, $|M_{\ell\ell}^{\text{SF-OS}} - M_Z| < 10 \text{ GeV}$, or $|M_{\ell\ell\ell} - M_Z| < 10 \text{ GeV}$

Central jets are those within $|\eta| < 2.5$ and the value for M_Z is taken as 91.2 GeV . The regions are further split by requiring the total charge to be positive or negative. The possibility to include jets with $p_T > 20 \text{ GeV}$ was considered to increase the acceptance of events where jets had borderline p_T that migrated within the $\approx 5 \text{ GeV}$ resolution of PFlow jets with $p_T = 25 \text{ GeV}$. This resulted in large off-diagonal migrations in the migration matrix that became especially large in high multiplicity events as shown in Figure 10.4. As a result of this and the added complexity of defining different binning between the particle-level and detector-level jet p_T , this selection was not kept and the nominal jet threshold of $p_T \text{ GeV}$ is used.

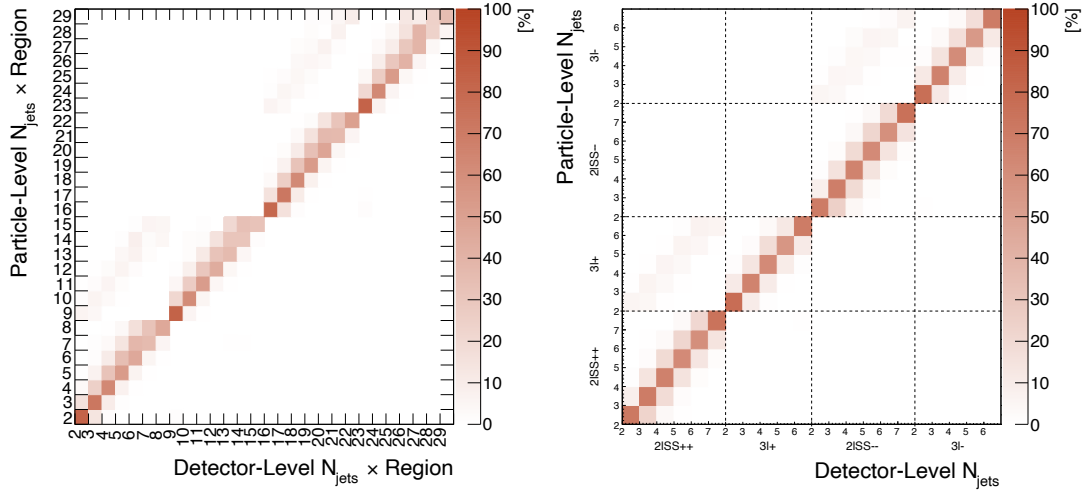


Figure 10.4: Differences of migration matrices for jet multiplicities defined with a p_T threshold of 20 GeV (left) and 25 GeV (right). Large off-diagonal migrations are observed in the 20 GeV case.

The overlap removal differs from the detector-level OR in two ways. The first step of the OR procedure which rejects electrons against muons (and vice-versa) is skipped because it is sensitive to whether or not the muon is reconstructed as a Calo-tagged muon and only happens when $\Delta R(e, \mu) < 0.1$. It is required due to the ambiguity in the reconstruction, which is not a consideration at the

particle-level. The rejection of jets against muons at the detector-level occurs when the muon is ghost-matched to the jet, it is not b -tagged, and the jet has fewer than 3 tracks having $p_T > 500$ MeV. Most jets in $t\bar{t}W$ production have more than 3 tracks and this rejection is infrequently triggered. Checks were done comparing the particle-level OR with and without this step, where at the particle-level jets are rejected against muons if the jet has no B-hadrons and $\Delta R_{\mu j} < 0.2^1$. The efficiency and acceptance corrections of the OR without jet-muon rejection were found to be 0.0% and -0.5% relative to the OR procedure using this step. The efficiency, acceptance, and migration matrices for N_{jets} and $N_{b\text{-jets}}$ are additionally shown in Figure 10.5, also demonstrating minimal differences. We therefore skip this step entirely in the final particle-level OR procedure.

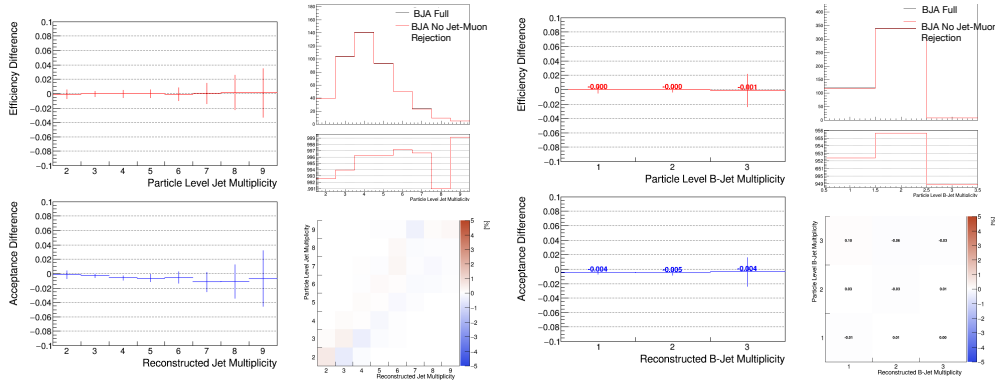


Figure 10.5: Differences of migration matrices, acceptance and efficiency corrections in N_{jets} and $N_{b\text{-jets}}$ of no-jet-rejection OR relative to the jet-rejection OR procedure at particle level.

An inclusive efficiency and acceptance correction can be calculated for each pair of fiducial region and channel. It is possible to perform the unfolding independently for each of these pairs. In this case, these corrections will be further from unity because there are nonzero cross-channel migrations from the fiducial regions. To model these explicitly, the unfolding can be done simultaneously with a roughly block-diagonal response matrix. Figure 10.7 shows the (un-)normalized migration

¹ This is more aggressive than what is done at the reconstruction-level because the jet truth particle multiplicity was not available for this study

matrices. There are migrations from the 3ℓ fiducial regions into the 2ℓ SS detector channels at the 10% level, which consist of events where the OS lepton has low- p_T and fails to be reconstructed or does not pass the lepton pre-selection/OR. Figure 10.6 shows the particle-level OS lepton p_T in the 3ℓ fiducial region separated by whether the event was reconstructed properly as a 3ℓ event or incorrectly as a 2ℓ SS event. Events in the 3ℓ fiducial region where one of the SS leptons fails reconstruction would be seen as 2ℓ OS events and are thus not captured in the signal regions. There are migrations from the 2ℓ SS fiducial regions to the 3ℓ detector channels at the permille level, where a fake lepton is found of opposite sign. There is a negligible number of events that migrate from fiducial regions to detector channels of opposite charge, demonstrating that $t\bar{t}W+$ and $t\bar{t}W-$ are very well isolated in the charge-separated detector channels. The migrations of particle-level events in the 3ℓ fiducial regions into the 3ℓ detector-level regions based on the number of SFOS leptons are modeled via a full non-square response matrix.

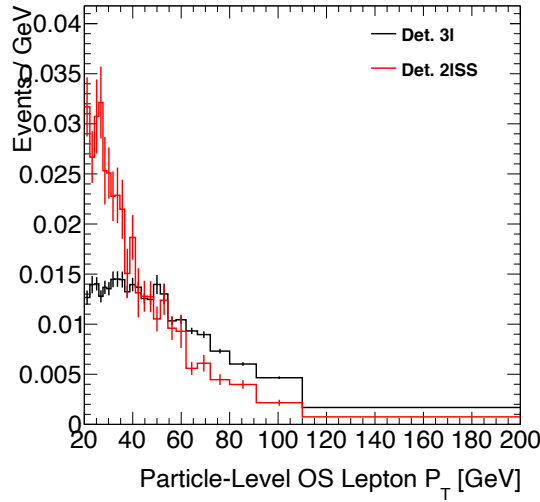


Figure 10.6: Normalized particle-level p_T in 3ℓ events that are reconstructed as 3ℓ events (black) and 2ℓ SS events (red).

Figure 10.8 shows the efficiency and acceptance corrections in the case of independent and si-

multaneous unfolding. The efficiency correction for the $3\ell+(3\ell^-)$ fiducial region decreases from 0.322 to 0.287 (0.324 to 0.291) when failing to account for cross-channel migrations, constituting a 10.9% (10.2%) relative decrease. This reflects the migration rate of 3ℓ fiducial events into 2ℓ SS detector channels of 10%. The efficiency correction in the 2ℓ SS channel is the same in the simultaneous unfolding case since the fraction of events in the 2ℓ SS fiducial region that migrate to the 3ℓ detector channel is very small. The acceptance correction for the 2ℓ SS+ $(2\ell$ SS-) detector channel decreases from 0.949 to 0.926 (0.949 to 0.925) when failing to account for cross-channel migrations, constituting a 2.4% (2.5%) relative decrease. This reflects the migration rate of 2ℓ SS detector events from 3ℓ fiducial regions. The acceptance correction for the $3\ell+(3\ell^-)$ detector channel decreases from 0.917 to 0.905 (0.923 to 0.909) when failing to account for cross-channel migrations, constituting a 1.3% (1.5%) relative decrease. This reflects the migration rate of 3ℓ detector channel events from 2ℓ SS fiducial regions. There is a greater improvement in the acceptance correction in the 2ℓ SS detector channels since the main effect is the migration of events into these from 3ℓ fiducial regions.

It is important to check that the unfolding performance is not negatively impacted by systematic uncertainties that may be larger when cross-channel migrations are explicitly modelled for simultaneous unfolding. Such effects could warrant unfolding each channel independently. This is checked by comparing the unfolded N_{jets} distribution in the two cases when unfolding Asimov pseudo-data from an alternate MC setup (MG5_AMC@NLO). A response matrix from this alternate setup is provided to the fit of N_{jets} as a systematic uncertainty. The unfolded result is very similar between the simultaneous and independent fits and simultaneous unfolding is selected as the nominal strategy.

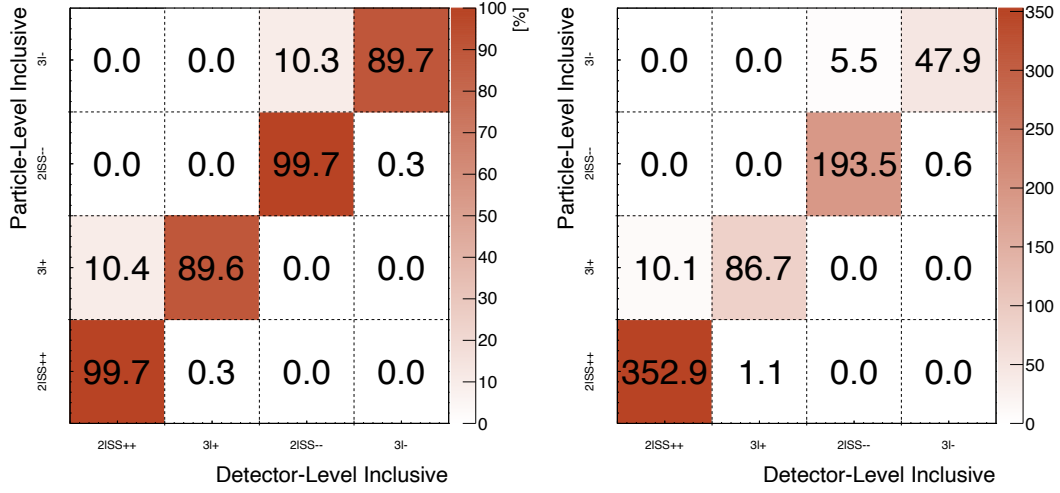


Figure 10.7: Normalised migration matrix (left) and non-normalised migration matrix (right) calculated in Sherpa 2.2.10 with EW corrections

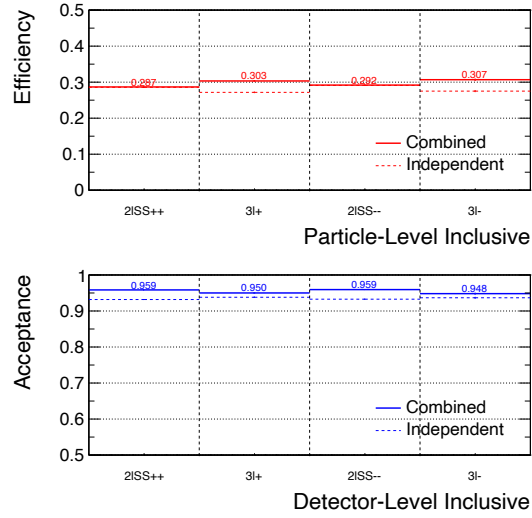


Figure 10.8: Efficiency and acceptance corrections in the case of independent and simultaneous unfolding calculated in Sherpa 2.2.10 with EW corrections

10.2 OBSERVABLES FOR DIFFERENTIAL MEASUREMENTS

A set of about 40 observables were originally considered for unfolding. In addition to the 10 observables discussed in Chapter 7, the list included kinematics (p_T and η) for all leptons in the event,

kinematics of the leading two jets, kinematics of the leading b -tagged jet, and maximum $|\eta|$ of all leptons. Observables formed from multiple objects included $|\Delta\eta|$, $|\Delta\phi|$, and $M_{\ell\ell}$ between all lepton combinations, ΔR between the leading two jets, minimum ΔR among all leptons and jets, E_T^{miss} , and visible H_T (defined as the scalar p_T sum of all leptons and b -jets). Finally, a set of three related observables were defined: the most forward jet (including $|\eta_{\text{jet}}| < 4.5$), the maximum di-jet invariant mass formed with the most forward jet, and the $|\Delta\eta|$ between the jets that form the maximum M_{jj} . This list is skimmed to the minimum number observables that capture the most salient features of $t\bar{t}W$ production and its modeling. The final selection of 10 observables will retain sensitivity to EW corrections, importance of multi-jet merging in modeling additional jet production, and physics of the $tW^+(\bar{t}W^-)$ system via SS leptons.

A bin optimization procedure is adopted for observables that take continuous values i.e. all excluding $N_{(b-)\text{jets}}$. The same binning is chosen at the particle-level and detector-level for simplicity and to ensure that the unfolded result is not under-constrained, as would be the case if $N_{\text{bins}}^{\text{Det}} < N_{\text{bins}}^{\text{Fid}}$ without additionally imposed constraints. The binning procedure requires that the statistical uncertainty of the expected signal-plus-background yields in each bin are below a specified maximum and that the fraction of events on the diagonal element of the migration matrix is at least 60% of the total number of events in that particle-level bin. The maximum statistical uncertainty across the bins is set to 10%, 12%, 15%, and 16% in the $2\ell\text{SS}^{++}$, $2\ell\text{SS}^{-}$, $3\ell^{+}$, and $3\ell^{-}$ regions and are optimized independently. These values are tuned by hand and affect observables that have low off-diagonal bin migrations for which the maximum statistical uncertainty effectively controls the number of final bins. Since the aforementioned regions have decreasing expected event yields, a variable maximum ensures a similar number of bins between regions. After the algorithm is run, the final

binning is then rounded by hand so that the $2\ell\text{SS}$ and 3ℓ regions use the same binning between the charge-split regions.

The optimization procedure begins by calculating a histogram for each observable over a range that covers the full phase space with 200 bins of uniform width. A second step is performed where the observable is re-binned uniformly with 200 bins in the cumulative distribution of expected events, yielding bins that capture a roughly equal fraction of the phase space. This adaptive binning step allows a fine binning to be used in dense regions of phase space and coarse binning in underpopulated regions. This reduces possible sensitivity to limited MC statistics in sparsely populated regions of phase space. These bins are sequentially merged from left to right (in increasing value of the observable) until the merged bin satisfies the bin criteria detailed above. Figure 10.9 illustrates the steps of the procedure for a single observable. The final set of observables and their bin definitions are given in Table 10.1.

The choice of endpoints is the only relevant choice for N_{jets} and $N_{b\text{-jets}}$, as their discrete values naturally fix the bin width. $t\bar{t}W$ production involves 2 light jets and 2 b -jets in $2\ell\text{SS}$ events and only 2 b -jets in 3ℓ . This motivates the lower bound of 2 and 1 jets for $2\ell\text{SS}$ and 3ℓ , respectively, as jet reconstruction inefficiencies lead to these bins being populated by $t\bar{t}W$ events. Similarly, the lower bound of $N_{b\text{-jets}}$ is set to 1. The upper bounds of N_{jets} in $2\ell\text{SS}$ and 3ℓ is as large as possible and is limited by the S/B ratio, which becomes dominated by $t\bar{t}Z$ and $t\bar{t}H$ at high multiplicities. The $N_{b\text{-jets}} = 3$ bin can be unfolded in $2\ell\text{SS}$ channels, but this bin in 3ℓ is dominated by $t\bar{t}t\bar{t}$ production and so is merged with the $N_{b\text{-jets}} = 2$ bin.

Figures 10.10-10.19 show the migration matrices, acceptance, and efficiencies for each unfolded observable. For most observables there is a ramping up of efficiency that reaches a plateau in the

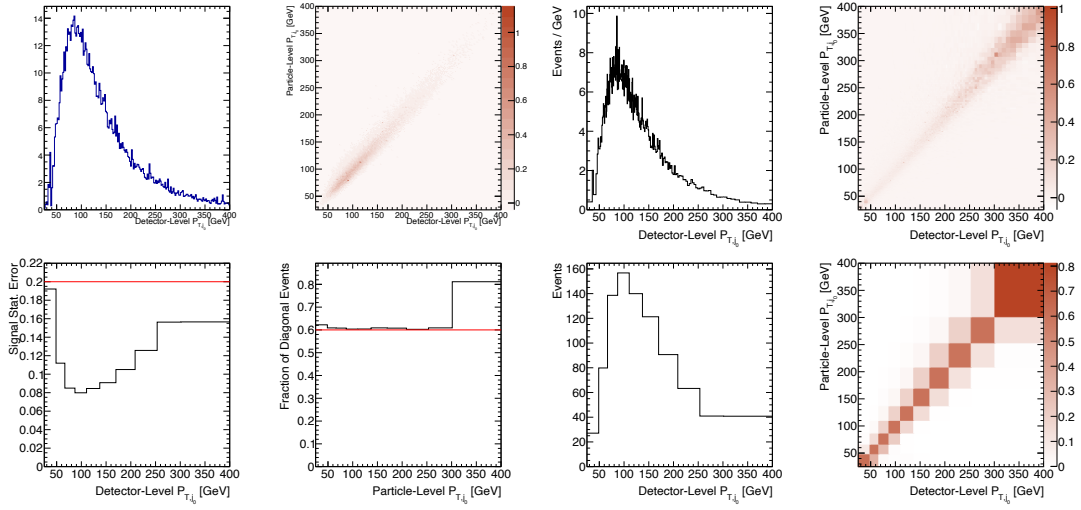


Figure 10.9: Illustration of binning optimisation procedure for $p_{T,j0}$ in the $2\ell\text{SS}++$ channel. Top row from left to right: initial fine binning for $t\bar{t}W$ at detector level, migration matrix with fine binning, $t\bar{t}W$ distribution with adaptive binning, migration matrix with adaptive binning. Bottom row from left to right: statistical uncertainty on S+B for the merged binning, diagonal fraction of migration matrix with merged binning, S+B distribution with merged binning, migration matrix with merged binning. Bin merging for this variable is dominated by detector resolution.

phase space where downward migrations have little effect on the event being accepted into a detector-level signal region. Migration matrices are mostly diagonal with slight asymmetries in the downward direction due to asymmetric losses in detection and reconstruction. Angular variables and leptonic variables generally have more diagonal migrations than momentum and jet variables due to the precision of their reconstruction. The efficiencies in 3ℓ fiducial regions is up to 5% higher than $2\ell\text{SS}$ regions partially because of the construction of the extended response matrix. This is also due in part to the higher reconstruction efficiency of leptons than jets and 3ℓ $t\bar{t}W$ production involves fewer jets. The acceptance differences across 3ℓ channels split by the number of SFOS leptons is due to the veto on SFOS leptons within 10 GeV of M_Z , such that fewer $t\bar{t}W$ events are accepted with increasing numbers of SFOS pairs.

