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TESI DOCTORAL

## Development of a likelihood-based top quark mass measurement using semileptonically decaying $t\bar{t}$ +jet events with the full Run 2 ATLAS dataset

Alberto Prades Ibáñez

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Sota la supervisió de  
Marcel Vos i Andrej Saibel

València, Desembre 2023





Dr. Marcel Vos, Investigador Científic del Consell Superior d'Investigacions Científiques.

Dr. Andrej Saibel, Investigador Postdoctoral del Consell Superior d'Investigacions Científiques.

Dr. Santiago González de la Hoz, Catedràtic d'Universitat del Departament de Física Atòmica, Molecular i Nuclear de la Universitat de València.

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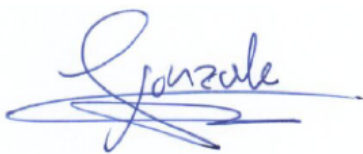
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Dr. Marcel Vos



Dr. Andrej Saibel



Dr. Santiago Gonzalez de la Hoz





# Dedication

In memory of Esteban Fullana Torregosa, whose passion for physics and dedication to his beloved family continue to inspire those who knew him. Esteban's support and contributions to the work presented in this thesis were one among his last contributions to particle physics. He will be deeply missed by all the people who were fortunate enough to have known him as a coworker and a friend.



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# Abstract

The top quark is the most massive elementary particle in the SM, which makes it play an important role in this theory and many of its extensions. This thesis presents the development status of a measurement of the top quark mass in the on-shell renormalization scheme, the top quark pole mass ( $m_t^{\text{pole}}$ ), using semileptonically decaying top quark pair events produced in association with at least one energetic jet ( $t\bar{t}+\text{jet}$ ). Additionally, the top quark mass parameter in the Monte Carlo simulation ( $m_t^{\text{MC}}$ ), is determined using semileptonically decaying top quark pair events produced in the lepton+4 jets channel, without additional jets ( $t\bar{t}$ ). The measurement is performed using the proton-proton collision data at 13 TeV collected by the ATLAS experiment at the LHC during Run 2 (2015-2018), corresponding to an integrated luminosity of  $140 \text{ fb}^{-1}$ .

Candidate  $t\bar{t}/t\bar{t}+\text{jet}$  events are required to contain one electron or muon, a significant amount of missing transverse momentum, and four or more jets, from which at least one is identified as a jet originating from the hadronization of a  $b$ -quark. To reconstruct the observables used in this analysis,  $\rho_s = 340 \text{ GeV}/\sqrt{s_{t\bar{t}+\text{jet}}}$  with  $\sqrt{s_{t\bar{t}+\text{jet}}} = m_{t\bar{t}+\text{jet}}$  and  $M_{lb}$ , a machine learning model implemented within the SPA-NET framework is used. The value of  $m_t^{\text{MC}}$ , and the corrected distribution of the parton level normalized cross section with respect to  $\rho_s$  are determined with a statistical model based on a profile likelihood fit. For the top quark pole mass, the methodology outlined in this thesis achieves an expected precision level of  $\Delta m_t^{\text{pole}}(\text{total}) \simeq {}^{+0.88}_{-0.78} \text{ GeV}$ , while the top quark Monte Carlo mass parameter in the simulation is expected to be determined with a precision of  $\Delta m_t^{\text{MC}}(\text{total}) \simeq 0.41 \text{ GeV}$ . At this precision, the top quark mass values extracted using this methodology would be positioned among the most precise determinations of these quantities to date.



# Contents

|          |                                                                                                     |           |
|----------|-----------------------------------------------------------------------------------------------------|-----------|
| <b>1</b> | <b>The Standard Model of particle physics</b>                                                       | <b>1</b>  |
| 1.1      | Elementary particles and their interactions . . . . .                                               | 2         |
| 1.1.1    | Fermions: Matter constituents . . . . .                                                             | 3         |
| 1.1.2    | Gauge bosons: Force mediators . . . . .                                                             | 6         |
| 1.1.3    | The Higgs boson . . . . .                                                                           | 7         |
| 1.2      | Quantum Electrodynamics . . . . .                                                                   | 8         |
| 1.2.1    | Derivation of the QED Lagrangian . . . . .                                                          | 8         |
| 1.2.2    | Perturbation theory for QED and Feynman diagrams . . .                                              | 11        |
| 1.3      | Electroweak Theory . . . . .                                                                        | 13        |
| 1.3.1    | Electroweak Unification . . . . .                                                                   | 13        |
| 1.3.2    | Electroweak Symmetry Breaking . . . . .                                                             | 16        |
| 1.3.3    | Masses of fermions . . . . .                                                                        | 19        |
| 1.4      | Quantum Chromodynamics . . . . .                                                                    | 21        |
| 1.4.1    | Mathematical description and motivation . . . . .                                                   | 21        |
| 1.4.2    | Ultraviolet divergencies, renormalization, and the running<br>of the couplings and masses . . . . . | 23        |
| 1.5      | Limitations of the Standard Model . . . . .                                                         | 26        |
| <b>2</b> | <b>The top quark and its mass</b>                                                                   | <b>29</b> |
| 2.1      | The physics of the top quark . . . . .                                                              | 30        |
| 2.1.1    | Top quark properties . . . . .                                                                      | 30        |
| 2.1.2    | Top quark production and decay . . . . .                                                            | 35        |