Table 10.1: Binning for final set of observables to be unfolded

Observable	Region	Binning
N_{jets}	2 ℓ SS	[2, 3, 4, 5, 6, 7, 8]
	3 ℓ	[1, 2, 3, 4, 5, 6]
$N_{\text{b-jets}}$	2 ℓ SS	[1, 2, 3, 4]
	3 ℓ	[1, 2, 3]
$H_{\text{T}}^{\text{lep}}$ [GeV]	2 ℓ SS	[40, 70, 85, 100, 115, 130, 150, 180, 220]
	3 ℓ	[40, 115, 145, 170, 200, 245, 325]
$H_{\text{T}}^{\text{jet}}$ [GeV]	2 ℓ SS	[50, 135, 185, 245, 305, 375, 500]
	3 ℓ	[50, 110, 165, 225, 300, 400]
$ \Delta\eta_{\ell_0^{\text{ss}}\ell_0^{\text{ss}}} $	2 ℓ SS	[0.0, 0.2, 0.4, 0.65, 0.9, 1.2, 1.6, 2.0]
	3 ℓ	[0.0, 0.25, 0.5, 0.8, 1.1, 1.5, 2.0]
$ \Delta\phi_{\ell_0^{\text{ss}}\ell_0^{\text{ss}}} /\pi$	2 ℓ SS	[0.0, 0.1]
	3 ℓ	[0.0, 0.2, 0.4, 0.55, 0.7, 0.85, 1.0]
$M_{\ell_0^{\text{ss}}\ell_1^{\text{ss}}}$ [GeV]	2 ℓ SS	[0, 44, 65, 85, 105, 125, 145, 180, 220]
	3 ℓ	[0, 50, 75, 100, 125, 160, 200]
$\Delta R(\ell_0, b_0)$	2 ℓ SS	[0.0, 0.9, 1.4, 1.8, 2.2, 2.55, 2.85, 3.1, 4.0]
	3 ℓ	[0.0, 1.1, 1.75, 2.3, 2.7, 3.0, 4.0]
$M_{j_0j_1}$ [GeV]	2 ℓ SS	[12, 90, 120, 165, 225, 300, 400, 600]
	3 ℓ	[15, 80, 130, 190, 250, 380, 600]
$M_{\ell_0b_0}$ [GeV]	2 ℓ SS	[12, 70, 100, 130, 180, 250, 600]
	3 ℓ	[15, 90, 120, 155, 215, 300, 600]

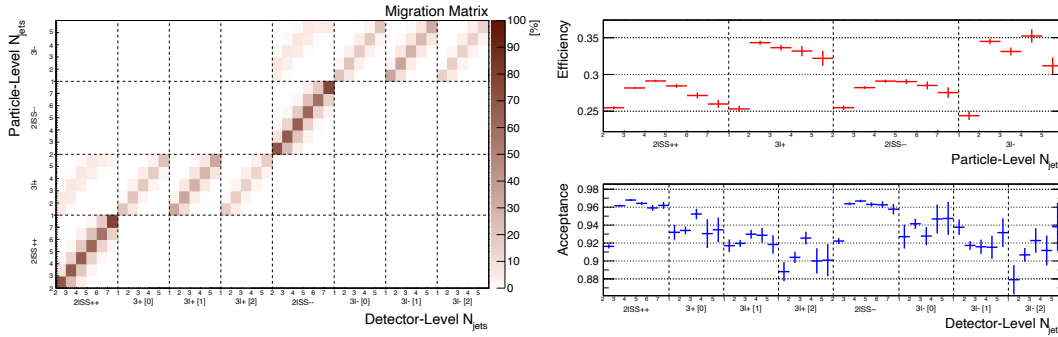


Figure 10.10: Components of response matrix for N_{jets} . The efficiency in the first bin of the 3 ℓ channels is reduced since this jet must be b -tagged. Efficiency in the 2 ℓ SS channel increases with N_{jets} as an increasing number of jets must fail to be reconstructed in order to fail the event selection. There is a decrease in efficiency with N_{jets} most likely due to more probable lepton removal in the OR procedure.

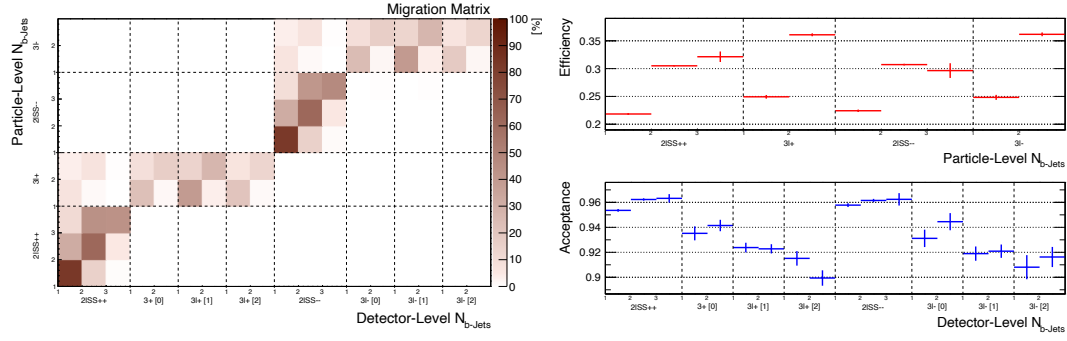


Figure 10.11: Components of response matrix for $N_{b\text{-jets}}$. The efficiency increase between the first two bins in each region is consistent with the 60% efficiency b -tagging WP chosen to define $N_{b\text{-jets}} = 1$ events at the detector-level.

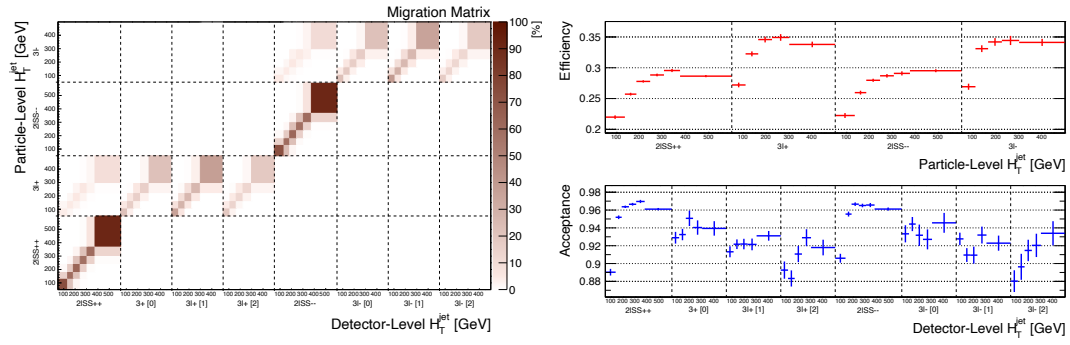


Figure 10.12: Components of response matrix for H_T^{jet}

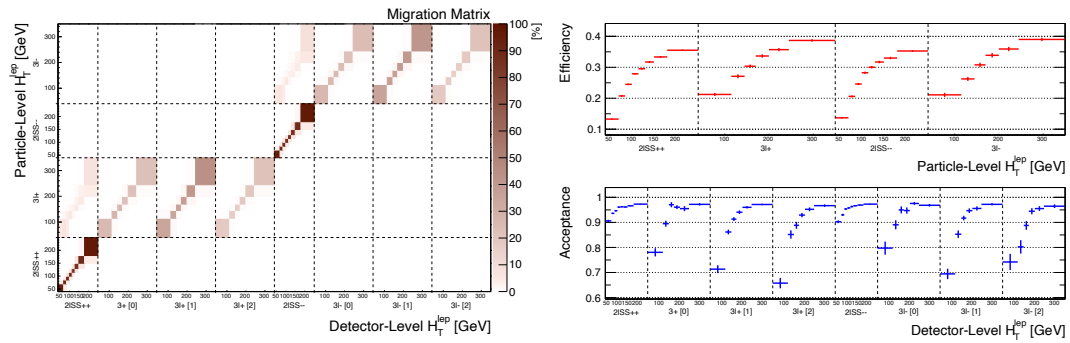


Figure 10.13: Components of response matrix for H_T^{lep}

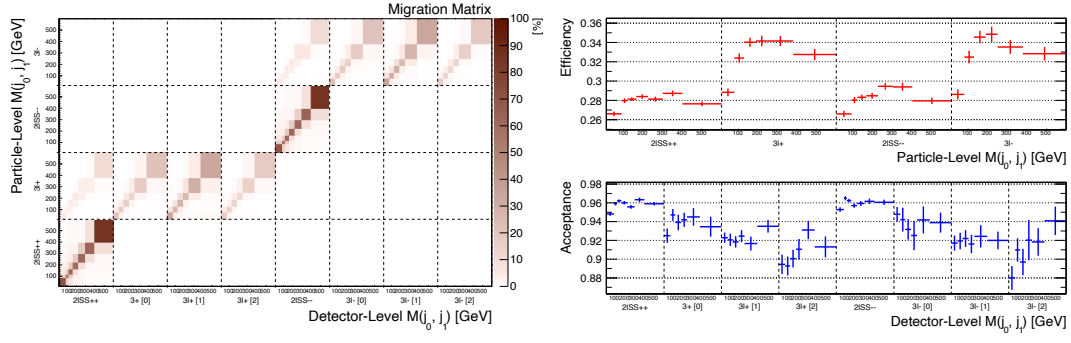


Figure 10.14: Components of response matrix for M_{jj}^{lead}

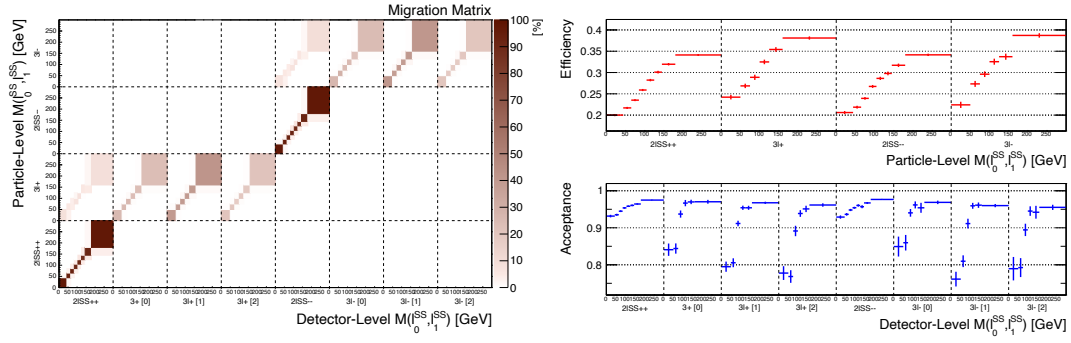


Figure 10.15: Components of response matrix for M_{ll}^{SS}

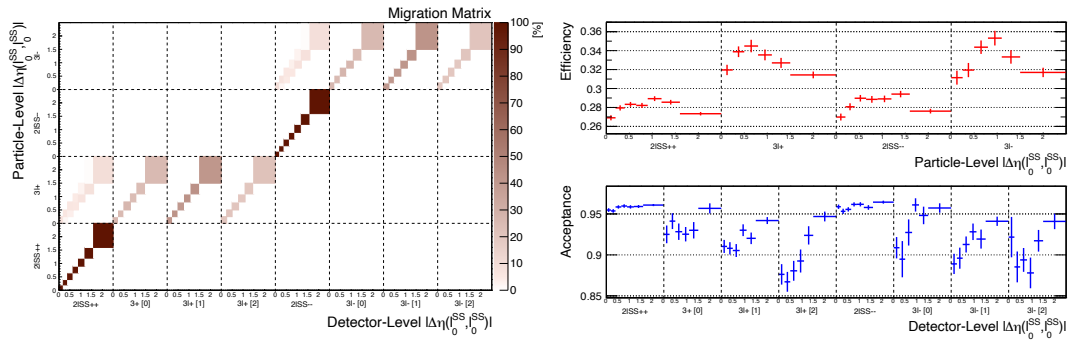


Figure 10.16: Components of response matrix for $\Delta\eta_{ll}^{SS}$

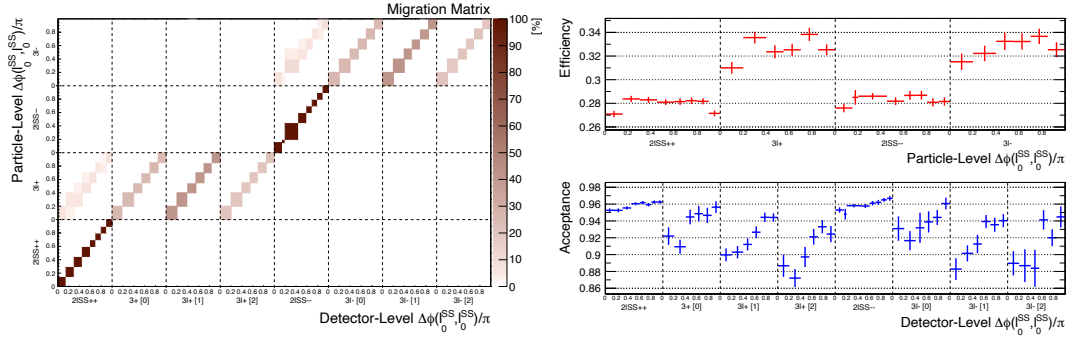


Figure 10.17: Components of response matrix for $\Delta\phi_{ll}^{SS}$

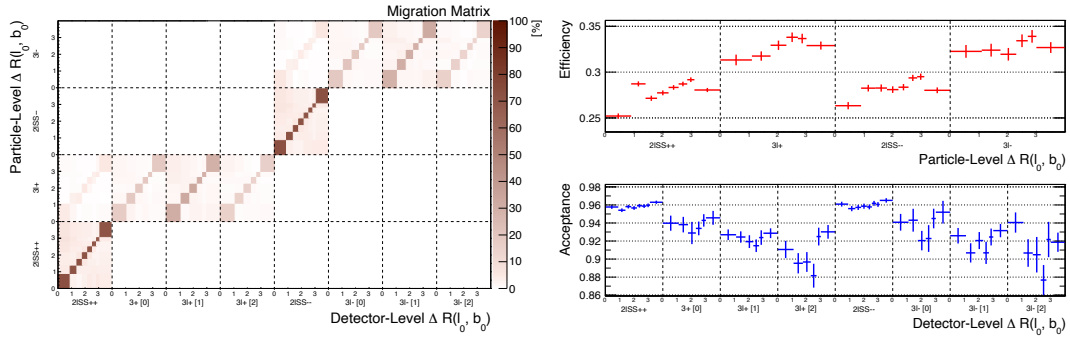


Figure 10.18: Components of response matrix for ΔR_{lb} . There is a roughly uniform pedestal of migrations away from the diagonal resulting from p_T -reordering that may occur after reconstruction, changing which leptons and b -jets are used to construct $\Delta R(lb)$.

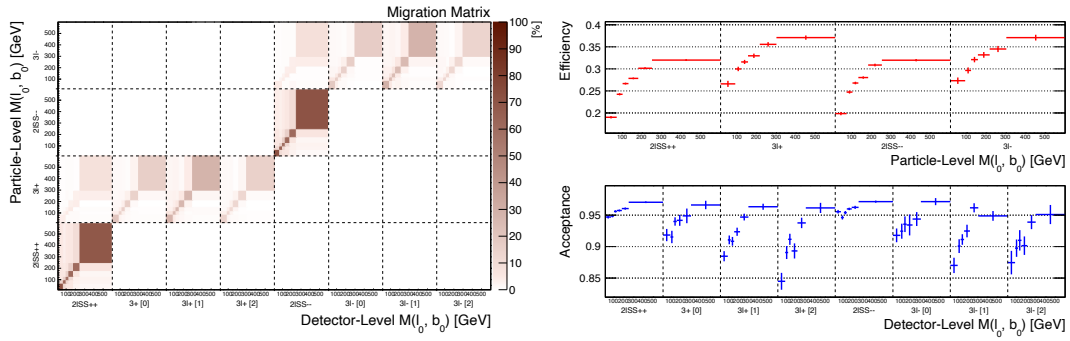


Figure 10.19: Components of response matrix for M_{lb} . There is a roughly uniform pedestal of migrations away from the diagonal resulting from p_T -reordering that may occur after reconstruction, changing which leptons and b -jets are used to construct $M(lb)$. Since the reordering happens asymmetrically by the leading object losing some p_T , the $M(lb)$ migrations are asymmetrically downward.

10.3 PROFILE LIKELIHOOD UNFOLDING

The method of IBU conceptually relies on Bayes' theorem, which provides a mathematical formalism for updating a probability distribution in light of new data. The algorithm iteratively updates a prior MC estimate for a given observable in light of measured data via

$$U_j^n = \frac{1}{\epsilon_j} \sum_i^{\text{Det}} \left[D_i \alpha_i \frac{M_{ij} U_j^{n-1}}{\sum_k^{\text{truth}} M_{ik} U_k^{n-1}} \right] \quad (10.2)$$

where U_j^n is the j^{th} truth-level bin of the unfolded distribution after n iterations, D_i is the observed data after background subtraction in the i^{th} detector-level bin, α_i is the acceptance of the i^{th} detector-level bin, and M_{ij} is the migration matrix giving the fraction of events in the j^{th} truth-level bin that migrate into the i^{th} detector-level bin. The fraction in the summation can be understood as the probability that a detector-level event in bin i migrated from particle-level bin j . The U_j^0 predictions are given by the initial MC estimate. The U^n distribution converges to the distribution given by matrix inversion in the limit $n \rightarrow \infty$. The algorithm is stopped after a fixed number of iterations ($n \approx 5$ is typical), which constitutes the regularization constraint.

A crucial feature of IBU is that it is a two-step procedure. The background composition must be estimated and subtracted from the data to compute D_i as a first step and iterative unfolding is performed as a second step. As argued in Chapter 9, the $t\bar{t}W$ signal strength and background estimation must be performed simultaneously. Extending the measurement strategy to unfold $t\bar{t}W$ simultaneously with background estimation requires the use of *profile likelihood-based unfolding* (PLU). An additional benefit is that the inclusive and differential measurements can be performed within the same statistical framework.

The PLU procedure works by applying normalization factors μ_j to each of the observable's particle-level bins. Each of the truth bins is folded to the detector-level, yielding a set N_{bins} detector-level sub-sample templates. The μ_j are freely floated in a fit to data and applied to the truth template to obtain the unfolded result. This method yields large anti-correlations among NFs of neighbouring bins, which is the manifestation of the typical issue of unregularized unfolding. Unregularized PLU is mathematically equivalent to matrix inversion. Regularization is imposed with a set of Tikhonov parameters τ_j in the likelihood function defined for the fit. The first of two options currently available in TREXFITTER imposes constraints on the individual truth bin NFs:

$$L'(\vec{\theta}, \vec{\mu}) = L(\vec{\theta}) \times \prod_{j=1}^{N_{\text{bins}}} \text{Gaus}(\mu_j | 1, 1/\tau_j) \quad (10.3)$$

The second imposes a constraint based on the discrete second derivative of the NFs:

$$\begin{aligned} L'(\vec{\theta}, \vec{\mu}) &= L(\vec{\theta}) \times \prod_{j=2}^{N_{\text{bins}}-1} \text{Gaus}(\mu_{j-1} - 2\mu_j + \mu_{j+1} | 0, 1/\tau_j) \\ &\equiv L(\vec{\theta}) \times \prod_{j=2}^{N_{\text{bins}}-1} \text{Gaus}(\Delta\mu_j - \Delta\mu_{j+1} | 0, 1/\tau_j) \end{aligned} \quad (10.4)$$

The second form of regularization is the more natural choice because it enforces smoothness in the unfolded distribution by imposing a linearity constraint on the μ_j NFs. In other words, as τ_j increases, the allowed difference in slope of the μ_j NFs around bin j is constrained. It is therefore unbiased against zeroth and first order differences between data and the prior for the signal distribution, i.e. normalization and linear shape effects. In the limit of infinitely large τ , the first regularization method fixes the unfolded distribution to the prior distribution, whereas the second method is equivalent to a linear parametric unfolding. A choice of regularization with moderate strength

will facilitate unfolding sensitive to some higher order shape effects in data while remaining robust against random statistical fluctuations. Second derivative constraints are preferred due to decreased risk of strong bias [160]. This is critical for the $t\bar{t}W$ measurement because it is known to have large normalization differences in data vs. MC. We adopt the second derivative regularization for all unfolded observables. Another important feature of Tikhonov regularization is that τ_j can be chosen differently bin-by-bin, whereas only a single choice of $N_{\text{iterations}}$ can be tuned for IBU. This is important for the simultaneous unfolding of multiple fiducial regions in $t\bar{t}W$, since regularization should not smooth the boundary between regions.

Systematic uncertainties are included in the form of alternate response matrices. These are used to fold the particle-level template to the detector-level. The differences between this forward-folded template and that obtained via the nominal response matrix is taken as a systematic uncertainty at the detector-level. Response matrices can be provided for one-sided or two-sided uncertainties, as well as other options already available in standard profile-likelihood fits. Uncertainties of MC predictions at the particle-level are not included as systematic uncertainties because MC is only needed to model the detector response. Uncertainties on the particle-level prediction should only be considered when comparing predictions to unfolded data.

10.3.1 REGULARIZATION OPTIMIZATION

After fixing the fiducial selection and binning for all observables, a regularization optimization procedure is performed based on statistical bootstrapping. The optimization procedure is performed on each of the 4 regions independently because each has different statistical properties and signal-to-background ratio. For each observable and detector-level channel, 2000 pseudo-data samples are

generated in the signal region from signal plus background smeared with Poisson statistics. Each pseudo-experiment is unfolded in a stat-only fit and a set of metrics are calculated. For each scanned value of τ , the median over the pseudo-experiments and mean over unfolded bins is calculated for each metric and plotted. The largest value of τ that does not increase the χ^2/N_{bins} relative to the true particle-level distribution is selected in order to maximally reduce the impact of statistical fluctuations without inducing a strong bias. Considered metrics are as follows:

- $\chi^2 = \Delta x_i V_{ij}^{-1} \Delta x_j$, where V is the covariance matrix of the truth bin NFs and Δx_i is the difference between the unfolded template and particle-level template in bin i . It is calculated by taking the particle-level template to be either the prior (SHERPA 2.2.10) or truth (MG5_AMC@NLO) and by taking V from TRExFitter or calculating it from the toys.
- Global correlation coefficient, which measures the diagonality of the covariance matrix calculated with toys:

$$\rho = \left\langle \sqrt{1 - (V_{ii} V_{ii}^{-1}) - 1} \right\rangle_{\text{bins}}$$

- Average relative uncertainty over all bins calculated with toys and with TRExFitter covariance matrix; standard deviation of relative uncertainties over all bins calculated with toys.
- Average absolute bias of unfolded distribution against prior and truth particle-level distribution calculated over all bins. The median over toys is taken either before or after the absolute value. In the case that the absolute value is taken before the median, it includes statistical effects, whereas statistical effects are marginalized when the median is taken before the absolute value and reproduces the results of an Asimov fit.
- Rate of unfolded results having at least one negative unfolded bin. Ideally this would be as low as possible.

The MG5_AMC@NLO $t\bar{t}W$ sample is used to generate the pseudo-data, either by considering the detector-level distribution of this sample directly (AltReco) or by folding the particle-level distribution with the response matrix from SHERPA 2.2.10 (AltTruth). The AltReco setup implicitly includes a bias from the different response matrix of the generators, which will be separately supplied to the unfolding fit as a systematic uncertainty. The AltTruth setup accounts only for the bias

induced by choosing a particle-level template from one MC over another, which is not accounted for by the inclusion of the response matrix of an alternate MC. The bias estimate for the choice of $\hat{\tau}$ is conservative enough if the assumption that the true $t\bar{t}W$ particle-level distribution in data does not have significantly larger second-order differences to the nominal MC prediction than the alternate MC prediction. If this assumption is not correct, then the bias term is underestimated.

Figures 10.20 and 10.21 show the regularization scans for N_{jets} and $N_{\text{b-jets}}$, respectively. In all regions, the value of τ at which the χ^2 begins to increase is similar between the AltTruth and AltReco configurations. We proceed with the regularization scans of the remaining variables in only the AltTruth configurations for simplicity. The choice of optimal regularization strength $\hat{\tau}$ for each of the regions is listed in Table 10.2.

Table 10.2: Optimized regularization parameter $\hat{\tau}$ for each observable and region

Observable	2ℓSS++	3ℓ+	2ℓSS--	3ℓ-
N_{jets}	3.0	1.0	1.5	1.0
$N_{\text{b-jets}}$	4.0	0.0	0.5	0.0
$H_{\text{T}}^{\text{jet}}$	2.0	1.5	1.5	1.0
$H_{\text{T}}^{\text{lep}}$	2.0	2.0	1.6	2.0
$M_{\ell\ell\text{ss}}$	3.5	1.0	2.5	1.5
$M_{\ell b}$	2.0	0.6	2.0	0.9
$M_{j_0 j_1}$	3.0	2.0	2.0	1.0
$ \Delta\eta_{\ell\ell\text{ss}} $	2.0	3.0	2.5	2.2
$ \Delta\phi_{\ell\ell\text{ss}} /\pi$	2.0	0.7	1.3	0.6
$\Delta R(\ell b)$	3.0	3.0	1.5	1.5

In the AltTruth configuration, the χ^2 becomes underestimated from TRExFitter due to over-estimation of uncertainties when $\tau > 0$, which will be discussed in detail in Section 10.3.3. The TRExFitter χ^2 calculated relative to the true distribution exhibits a local minimum at a large value of τ in some regions because the competing effects of uncertainty underestimation and bias turns

over. However, since the second derivative regularisation is unbiased to first and second order, the χ^2 remains small at high τ . The global correlation coefficient is minimized at low τ . At $\hat{\tau}$, the average bin uncertainties and rate of having at least 1 negative unfolded bin are close to their minimal values, suggesting that the unfolding is as robust as possible to statistical fluctuations while inducing minimal bias.

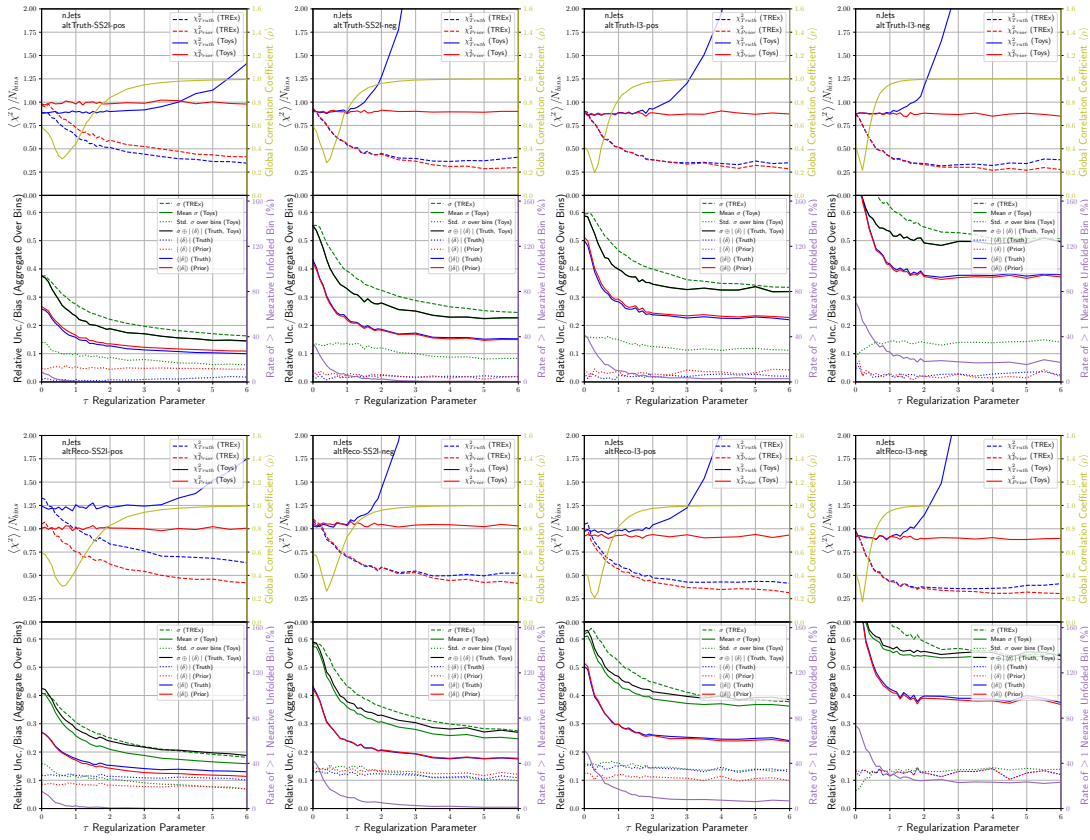


Figure 10.20: Regularisation scans for N_{jets} in the (from left to right) $2l\text{SS}^{++}$, $2l\text{SS}^{--}$, $3l^{+}$, and $3l^{-}$ regions in AltTruth (top) and AltReco (bottom) fit configurations

To demonstrate the effect of the chosen regularization, a single stat-only toy unfolding fit of N_{jets} is performed on Poisson-smear pseudo-data generated in the AltTruth setup. The pre-fit plots and unfolded distributions are shown in Figure 10.22. One can see that imposing the regularization

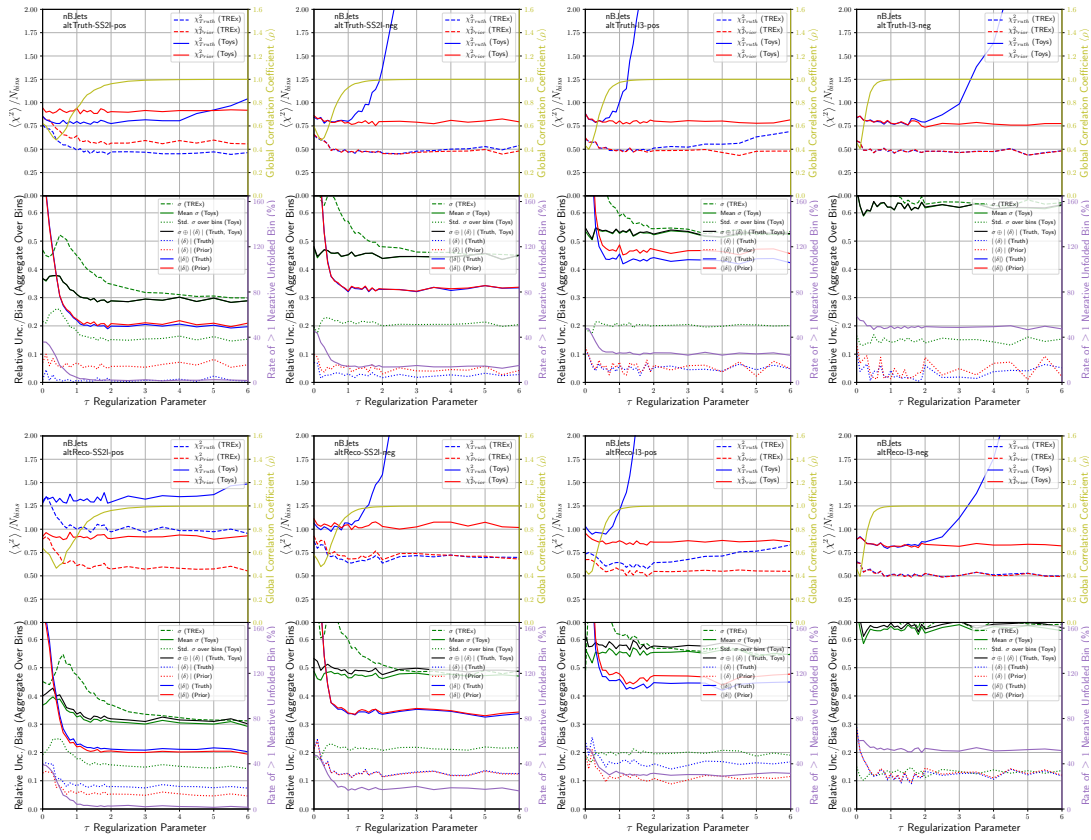


Figure 10.21: Regularisation scans for $N_{b\text{-jets}}$ in the (from left to right) $2lSS++$, $2lSS-$, $3l+$, and $3l-$ regions in AltTruth (top) and AltTruth (bottom) fit configurations

corrects four unfolded bins that have negative bin content, generally smooths the unfolded distribution, and reduces the total uncertainty. In this particular example, there appears to be a trend in the $2lSS++$ by luck, and it is seen in the unfolded distribution. Since the uncertainty is stat-only, the difference between the unfolded distribution and the prediction from aMCNLO/MG should be mostly covered by the uncertainty band, which it is.

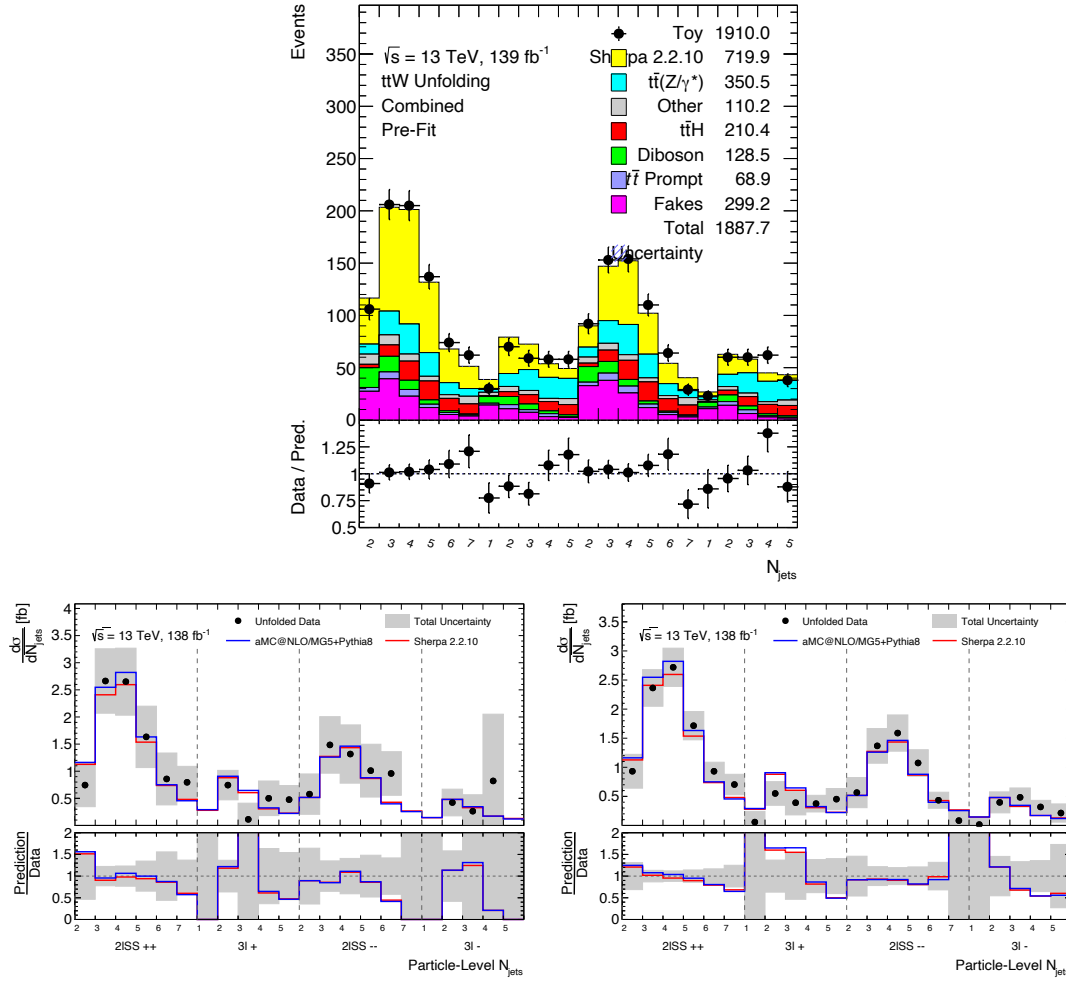


Figure 10.22: A single toy unfolding fit to N_{jets} , from top to bottom-right: pre-fit plot, unregularized result, and regularized result

10.3.2 STRESS TESTS AND NON-CLOSURE

We perform stress tests to ensure the robustness of the fit. It is expected that the second derivative regularization is unbiased up to first order shape differences between data and MC. We verify this by unfolding pseudo-data in N_{jets} obtained by applying 1) a $\pm 40\%$ normalization into the $2\ell\text{SS}$ and 3ℓ channels separately and 2) a $\pm 20\%$ slope into the particle-level templates obtained from SHERPA 2.2.10. The unfolded results for these stress tests are shown in Figure 10.23. Exact closure is ob-

tained in all unfolded bins, confirming the model’s robustness to normalization and linear shape effects. The closure in stress tests are also confirmed in other observables with different migration patterns.

Closure checks are performed using the alternate MC sample (MG₅_AMC@NLO) in the Alt-Truth setup, which are shown in Figure 10.24 and tabulated in Tables 10.3 and 10.4. The non-closure in the AltTruth fit is due entirely to regularization. Non-closure uncertainties are derived for each observable in a statistics-only fit in the signal region with fixed backgrounds. They are quoted separately from other uncertainties and can be added in quadrature for the total uncertainty. This fit setup produces a more conservative estimate of the non-closure uncertainty because small pulls in nuisance parameters and background normalization factors can absorb the difference between the nominal and alternate signal samples. The non-closure is not included in the likelihood fit so that the unfolded result can be reported with and without non-closure uncertainties applied².

² Another reason to separate non-closure uncertainties is that its interpretation as a Gaussian uncertainty in the fit is questionable

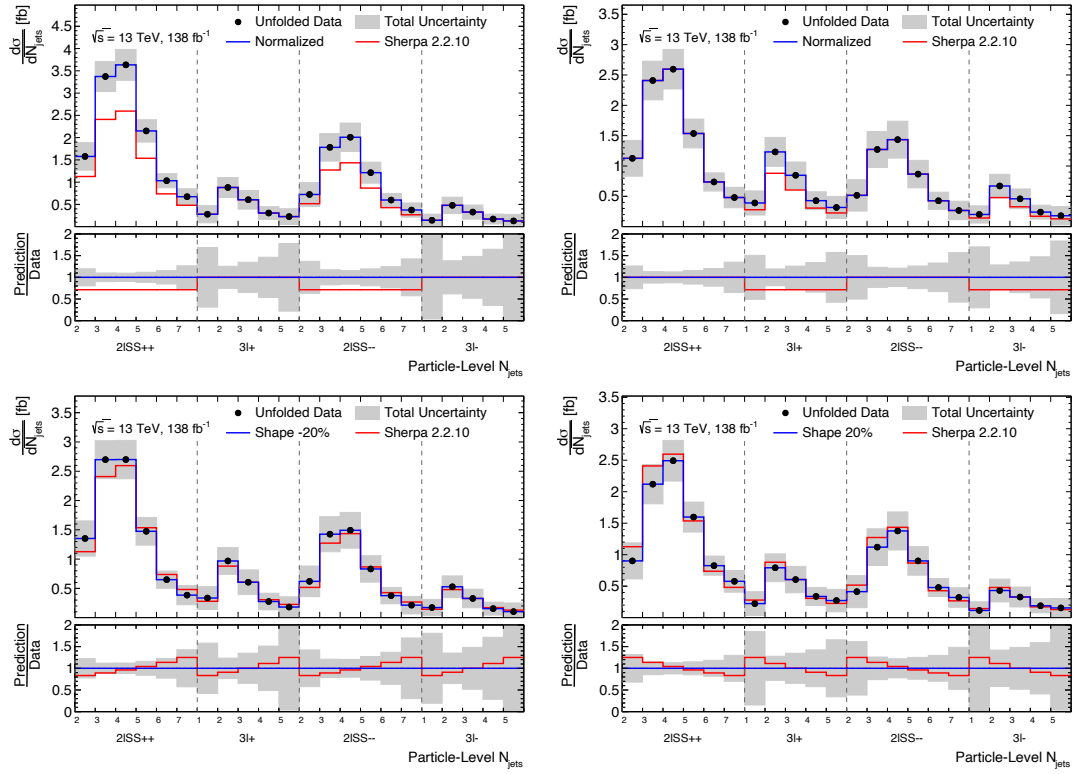


Figure 10.23: Unfolded distributions for N_{jets} in simplified template fit unfolding stress tests with +40% normalization to $2\ell\text{SS}$ and 3ℓ channels (top) and $\pm 20\%$ linear shape (bottom)

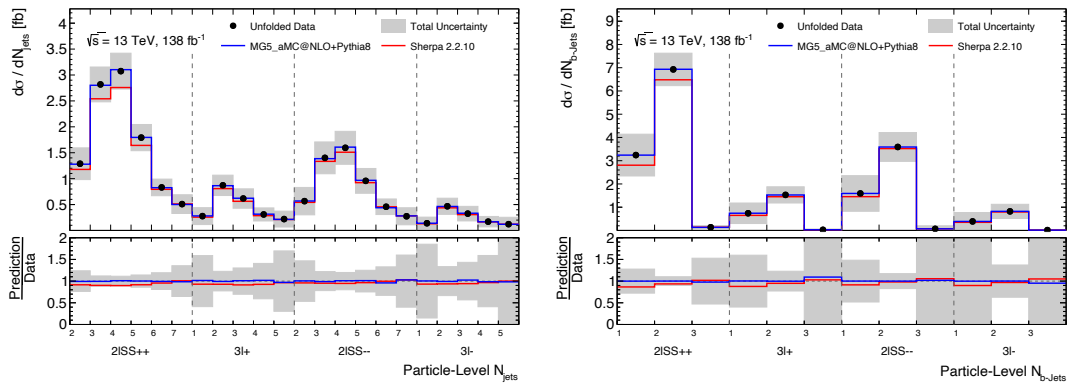


Figure 10.24: Unfolded distributions in simplified template fit unfolding closure tests in the AltTruth pseudo-data setups

Table 10.3: Tabulated unfolding result with non-closure against the aMC@NLO sample (fifth column), which can be taken as non-closure uncertainties

Channel	Bin	N_{jets}		
		$d\sigma/dX$ [fb]		
		Data	SHERPA 2.2.10 - Data	MG5_AMC@NLO - Data
$2\ell\text{SS}++$	[2,3)	1.29 ± 0.31	0.11	0.01
	[3,4)	2.82 ± 0.34	0.28	0.02
	[4,5)	3.07 ± 0.35	0.32	0.03
	[5,6)	1.79 ± 0.25	0.15	0.00
	[6,7)	0.83 ± 0.16	0.04	0.01
	[7,8)	0.51 ± 0.18	0.00	0.01
$3\ell+$	[1,2)	0.28 ± 0.16	0.02	0.00
	[2,3)	0.87 ± 0.20	0.06	0.01
	[3,4)	0.62 ± 0.19	0.05	0.01
	[4,5)	0.31 ± 0.13	0.02	0.01
	[5,6)	0.22 ± 0.15	0.01	0.01
$2\ell\text{SS}-$	[2,3)	0.57 ± 0.26	0.02	0.00
	[3,4)	1.40 ± 0.31	0.07	0.02
	[4,5)	1.59 ± 0.32	0.09	0.01
	[5,6)	0.96 ± 0.24	0.03	0.01
	[6,7)	0.46 ± 0.15	0.00	0.02
	[7,8)	0.27 ± 0.16	0.01	0.01
$3\ell-$	[1,2)	0.14 ± 0.12	0.01	0.00
	[2,3)	0.47 ± 0.16	0.03	0.00
	[3,4)	0.32 ± 0.14	0.02	0.01
	[4,5)	0.17 ± 0.10	0.01	0.00
	[5,6)	0.12 ± 0.13	0.00	0.00

Table 10.4: Tabulated unfolding result with non-closure against the aMC@NLO sample (fifth column), which can be taken as non-closure uncertainties

N_{b-jets}				
Channel	Bin	$d\sigma/dX$ [fb]		
		Data	SHERPA 2.2.10 - Data	MG ₅ _aMC@NLO - Data
$2\ell SS++$	[1,2)	3.24 ± 0.90	0.44	0.00
	[2,3)	6.93 ± 0.70	0.45	0.01
	[3,4)	0.14 ± 0.07	0.00	0.00
$3\ell+$	[1,2)	0.74 ± 0.44	0.09	0.00
	[2,3)	1.53 ± 0.35	0.08	0.00
	[3,4)	0.03 ± 0.04	0.00	0.00
$2\ell SS-$	[1,2)	1.59 ± 0.77	0.14	0.00
	[2,3)	3.59 ± 0.62	0.07	0.00
	[3,4)	0.07 ± 0.13	0.00	0.00
$3\ell-$	[1,2)	0.39 ± 0.38	0.04	0.00
	[2,3)	0.82 ± 0.30	0.03	0.00
	[3,4)	0.01 ± 0.03	0.00	0.00

10.3.3 STATISTICAL PROPERTIES

The uncertainty estimation from TREXFITTER is provided by the HESSE algorithm based on the Hessian matrix error estimation under the Gaussian hypothesis. Considering Equations 9.6 and 10.4, the uncertainty returned by HESSE is given by:

$$\hat{\Sigma}_{\alpha_i \alpha_j}^{-1} = -\frac{\partial^2}{\partial \alpha_i \partial \alpha_j} \left(\log \mathcal{L}(\mathbf{n}|\boldsymbol{\alpha}) - \frac{1}{2} \sum_{j=2}^{N_{\text{bins}}-1} \tau_j^2 (\mu_{j-1} - 2\mu_j + \mu_{j+1})^2 \right) \bigg|_{\boldsymbol{\alpha}=\hat{\boldsymbol{\alpha}}} \quad (10.5)$$

The effect of the regularization is to overestimate the uncertainties of the unfolded bins. The severity of the overestimation can be evaluated using toy pseudo-experiments where the best-fit value of each fit POI is aggregated and fit with a Gaussian to extract the mean and uncertainty. The procedure and results for a statistics-only Asimov fit with 20k toys are shown in Figure 10.25. One can see that the mean values agree in the regularized case, but the uncertainties are overestimated by up to 10% relative to the true uncertainty. This reduced to the level of approximately 5% when the dominant uncertainties are included in the fit. This is considered to be within the range of tolerability for the measurement such that an effort to correct for this effect is not pursued.

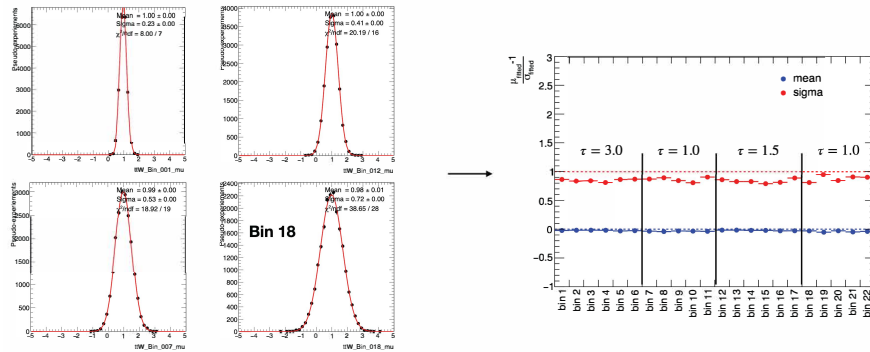


Figure 10.25: Results of per-bin N_{jet} unfolding estimate using toys compared to the nominal fit uncertainty and central values

10.4 RELATIVE CHARGE ASYMMETRY MEASUREMENTS

Along with inclusive and differential cross section measurements of the $t\bar{t}W$ process, it is also interesting to measure the relative charge asymmetry defined by

$$A_C^R = \frac{N^+ - N^-}{N^+ + N^-} = \frac{\sigma(t\bar{t}W^+) - \sigma(t\bar{t}W^-)}{\sigma(t\bar{t}W^+) + \sigma(t\bar{t}W^-)}$$

where $N^\pm$ is the number of $t\bar{t}W$ signal events split by the total charge of the leptons in the event.

This observable probes the differences between cross sections for $t\bar{t}W^\pm$ production and is expected to be less sensitive to some correlated systematic uncertainties of $\sigma(t\bar{t}W^\pm)$ (e.g. luminosity uncertainty). Furthermore, A_C^R can be extracted inclusively in each of the 2ℓ SS and 3ℓ regions and also differentially. One particularly interesting observable for the differential measurement is N_{jets} , where the ATLAS $t\bar{t}t\bar{t}$ analysis team has observed deviations in A_C^R in $t\bar{t}W$ at the detector level. It should also be noted that this definition is distinct from the $t\bar{t}W$ lepton charge asymmetry, defined by

$$A_C^\ell = \frac{N(\Delta_\eta^\ell < 0) - N(\Delta_\eta^\ell > 0)}{N(\Delta_\eta^\ell < 0) + N(\Delta_\eta^\ell > 0)} \quad (10.6)$$

which is within the scope of a separate dedicated ATLAS analysis.

With the inclusive and differential cross section measurements to be reported by the analysis, it is in principle possible to manually compute A_C^R . This would not only require a highly granular description of systematic uncertainties but also a careful treatment of their combination considering their correlations. Non-Gaussian uncertainties would in particular be non-trivial to handle. A solution to this problem is to reparametrize the likelihood function in the PLU fit in terms of A_C^R and

charge-inclusive normalization factors instead of per-bin normalization factors (NF) at the fiducial level. This would leverage the likelihood fit itself to handle the non-trivial systematic uncertainties calculation for A_C^R . Such reparametrized fits produce the same unfolded distributions as the nominal unfolding fits. They provide A_C^R measurements at the particle-level in each of the $2\ell SS$ and 3ℓ fiducial volumes.

10.4.1 PARAMETRIZATION SETUPS

There are four parametrization setups for each observable. Setups 1-2 are analogous to 3-4, where 3-4 allow for the extraction of A_C^R . The redefinitions in the likelihood function are achieved via the Expressions block of TRExFitter.

1. The first is the standard configuration with per-bin NFs in each of the 4 fiducial regions:

$$\{\mu_i^{2\ell SS++}\}_{i=1}^m, \{\mu_i^{2\ell SS--}\}_{i=1}^m, \{\mu_i^{3\ell+}\}_{i=1}^m, \{\mu_i^{3\ell-}\}_{i=1}^m$$

where m denotes the total number of bins per region (but need not be the same between $2\ell SS$ and 3ℓ). This is the standard unfolding setup in TRExFitter.

2. The second configuration is defined by the redefinition of the NF of the first bin in each region in terms of per-channel NFs, such that the parameters of interest (POI) are:

$$\{\mu_i^{2\ell SS++}\}_{i=2}^m, \{\mu_i^{2\ell SS--}\}_{i=2}^m, \{\mu_i^{3\ell+}\}_{i=2}^m, \{\mu_i^{3\ell-}\}_{i=2}^m$$

$$\mu^{2\ell SS++}, \mu^{2\ell SS--}, \mu^{3\ell+}, \mu^{3\ell-}$$

The redefinition is defined with the mathematical formula

$$\mu_1 = \frac{1}{N_1} \left(\mu N - \sum_{i=2}^m \mu_i N_i \right)$$

where μ_i is the NF of the i^{th} bin in a given fiducial region and μ is the inclusive NF for that region. The variables $N_{(i)}$ are the corresponding number of events in the nominal signal

template used in the PLU. This equation can be derived from the following relation:

$$\mu = \frac{1}{N} \left(\sum_{i=1}^m \mu_i N_i \right)$$

3. For a given set of fiducial region separated by charge (i.e. either $2\ell SS$ or 3ℓ), A_C^R is defined by

$$A_C^R = \frac{\mu^+ N^+ - \mu^- N^-}{\mu^+ N^+ + \mu^- N^-}$$

From this, one can redefine the per-bin NFs in the charge-split regions by:

$$\mu_i^- = \frac{1}{2} \mu_i \left(1 - \frac{N_i^+}{N_i^-} \right) (1 - A_{C,i}^R)$$

$$\mu_i^+ = \frac{1}{2} \mu_i \left(1 - \frac{N_i^-}{N_i^+} \right) (1 + A_{C,i}^R)$$

This redefinition also allows the charge-inclusive rates to be extracted via μ_i . Note that the binning for the given observable must be the same in the charge-split regions. The POI for this configuration are then

$$\{\mu_i^{2\ell SS}\}_{i=1}^m, \{A_{C,i}^{R,2\ell SS}\}_{i=1}^m, \{\mu_i^{3\ell}\}_{i=1}^m, \{A_{C,i}^{R,3\ell}\}_{i=1}^m$$

A POI configuration where μ_i^- is redefined in terms of μ_i^+ was also studied via the formula

$$\mu_i^- = \frac{\mu_i^+ N_i^+ (1 - A_{C,i}^R)}{N_i^- (1 + A_{C,i}^R)}$$

but this configuration does not provide a measurement for the charge-inclusive rate. Tested PLU fits also do not stably converge, likely a result of the presence of A_C^R in the denominator causing issues during the internal POI transformation performed by MINUIT.

4. The NF for the first bin of each unfolded distribution can be redefined in terms of A_C^R analogously to parametrization 2 as follows:

$$\mu_1^- = \frac{1}{2N_1^-} \left[\mu N (1 - A_C^R) - \sum_{i=2}^m \mu_i N_i (1 - A_{C,i}^R) \right]$$

$$\mu_1^+ = \frac{1}{2N_1^+} \left[\mu N (1 + A_C^R) - \sum_{i=2}^m \mu_i N_i (1 + A_{C,i}^R) \right]$$

The set of POI in this configuration is given by

$$\{\mu_i^{2\ell SS}\}_{i=2}^m, \{A_{C,i}^{R,2\ell SS}\}_{i=2}^m, \{\mu_i^{3\ell}\}_{i=2}^m, \{A_{C,i}^{R,3\ell}\}_{i=2}^m$$

$$\mu^{2\ell SS}, A_C^{R,2\ell SS}, \mu^{3\ell}, A_C^{R,3\ell}$$

11

Results

With the statistical analysis strategy and unfolding methodology outlined, we turn now to the analysis of expected and observed measurements. The measurement considers an integrated luminosity of 139 fb^{-1} data collected by the ATLAS detector during good detector operations between 2015 and 2018. The analysis strategy has been developed without performing any fits to real data in the SRs. This blinding strategy aims to reduce the likelihood of bias by the analyzers in shaping the measurement result. This would be a particular concern for tuning of the unfolding regularization.

The chapter will proceed as follows. Section [11.1](#) shows the results of fits to data in the CRs

alone, which has been performed throughout the analysis development. Section ?? shows the results of hybrid Asimov fits to evaluate the expected measurement precision under the nominal $t\bar{t}W$ prediction. Finally, Section 11.2 shows the results of fully unblinded fits to data in all regions.

11.1 CONTROL REGION FITS TO DATA

Fits to data in the CRs are performed with the $t\bar{t}W$ yields fixed to the Asimov prediction. Minor systematic uncertainties are pruned to reduce the complexity of the fit while accurately estimating uncertainties using the most dominant systematics. This is evaluated separately for normalization and shape components of instrumental and theoretical uncertainties and also for MC statistical uncertainties modeled by γ factors in the likelihood. Normalization components of uncertainties applied to specific samples are dropped if they are below the 1% threshold and the shape component of systematics is dropped if no uncertainties of bin yields are larger than 1%. Similarly, γ factors for MC statistical uncertainties are dropped if the relative uncertainty in the given bin is below 1%.

Pre-fit and post-fit data/MC comparisons are shown in Figures 11.1-11.3 with the corresponding background normalization factors obtained from the fit are given in Figure 11.4. The agreement between data and MC is generally good pre-fit, with some mis-modeling in the low- p_T bins of the HFe/μ TM CRs. The agreement is very good post-fit, where all MC yields are consistent with data within statistical and systematic uncertainties. The post-fit background normalizations are generally consistent with unity, with slight preference for larger yields.

The nuisance parameter pulls and post-fit constraints are shown in Figure ?. Instrumental uncertainty NPs are generally not pulled, with some downward pulls on the JES pileup ρ -calibration

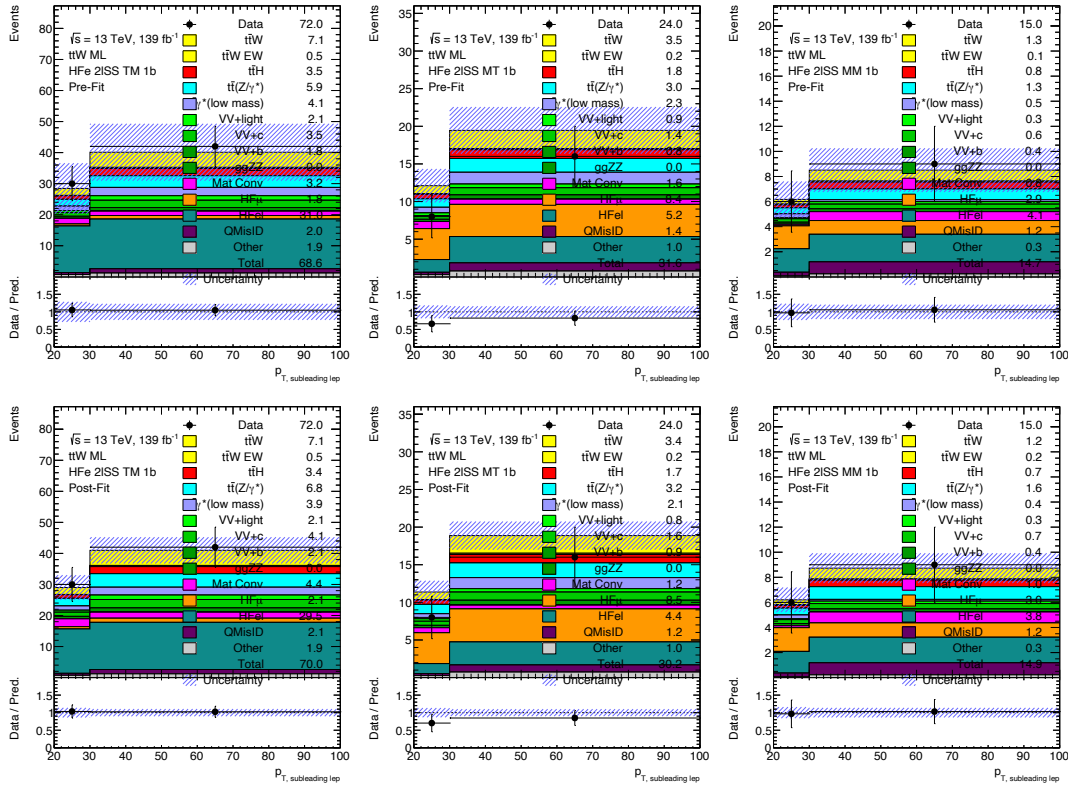


Figure 11.1: Data/MC comparisons in HFe CRs pre-fit (top) and post-fit (bottom).

uncertainty¹ and the leading two components of the b -tagging uncertainties. No NP pulls are seen for uncertainties on the DD QMisID estimate or the lepton PLIV uncertainties. Some pulls are seen in NPs relating to the $t\bar{t}Z$ modeling, where a preference for the alternate $t\bar{t}Z$ showering algorithm is seen. There is also a preference for larger $t\bar{t}Z$ +HF production of approximately 20%. Some minor pulls are seen on the NPs controlling non-closure in PLIV observables. All NPs retain similar post-fit uncertainties to their pre-fit values, indicating that the fit does not constrain any of the NPs. Figure 11.6 shows the pulls on γ NP that are consistent with unity except for a slight upward pull in the high- p_T bin of the TM HFe μ CR. Finally, Figure 11.7 shows the correlation matrix of all parameters included in the fit, where NPs with no correlations above 20% are shown. Anti-correlations

¹Here ρ refers to the jet p_T density and is corrected to data in the presence of pileup

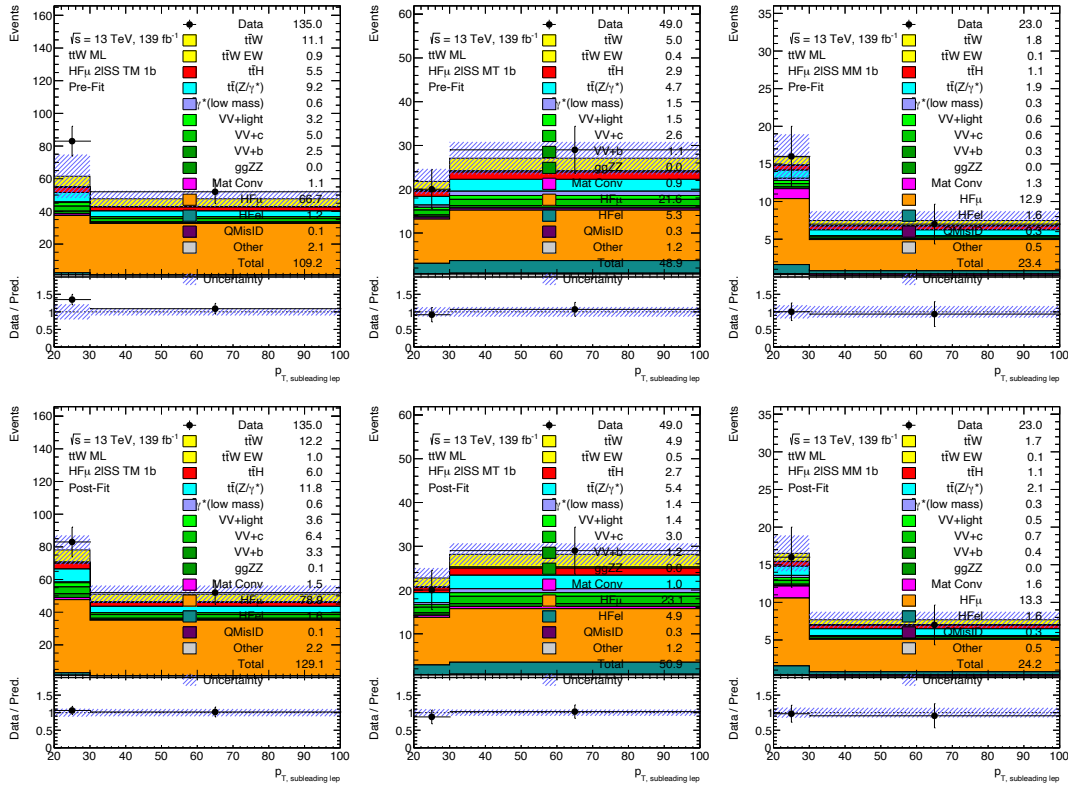


Figure 11.2: Data/MC comparisons in $HF\mu$ CRs pre-fit (top) and post-fit (bottom).

are typical between NFs and NPs that control the normalization of different components of a given process or control normalizations for backgrounds in overlapping phase spaces. For example, the NFs for $VV + HF$ and $t\bar{t}Z + \text{light}$ have a -60% correlation. Some correlations between instrumental NPs and background NFs are also seen. These are expected to occur sometimes due to the large number of uncertainties included in the fit and is not expected to impact the precision or stability of the fit.

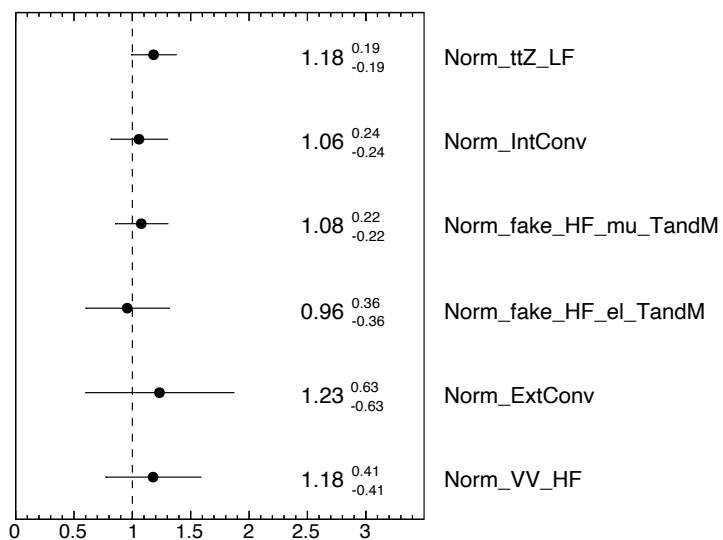
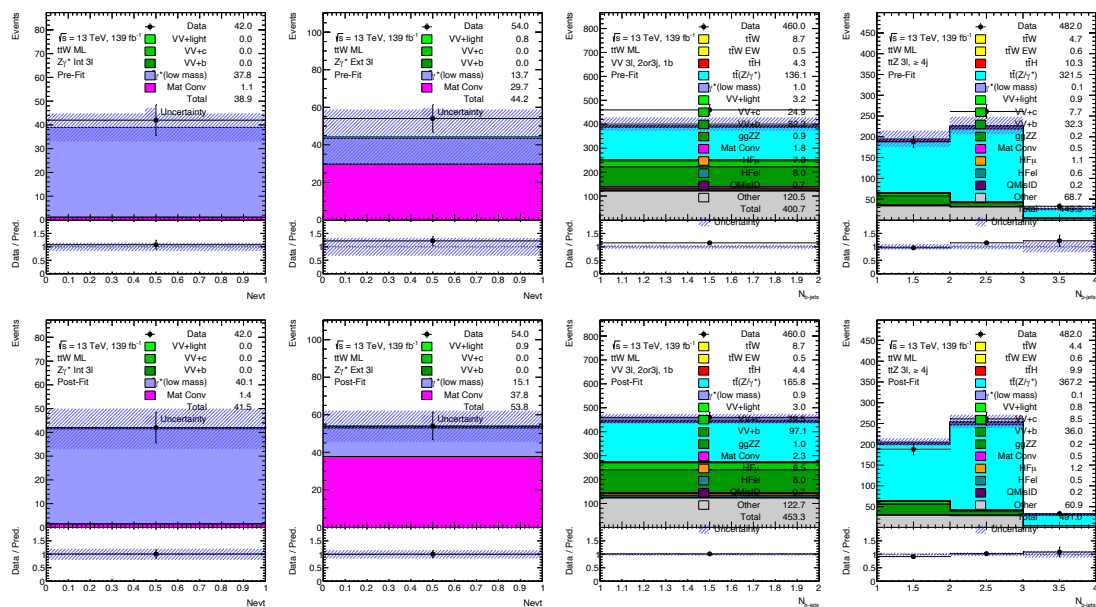


Figure 11.4: Post-fit values and uncertainties for backgrounds normalization factors.

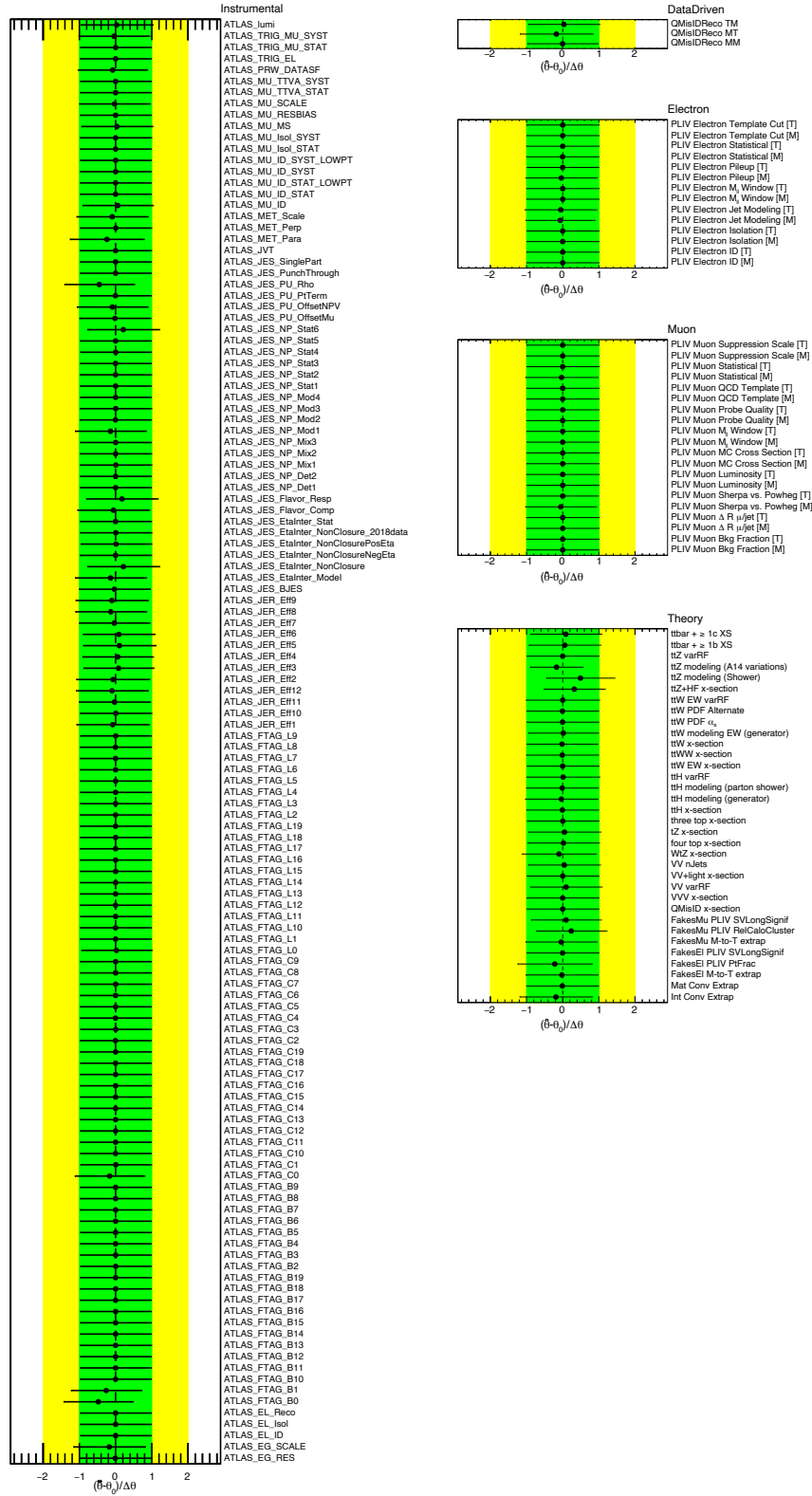


Figure 11.5: Pull plot for all nuisance parameters split by category.

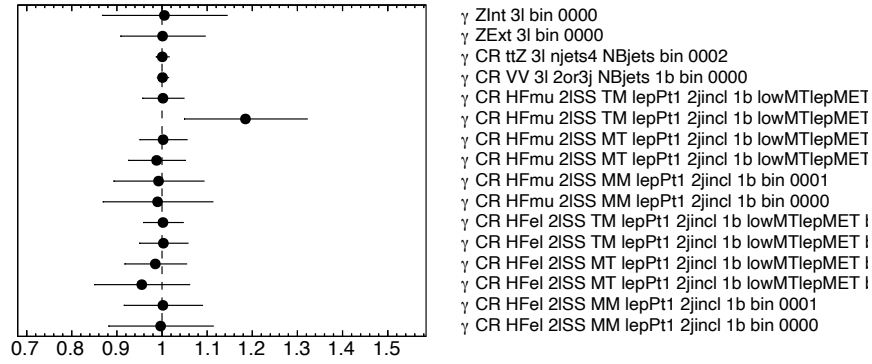


Figure 11.6: Post-fit values for γ uncertainties for limited MC statistics.

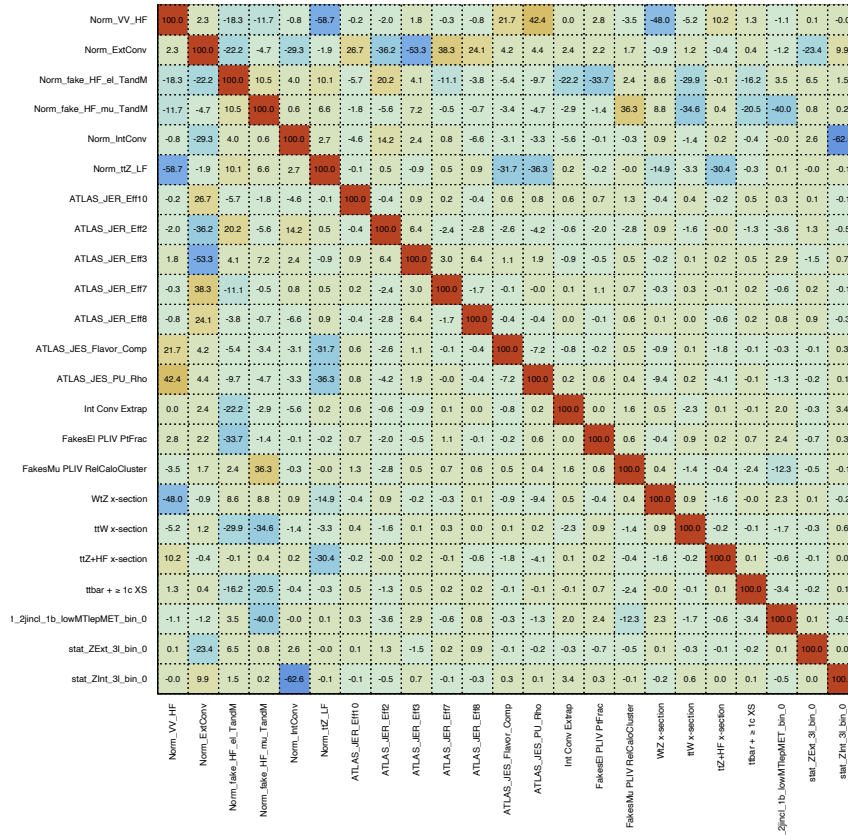


Figure 11.7: Correlation matrix for all nuisance parameters.

11.2 DIFFERENTIAL MEASUREMENTS

We now turn to the results of fully unblinded fits performed simultaneously in signal and control regions. Inclusive fiducial cross sections and relative charge asymmetries extracted from fits to the N_{jets} distribution are quoted in Tables 11.1 and 11.2. These values are consistent between fits of other observables in the SR, but the N_{jets} distribution offers slightly higher precision. These results are also shown graphically in Figure 11.8 with nominal predictions from other $t\bar{t}W$ MC samples. The fiducial cross sections in $2\ell\text{SS}$ channels are measured at roughly 1.25 times the theoretical expectation while in 3ℓ channels they are measured at 1.15 times the theoretical expectation. A_C^R measured in the $2\ell\text{SS}$ regions is larger than the prediction, while in 3ℓ the measured value is smaller. Note that while the charge-inclusive fiducial cross sections are dominated by systematic uncertainties, A_C^R is limited by statistical uncertainties (as expected). Predictions are consistent with measurement at the level of two standard deviations.

Table 11.1: Inclusive fiducial cross sections for $t\bar{t}W^\pm$ production extracted from fits to the N_{jets} distribution. Theory predictions are derived from Sherpa 2.2.10 with PDF and scale uncertainties included.

Fiducial Region	Measured Cross Section [fb]	Theory [fb]
$2\ell\text{SS}^{++}$	$12.9 \pm 1.6 [\pm 0.7 \text{ (stat)} \pm 1.4 \text{ (syst)}]$	9.4 ± 2.5
$2\ell\text{SS}^{--}$	$5.6 \pm 1.1 [\pm 0.6 \text{ (stat)} \pm 0.8 \text{ (syst)}]$	5.0 ± 1.5
$3\ell^+$	$2.4 \pm 0.6 [\pm 0.4 \text{ (stat)} \pm 0.4 \text{ (syst)}]$	2.1 ± 0.6
$3\ell^-$	$1.4 \pm 0.6 [\pm 0.3 \text{ (stat)} \pm 0.3 \text{ (syst)}]$	1.2 ± 0.3
$2\ell\text{SS}$	$18.4 \pm 2.4 [\pm 0.9 \text{ (stat)} \pm 2.2 \text{ (syst)}]$	14.5 ± 4.0
3ℓ	$4.1 \pm 0.9 [\pm 0.5 \text{ (stat)} \pm 0.7 \text{ (syst)}]$	3.3 ± 0.9

The breakdown of uncertainties for the inclusive measurements are shown in Figure 11.9. The leading uncertainties pertain to $t\bar{t}W$ modeling, almost entirely from the difference between response modeling between SHERPA and MG5_AMC@NLO. The efficiency corrections derived

Table 11.2: Relative charge asymmetries in 2ℓ SS and 3ℓ fiducial regions extracted from fits to the N_{jets} distribution. Theory predictions are derived from Sherpa 2.2.10 with PDF and scale uncertainties included.

Fiducial Region	Measured A_C^R	Theory [fb]
2ℓ SS	$0.39 \pm 0.06 [\pm 0.05 \text{ (stat)} \pm 0.03 \text{ (syst)}]$	0.30 ± 0.02
3ℓ	$0.21 \pm 0.13 [\pm 0.12 \text{ (stat)} \pm 0.04 \text{ (syst)}]$	0.29 ± 0.02

in MG₅_AMC@NLO are lower than the nominal SHERPA prediction by 5% uniformly across the 10 observables chosen for unfolding. The next leading source of uncertainty come from the semi-data-driven background estimation. The balance of background uncertainties vs $t\bar{t}W$ modeling uncertainties varies by fiducial region, tracking with the ratio of signal to background in each. The next most leading uncertainty are the instrumental uncertainties from JES and JER, but these are significantly subdominant. Further uncertainties related to heavy flavor tagging, PLIV, trigger, luminosity, lepton reconstruction, and E_T^{miss} reconstruction are small. Uncertainties from finite MC statistics are notably not the least significant uncertainty. Finally, it is plain that statistical uncertainties are very dominant in the extraction of A_C^R , particularly for 3ℓ channels. Among the subdominant systematic uncertainties, uncertainties from $t\bar{t}W$ model are very low.

Differential measurements of the 10 observables of interest and the breakdown of their uncertainties are shown in Figures 11.10-11.29. The most precise measurements of the $t\bar{t}W$ process come in the 2ℓ SS++ channel, where there is the least relative contribution from backgrounds. The excess events are localized to 2ℓ SS++ events with 2 or 3 jets, high H_T^{lep} and large $M_{\ell\ell}^{SS}$, and large dijet invariant mass of the leading jets. Enhancements in $t\bar{t}W$ rates are otherwise not strongly dependent on phase space. The differences between $t\bar{t}W^+$ and $t\bar{t}W^-$ production can be seen in the A_C^R fit results, which are predicted to be roughly constant across all regions of phase space.

Uncertainties at the differential level are dominated by statistical uncertainties, which is a com-

mon scenario for differential measurements. The leading systematic uncertainties remains the $t\bar{t}W$ model and background estimation. The JES/JER and flavor tagging uncertainties become important in N_{jets} and $N_{b\text{-jets}}$, respectively, as would be expected.

11.2.1 IMPLICATIONS

While the $t\bar{t}H$ and $t\bar{t}W$ phase spaces are overlapping, the measurement reported in this thesis accounts for multiple sources of uncertainty for the $t\bar{t}H$ model. Additionally, the $t\bar{t}H$ background is small compared to the signal. Therefore, the differential $t\bar{t}W$ measurements can be used to constrain the $t\bar{t}W$ background predictions for a measurement of $t\bar{t}H$ in multi-lepton channels. The most recent $t\bar{t}H$ multi-lepton measurement performed by the ATLAS collaboration is limited by the uncertainty in background estimation for the $t\bar{t}W$ process. That measurement allowed the normalization of $t\bar{t}W$ to float independently in 2ℓ SS events with 2-3 jets, 2ℓ SS events with ≥ 4 jets, and 3ℓ events; in these regions, the $t\bar{t}W$ normalization was found to be approximately 1.4, 1.2, and 1.7, respectively. We see that $t\bar{t}W$ is significantly pulled upward in 2ℓ SS events with 2 or 3 jets. However, in events with ≥ 4 jets the prediction from SHERPA is quite accurate. The 3ℓ fiducial region also shows a cross section consistent with the SHERPA prediction with an enhancement of only 20%. These inputs motivate a more precise treatment of the $t\bar{t}W$ background in a subsequent $t\bar{t}H$ measurement.

In addition to constraining $t\bar{t}W$ as a background, these measurements can be analyzed and possibly interpreted in the context of EFT operators. It is possible that the excess can be associated to tW scattering processes, where could expect an enhancement in $M_{\ell\ell}^{SS}$ that is sensitive to the kinematics of the tW system. However, these events seemly have a low number of jets. It is therefore not obvi-

ous what processes might be causing the deviations. These measurements are, however, invaluable feedback to phenomenologists working on explaining the anomalous behavior of $t\bar{t}W$.

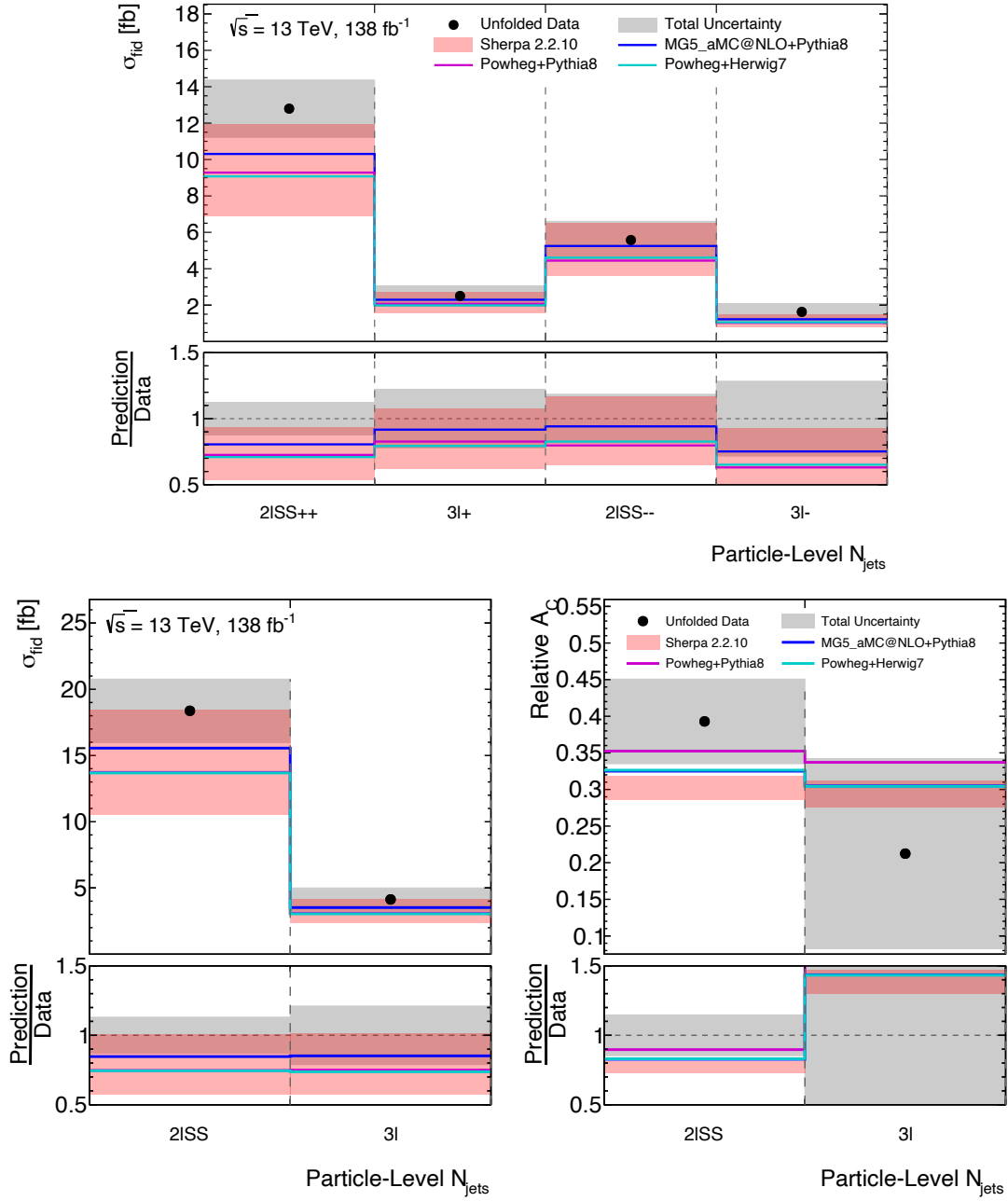


Figure 11.8: Inclusive fiducial cross section measurements compared to MC predictions.

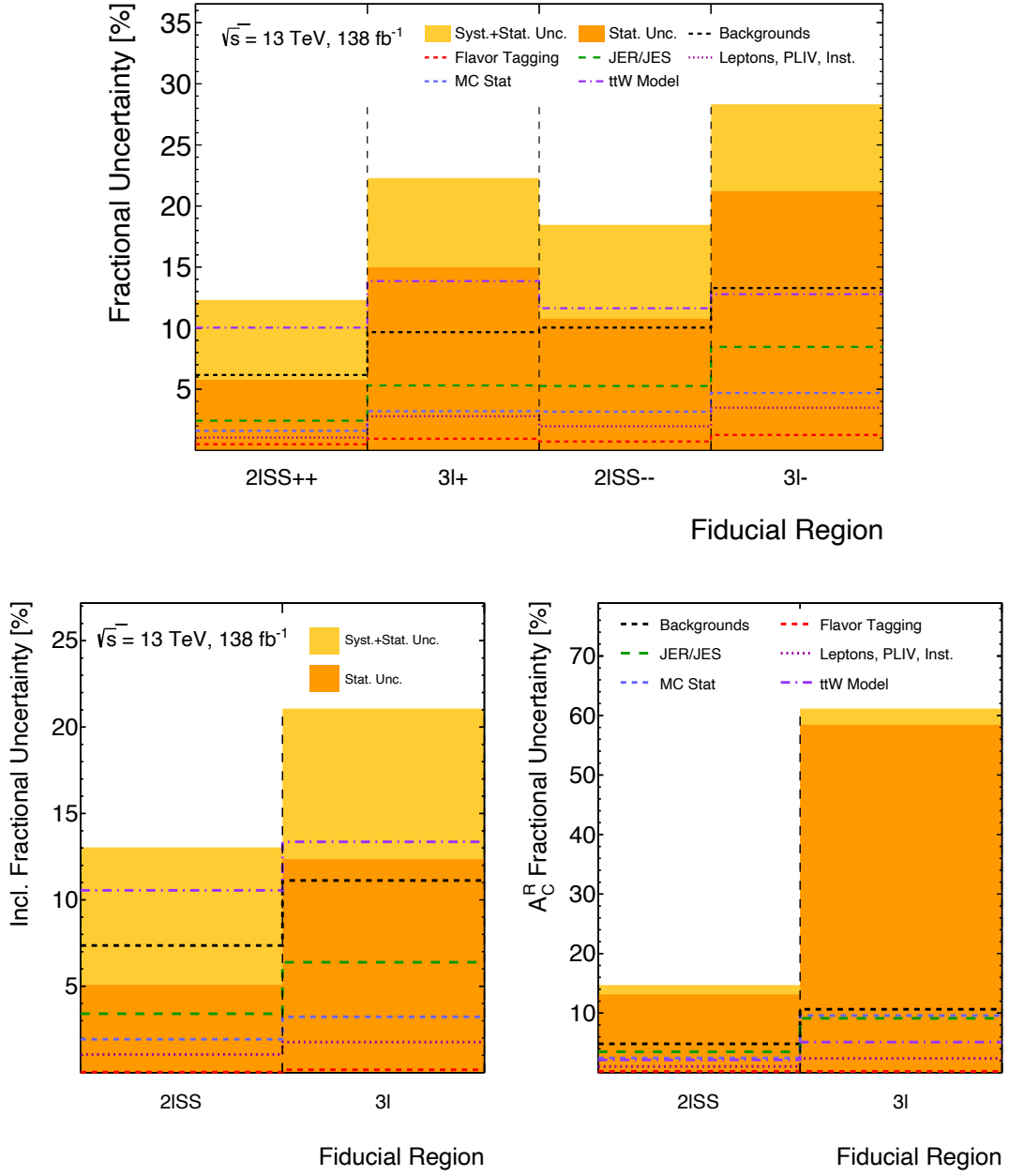


Figure 11.9: Breakdown of uncertainties for inclusive fiducial cross section measurements.

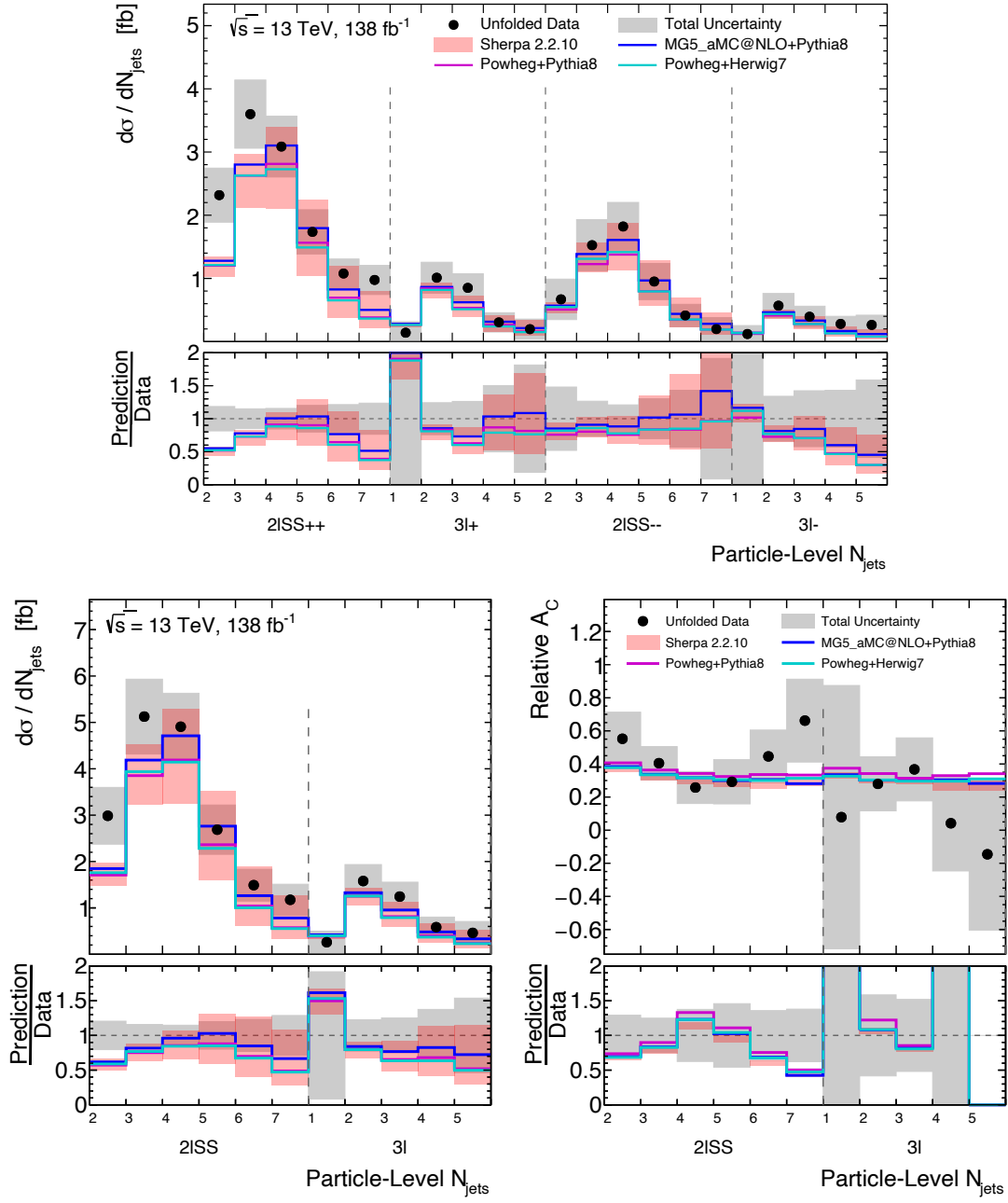


Figure 11.10: N_{jets} differential cross section measurements compared to MC predictions.

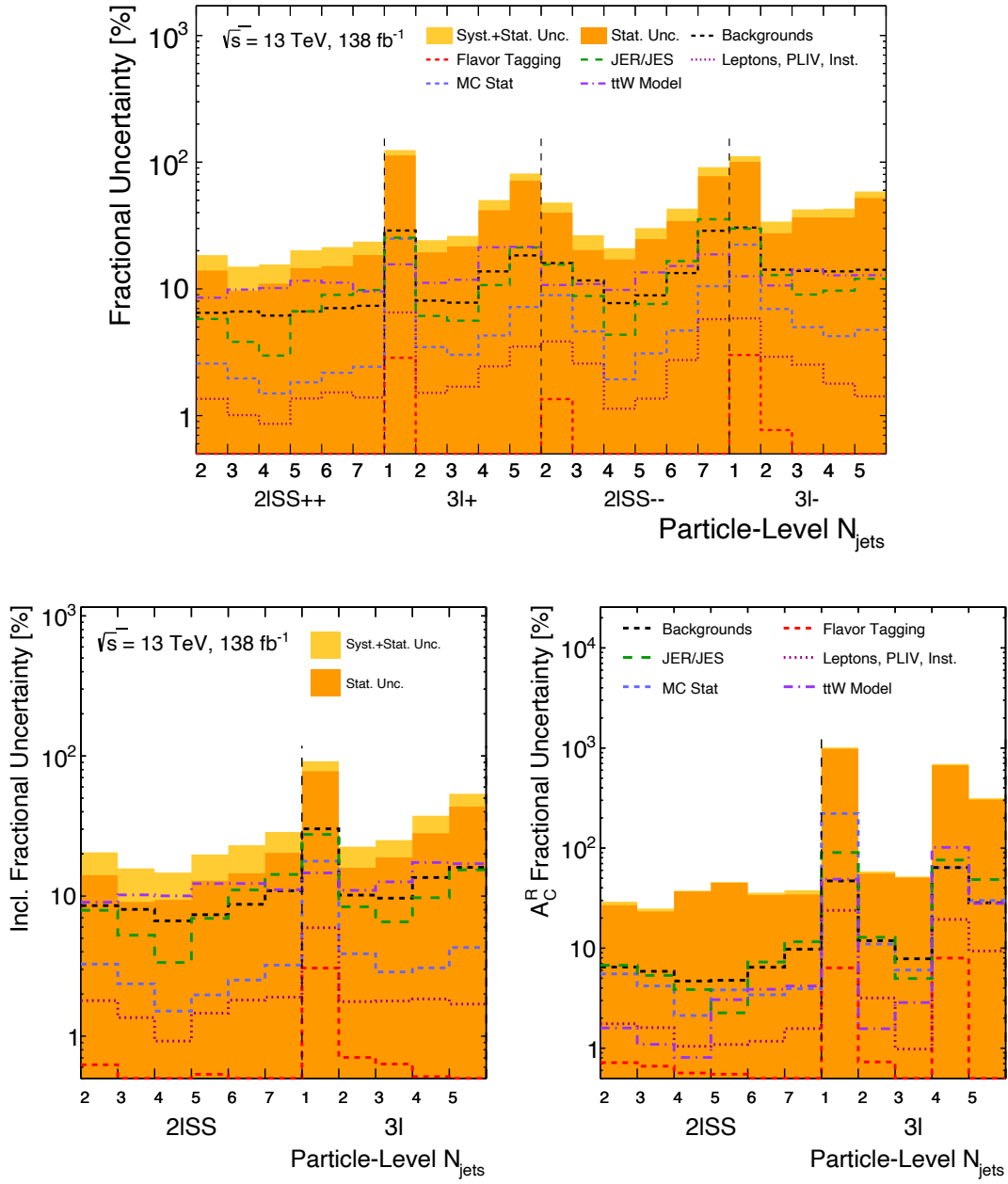


Figure 11.11: Breakdown of uncertainties for N_{jets} differential cross section measurements.

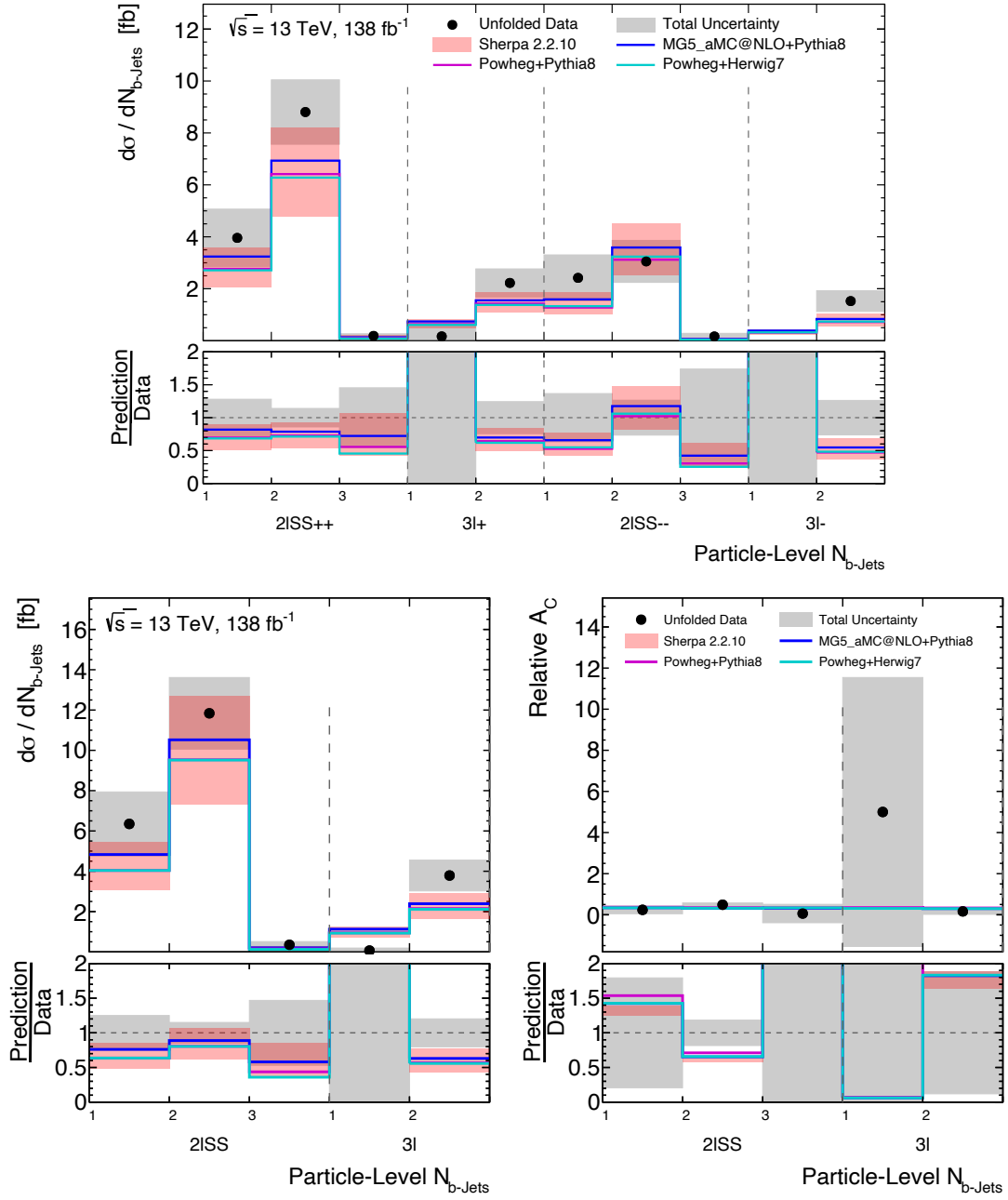


Figure 11.12: $N_{b\text{-jets}}$ differential cross section measurements compared to MC predictions.

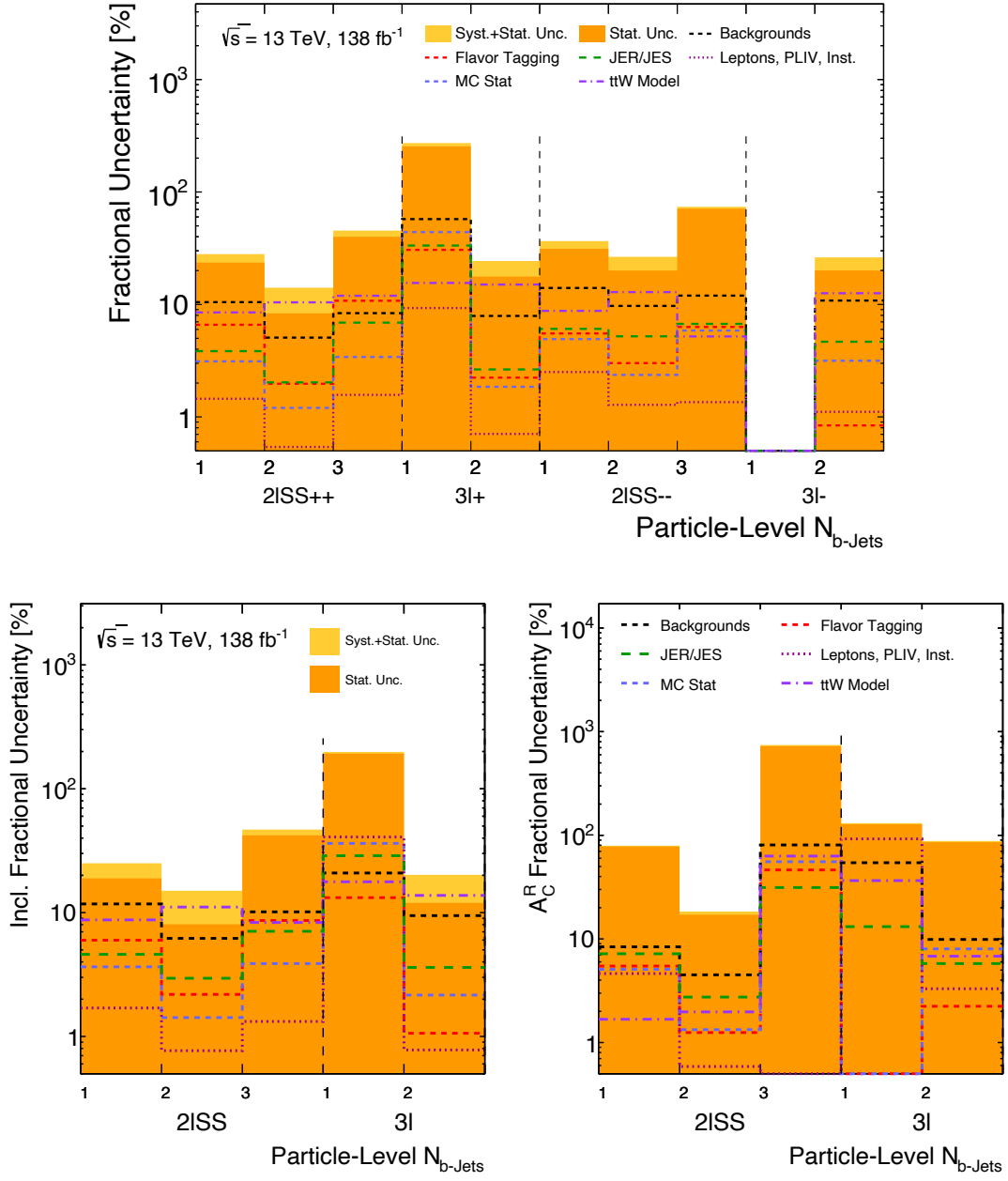


Figure 11.13: Breakdown of uncertainties for $N_{b\text{-jets}}$ differential cross section measurements.

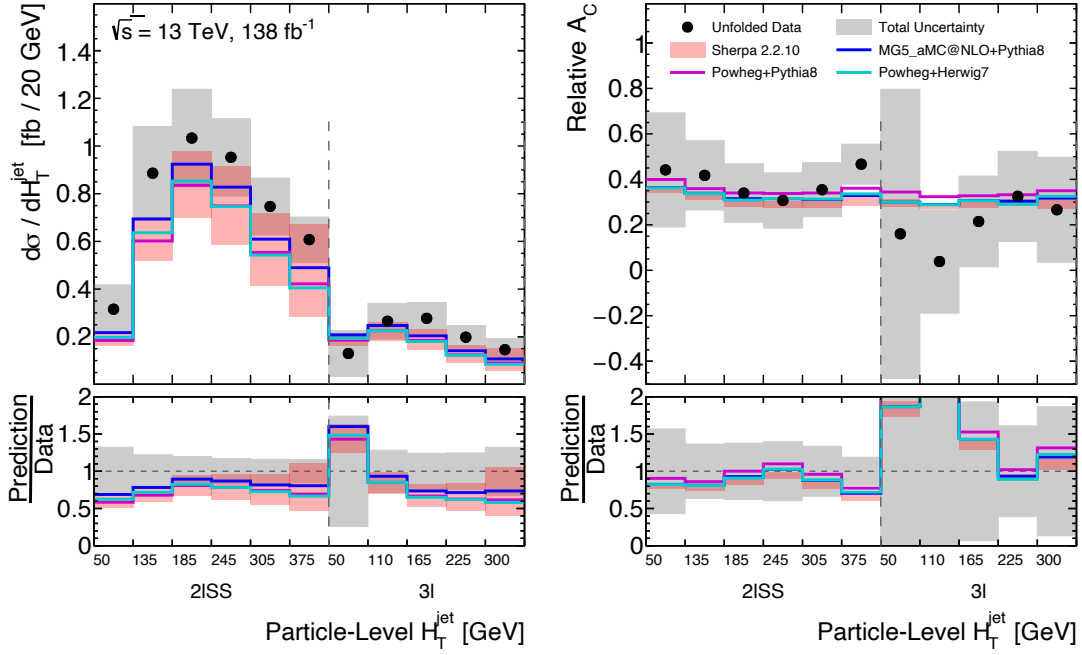
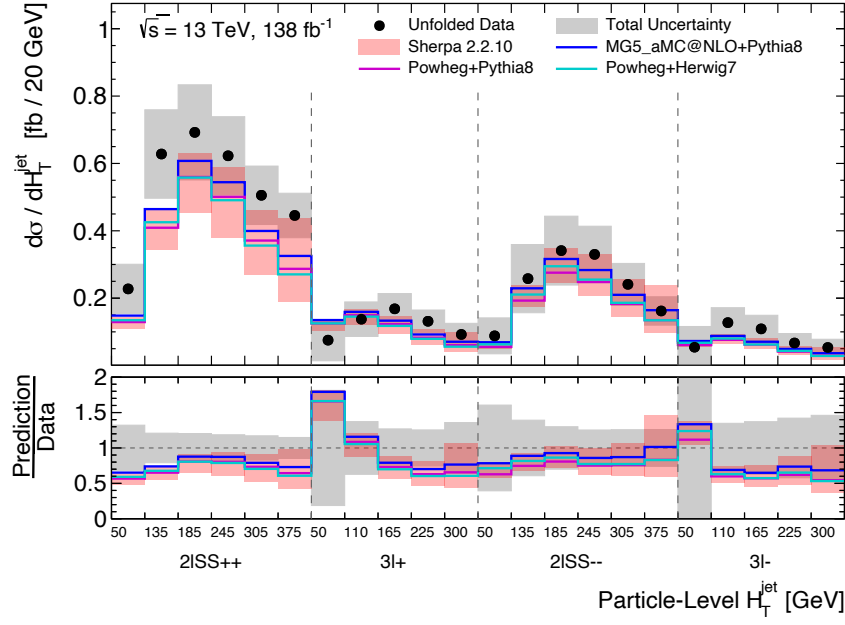


Figure 11.14: H_T^{jet} differential cross section measurements compared to MC predictions.

Figure 11.15: Breakdown of uncertainties for H_T^{jet} differential cross section measurements.

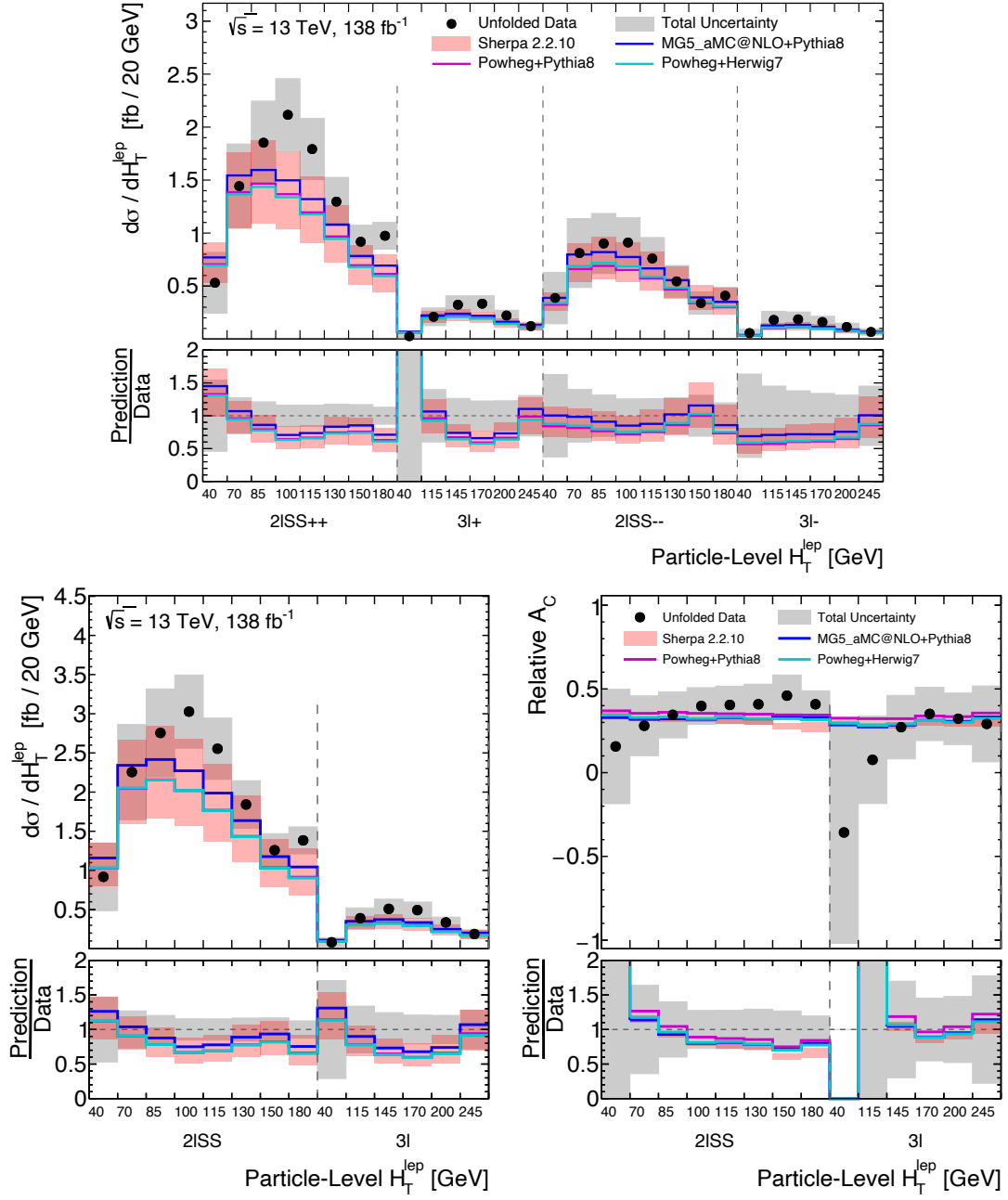


Figure 11.16: H_T^{lep} differential cross section measurements compared to MC predictions.

Figure 11.17: Breakdown of uncertainties for H_T^{lep} differential cross section measurements.

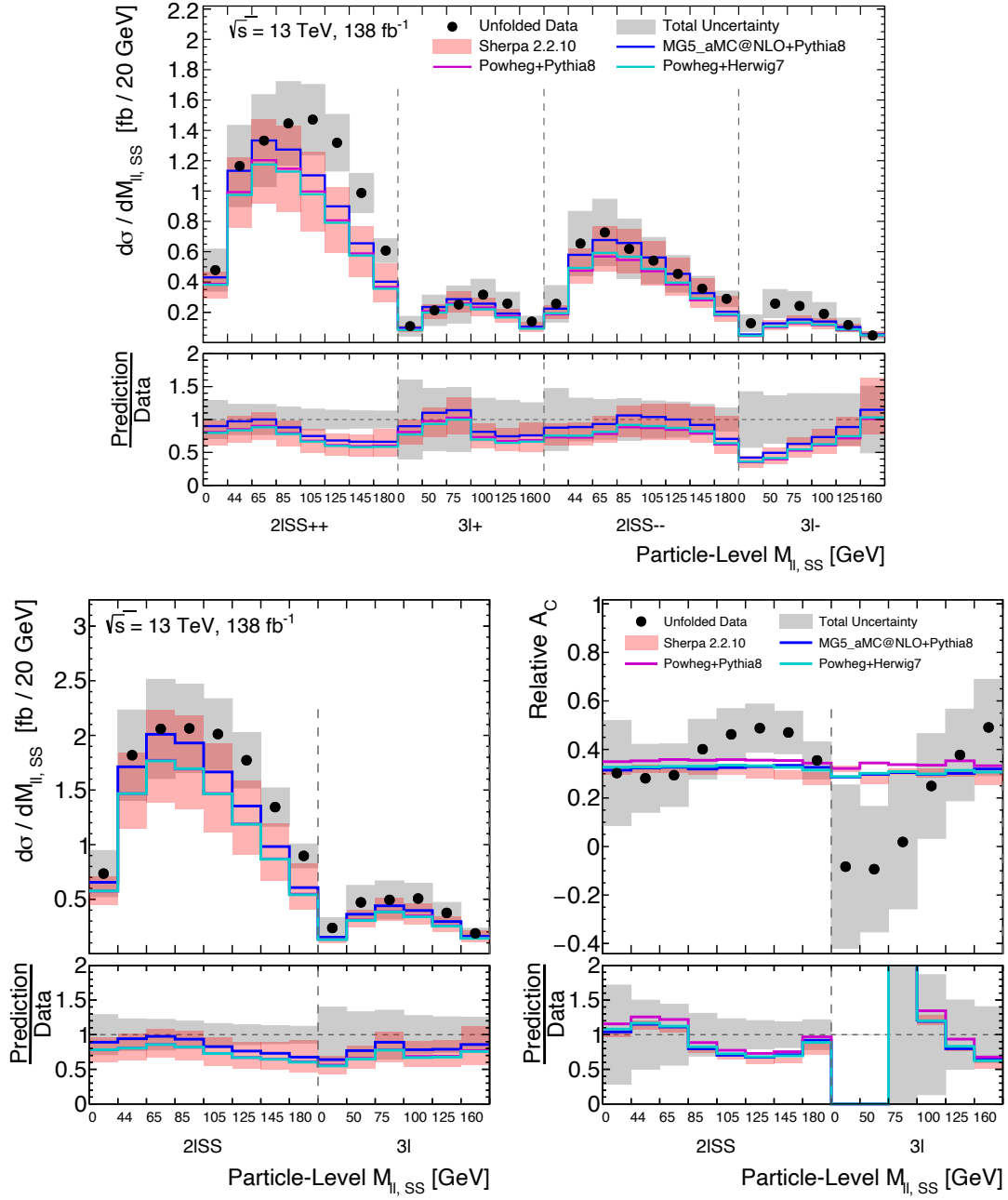


Figure 11.18: $M_{\ell\ell}^{SS}$ differential cross section measurements compared to MC predictions.

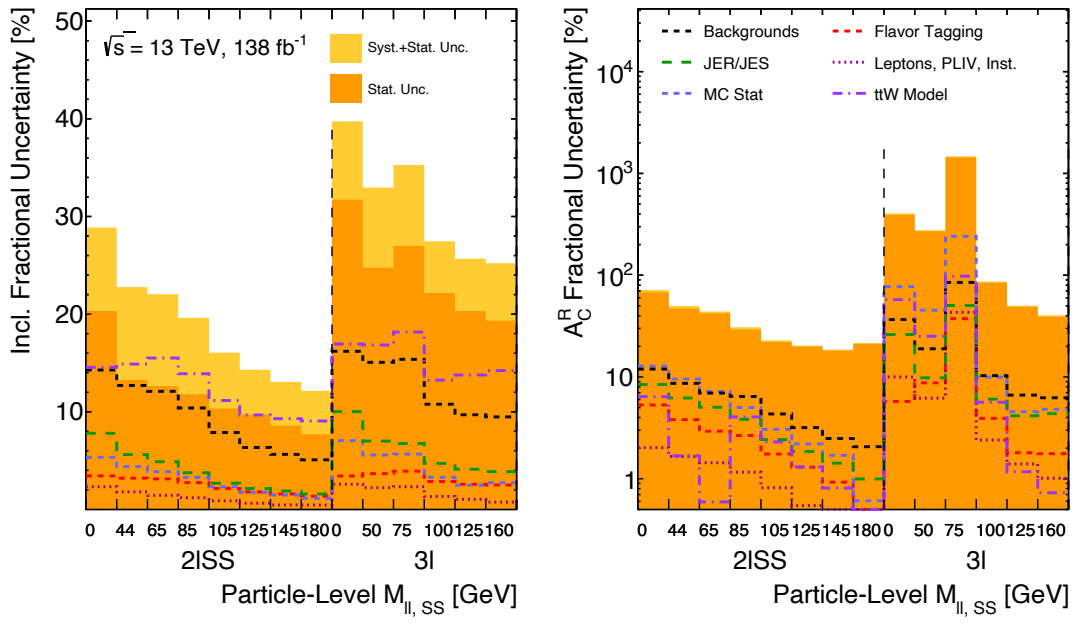


Figure 11.19: Breakdown of uncertainties for $M_{\ell\ell}^{SS}$ differential cross section measurements.

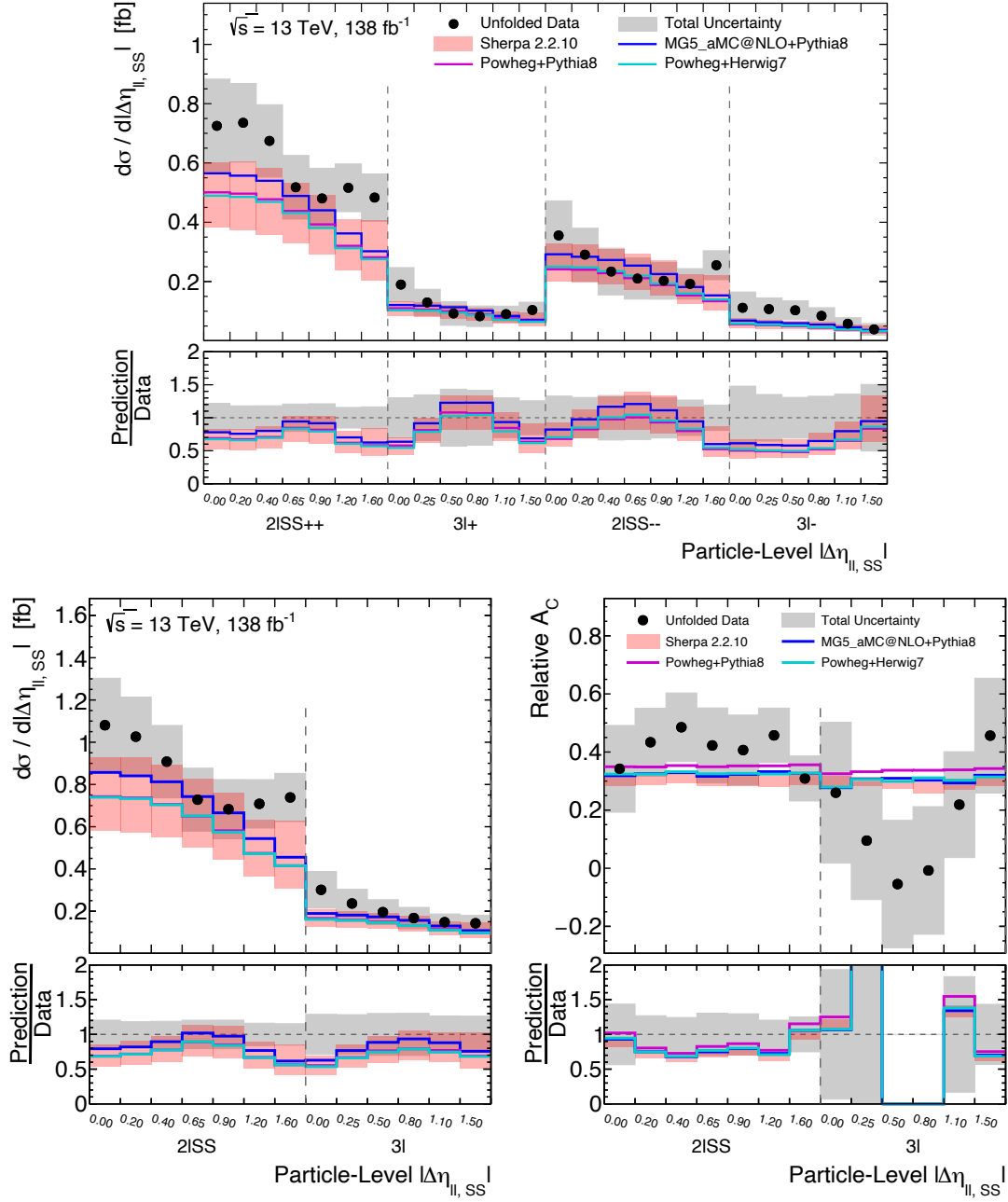


Figure 11.20: $|\Delta\eta_{\ell\ell}^{SS}|$ differential cross section measurements compared to MC predictions.

Figure 11.21: Breakdown of uncertainties for $|\Delta\eta_{\ell\ell}^{SS}|$ differential cross section measurements.

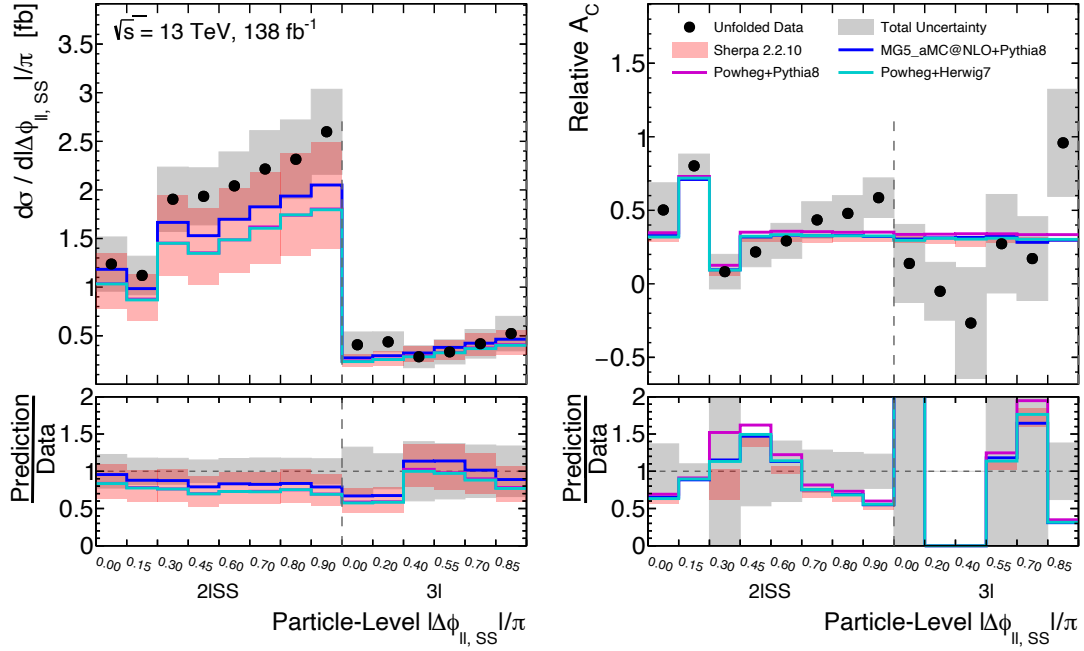
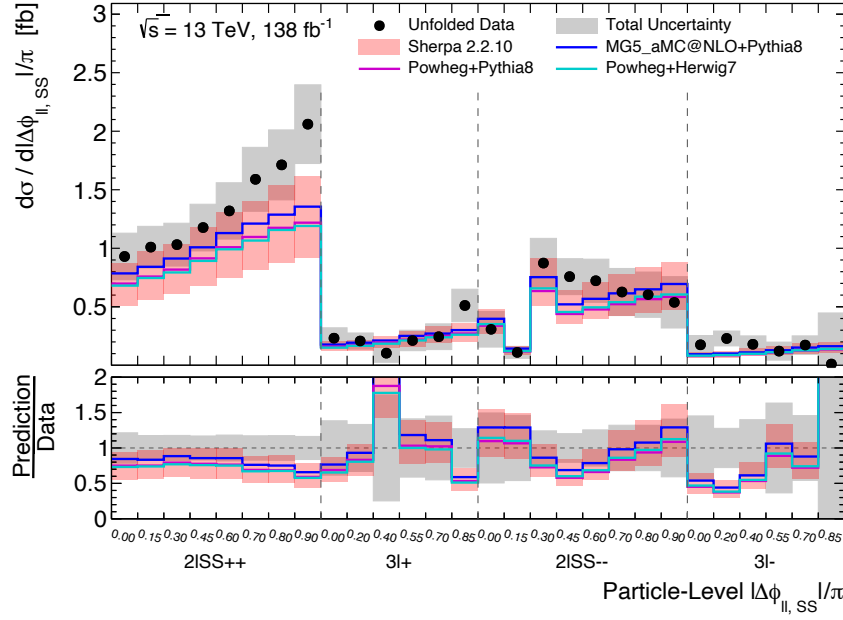


Figure 11.22: $|\Delta\phi_{\ell\ell}^{SS}|$ differential cross section measurements compared to MC predictions.

Figure 11.23: Breakdown of uncertainties for $|\Delta\phi_{\ell\ell}^{SS}|$ differential cross section measurements.

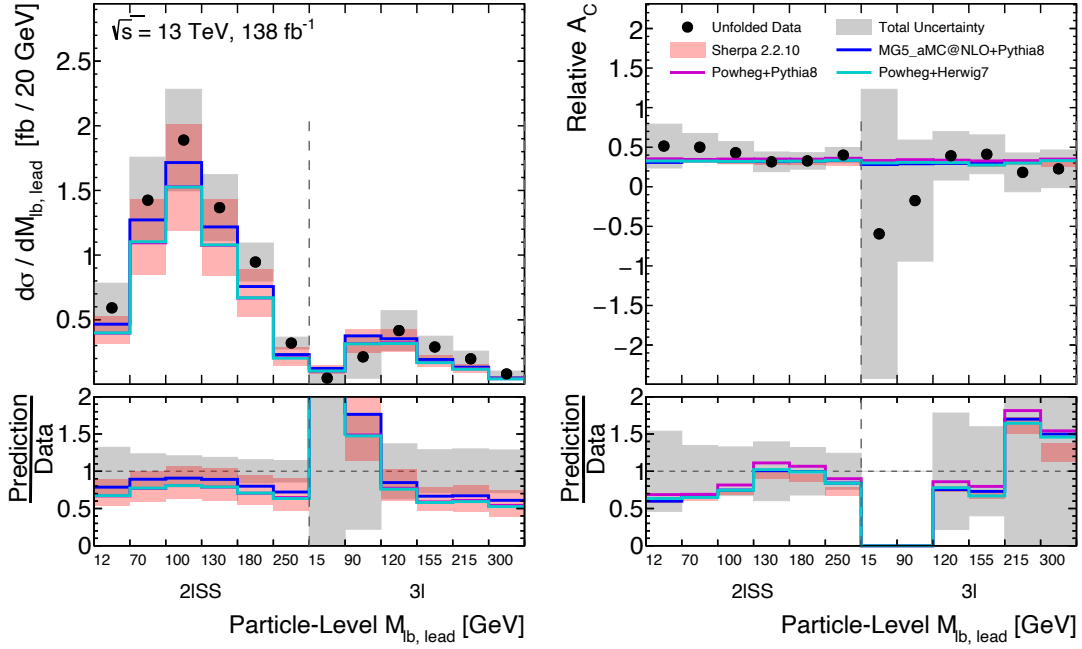
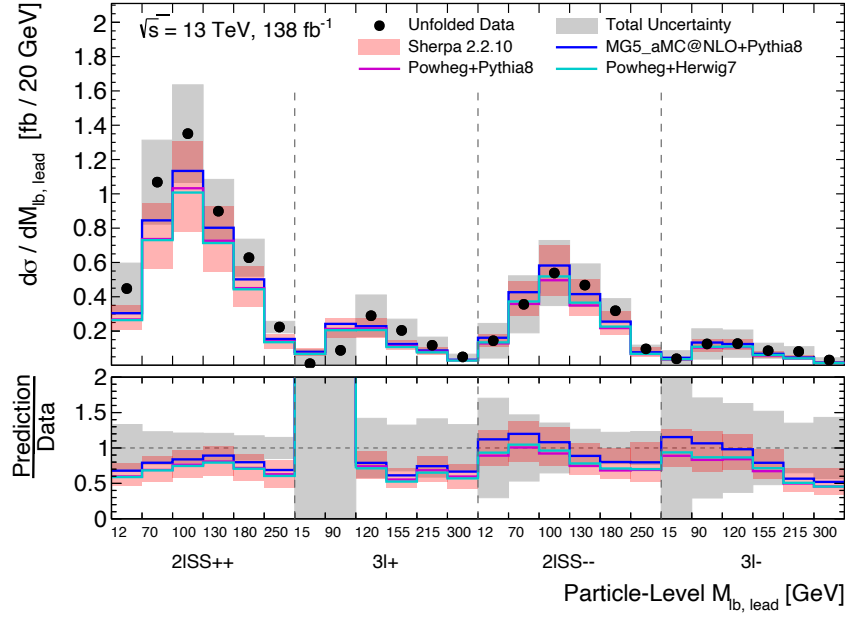


Figure 11.24: M_{lb} differential cross section measurements compared to MC predictions.

Figure 11.25: Breakdown of uncertainties for M_{lb} differential cross section measurements.

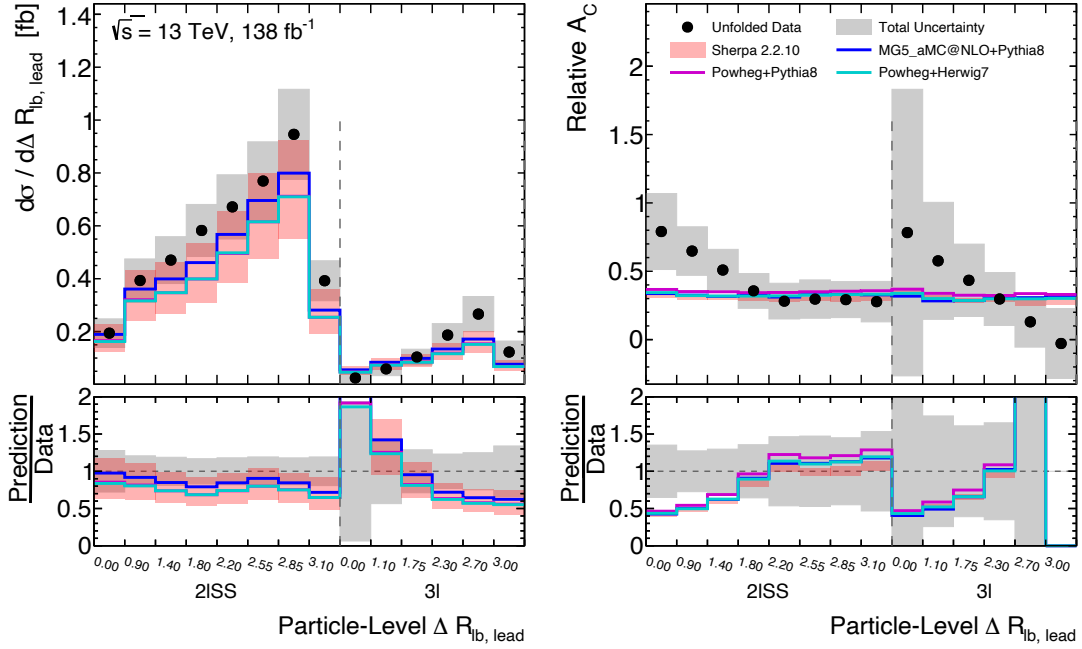
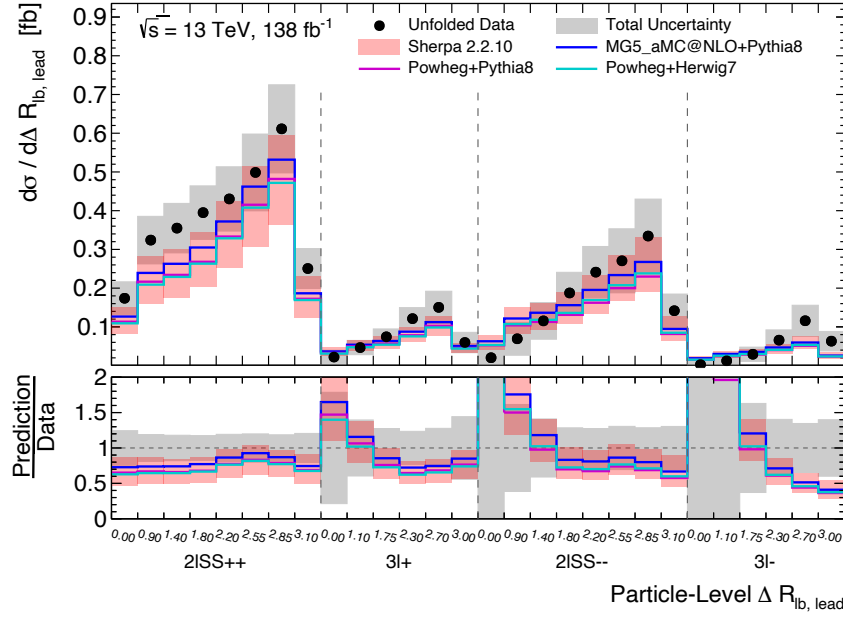


Figure 11.26: ΔR_{lb} differential cross section measurements compared to MC predictions.

Figure 11.27: Breakdown of uncertainties for ΔR_{lb} differential cross section measurements.

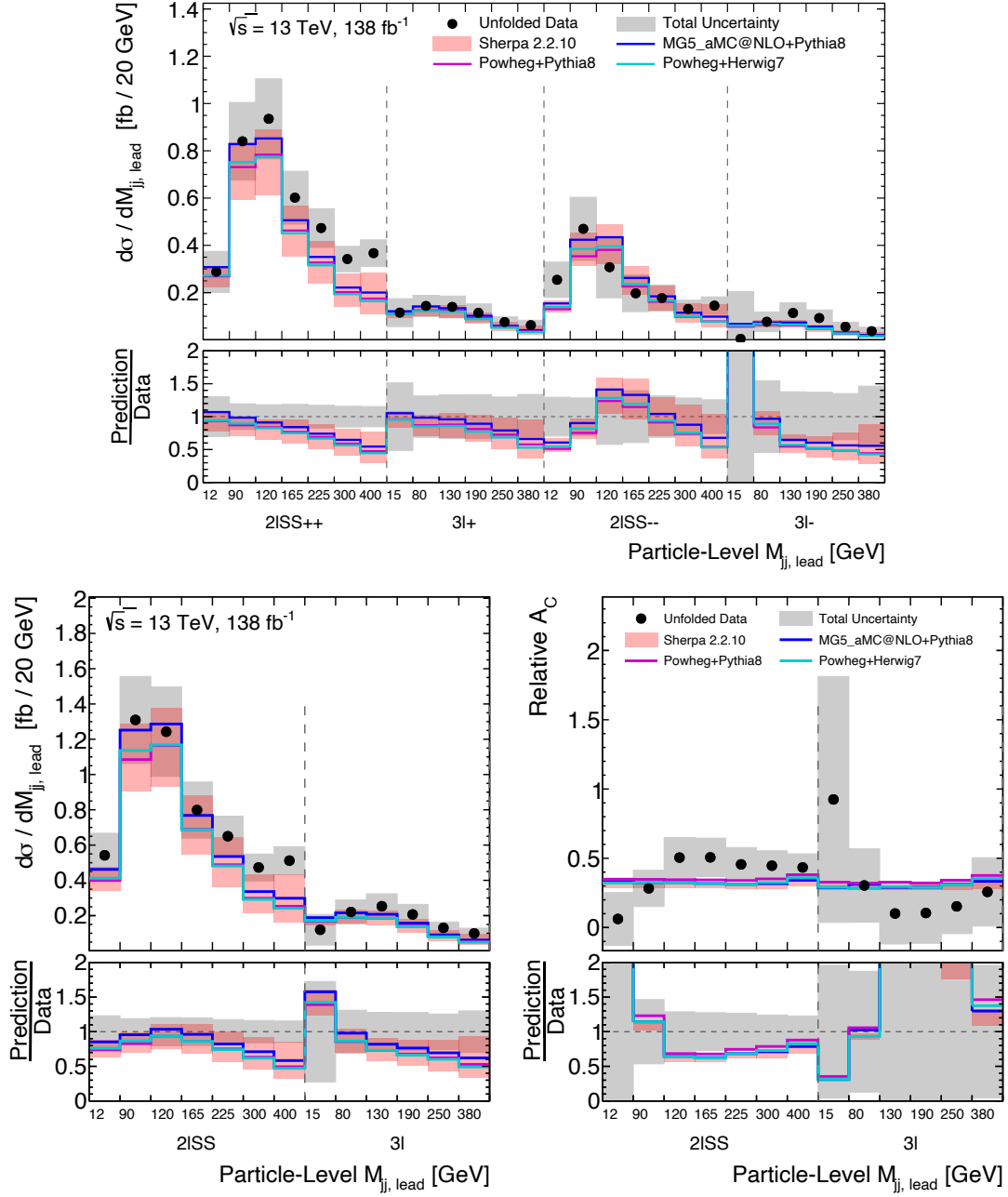


Figure 11.28: ΔM_{jj} differential cross section measurements compared to MC predictions.

Figure 11.29: Breakdown of uncertainties for M_{jj} differential cross section measurements.

Part V

Conclusions

12

Summary and Outlook

The field of particle physics underwent a sea change after the discovery of the Higgs boson at the LHC. In earlier times, there had either been an abundance of experimental signatures that could be studied (as in the case in the 1970s) or a clearly motivated particle predicted by theorists that could be sought after and, very frequently, found. This ended with the discovery of the Higgs boson. Now, the preeminent theory of particle physics, the Standard Model, has been experimentally verified to the utmost precision and is theoretically consistent and UV complete, offering little in the way of additional threads that can be pulled to unravel any of its many apparent deficiencies.

After its first long shutdown, the LHC began a second data-taking run colliding protons at nearly double the energy and 10 times the luminosity than what was used to discover the Higgs boson at the ATLAS and CMS experiments. With the trove of data collected during Run II, the physics reach of ATLAS has been greatly extended. In many cases, the increase in statistics has facilitated the measurement of rare Higgs production processes like $t\bar{t}H$, providing sensitivity to the top quark Yukawa coupling. This is one of many properties of the Higgs boson that has been probed in order to verify that the scalar boson observed 10 years ago at the LHC is indeed the Higgs boson of the Standard Model.

There have also been a handful of anomalous measurements performed at the LHC over the last decade. One that has done little more than to detract from the sensitivity to the more high-profile searches for $t\bar{t}H$ and $t\bar{t}t\bar{t}$ production in multi-lepton channels is the production of $t\bar{t}$ in association with a W boson. At face value it is an uninteresting process. With no sensitivity to the $t - W$ coupling, $t\bar{t}W$ offers no handle on EW dynamics with the heaviest fermion. It was only when the production rate of $t\bar{t}W$ was consistently shown to be larger than expected by the most precise theoretical calculations did the theory community take a greater interest in this process. They quickly determined that this process can indeed offer some sensitivity to the UV behavior of EW couplings due to subtle effects that initially had been overlooked. Advanced techniques in MC simulation were extended the modeling of $t\bar{t}W$ in an effort to ease the tension between data and prediction. To date, these efforts have eased this tension but have not offered a complete explanation for the higher than expected rate of $t\bar{t}W$ production.

The vast cache of data collected by ATLAS during Run II allows the $t\bar{t}W$ process to be measured with the utmost precision. For the first time, $t\bar{t}W$ production is measured differentially across

a comprehensive set of observables. This has been achieved by extending the commonly used statistical formalism of the profile likelihood to the task of unfolding data to the particle-level. The profile likelihood unfolding method, along with machine learning tools capable of identifying challenging backgrounds, have been used to build a statistical model capable of extracting differential distributions for $t\bar{t}W$ production while controlling background rates. The result is a collection of measurements that comprehensively characterize $t\bar{t}W$ production to an unprecedented precision. These results will be used to correct the modeling of $t\bar{t}W$ production as backgrounds for measurements of $t\bar{t}H$ and $t\bar{t}t\bar{t}$ production in the multi-lepton final states, extending the sensitivity of these measurements to the top Yukawa coupling and contact interactions in the SMEFT framework.

As these results are digested by the theory community and checked against a differential measurement that CMS may perform, one of two scenarios will unfold. One possibility is that theorists will crack the code and achieve a more precise $t\bar{t}W$ calculation, possibly through a NNLO QCD calculation, and provide predictions on $t\bar{t}W$ differential production that agree well with data. A more interesting possibility is that new precision methods will be developed that do not conform to the best experimental measurements or predict new features of $t\bar{t}W$ production that can be further studied at the LHC. In any case, the interest in the $t\bar{t}W$ process is unlikely to subside until its mysteries have been resolved.

The LHC is actively preparing for Run III with beam circulation tests at 450 GeV threshold energy and will soon have first collisions at a record center of mass energy of 13.6 TeV. Run III is slated to provide 200 fb⁻¹ of data which, in combination with Run II data, will greatly enhance the sensitivity of ATLAS to rare processes involving the top quark in association with gauge and scalar bosons, which have greatly overlapping phase spaces. The profile likelihood unfolding method will

likely see increased use in this suite of measurement efforts as it can be readily extended to unfold multiple overlapping signal processes. At the same time, MC modeling techniques including those leveraging machine learning are being deployed to enhance the quality of detector simulation. This will allow analyses to adopt more MC-driven background estimation techniques for challenging backgrounds like fake lepton production. The net result is the following. Differential cross section measurements of processes that have small and simple backgrounds will continue using IBU and migrate to methods like OMNIFOLD, which promises unbinned differential cross sections measured simultaneously in the full phase space using machine learning. For those measurements that are less cleanly isolated, either through contamination by challenging backgrounds or through overlap with other processes that can offer boosted sensitivity if measured together, profile likelihood unfolding will be the preferred technique.

We are now in the precision age of particle physics. Facing a confoundingly consistent theory, the HEP community has developed sophisticated new techniques to analyze the most complex datasets ever collected to find even the most subtle of hints of where the SM will yield to the supremacy of Nature. As the LHC begins delivering physics data in Run III and continues upgrade efforts toward the High Luminosity LHC, physicists will continue to develop and deploy these and other new techniques. Perhaps in the next decade we see a new picture of particle physics emerge. Perhaps the dam will break and a new age will be ushered in, an age in which the nature of the universe will be revealed to be even more strange and beautiful than we can currently imagine.

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