|          |                                                                                                                 |           |
|----------|-----------------------------------------------------------------------------------------------------------------|-----------|
| 2.2      | Testing the Standard Model consistency using the top quark mass                                                 | 40        |
| 2.3      | Top quark mass measurements . . . . .                                                                           | 45        |
| 2.3.1    | Direct measurements . . . . .                                                                                   | 45        |
| 2.3.2    | Indirect measurements: top quark mass determination from<br>inclusive and differential cross sections . . . . . | 47        |
| 2.3.3    | Top quark pole mass measurements from $t\bar{t}$ +jet topologies                                                | 50        |
| <b>3</b> | <b>The LHC and the ATLAS experiment</b>                                                                         | <b>57</b> |
| 3.1      | The LHC acceleration complex . . . . .                                                                          | 57        |
| 3.2      | The ATLAS experiment . . . . .                                                                                  | 60        |
| 3.2.1    | Coordinate system . . . . .                                                                                     | 62        |
| 3.2.2    | Tracking system . . . . .                                                                                       | 63        |
| 3.2.3    | Calorimeter system . . . . .                                                                                    | 65        |
| 3.2.4    | Muon spectrometers . . . . .                                                                                    | 67        |
| 3.2.5    | Magnet system . . . . .                                                                                         | 69        |
| 3.2.6    | Luminosity measurement and forward detectors . . . . .                                                          | 70        |
| 3.2.7    | Trigger system and data storage . . . . .                                                                       | 72        |
| 3.2.8    | Data quality . . . . .                                                                                          | 73        |
| <b>4</b> | <b>Objects definition and event reconstruction in ATLAS</b>                                                     | <b>77</b> |
| 4.1      | Tracks and vertices . . . . .                                                                                   | 79        |
| 4.2      | Electrons . . . . .                                                                                             | 81        |
| 4.3      | Muons . . . . .                                                                                                 | 82        |
| 4.4      | Jets . . . . .                                                                                                  | 84        |
| 4.5      | Identification of $b$ -jets . . . . .                                                                           | 87        |
| 4.6      | Missing transverse energy . . . . .                                                                             | 88        |
| 4.7      | Object overlap removal . . . . .                                                                                | 89        |
| 4.8      | Large- $R$ jet definition, calibration, and uncertainties in ATLAS . .                                          | 90        |
| 4.8.1    | Calibration sequence for large- $R$ jets . . . . .                                                              | 92        |



|          |                                                                                                                             |            |
|----------|-----------------------------------------------------------------------------------------------------------------------------|------------|
| 4.8.2    | The forward folding method . . . . .                                                                                        | 96         |
| 4.8.3    | Measurement of the JMS and JMR for large- $R$ jets using<br>the $Z/W$ mass peak . . . . .                                   | 97         |
| 4.8.4    | Implementation of the large- $R$ jets JMR uncertainties in the<br>ATLAS software framework . . . . .                        | 100        |
| <b>5</b> | <b>Top quark mass measurement in semileptonic <math>t\bar{t}</math>+jet events:<br/>Analysis overview</b>                   | <b>103</b> |
| <b>6</b> | <b>Data and simulated samples</b>                                                                                           | <b>107</b> |
| 6.1      | Data samples . . . . .                                                                                                      | 108        |
| 6.2      | Simulated samples . . . . .                                                                                                 | 108        |
| 6.2.1    | Nominal simulated samples . . . . .                                                                                         | 110        |
| 6.2.2    | Alternative simulated samples . . . . .                                                                                     | 112        |
| 6.3      | Fake and non-prompt leptons background . . . . .                                                                            | 114        |
| <b>7</b> | <b>Event selection and reconstruction using SPA-Net</b>                                                                     | <b>117</b> |
| 7.1      | Data quality requirements and object definitions. . . . .                                                                   | 118        |
| 7.1.1    | Data quality requirements . . . . .                                                                                         | 118        |
| 7.1.2    | Object selection . . . . .                                                                                                  | 119        |
| 7.2      | Event preselection . . . . .                                                                                                | 121        |
| 7.3      | Reconstruction of the $t\bar{t}$ and $t\bar{t}$ +jet systems using SPA-NET . . .                                            | 126        |
| 7.3.1    | Introduction to SPA-NET . . . . .                                                                                           | 126        |
| 7.3.2    | Implementation of SPA-NET in $t\bar{t}$ +jet event topologies<br>and the $M_{lb}$ observable . . . . .                      | 128        |
| 7.4      | Performance of the SPA-NET model and final event selection . . .                                                            | 135        |
| 7.5      | Summary of the event selection used in the analysis . . . . .                                                               | 149        |
| <b>8</b> | <b>Extraction of the top quark MC mass and the <math>t\bar{t}</math>+jet differential<br/>cross section at parton level</b> | <b>151</b> |
| 8.1      | Introduction to the profile maximum likelihood techniques . . . . .                                                         | 152        |

|           |                                                                                                                                                              |            |
|-----------|--------------------------------------------------------------------------------------------------------------------------------------------------------------|------------|
| 8.2       | Uncertainties in the profile likelihood fit . . . . .                                                                                                        | 158        |
| 8.2.1     | Statistical uncertainties . . . . .                                                                                                                          | 158        |
| 8.2.2     | Systematic uncertainties . . . . .                                                                                                                           | 158        |
| 8.3       | Definition of the statistical model . . . . .                                                                                                                | 173        |
| 8.4       | Fit validation and expected precision using the Asimov dataset . .                                                                                           | 179        |
| <b>9</b>  | <b>Extraction of the top quark pole mass</b>                                                                                                                 | <b>193</b> |
| 9.1       | Top quark pole mass extracted from the nominal Asimov dataset<br>and its associated fit uncertainty . . . . .                                                | 194        |
| 9.2       | Theory uncertainties . . . . .                                                                                                                               | 198        |
| 9.3       | Measurement of the top quark pole mass: Expected precision . . .                                                                                             | 203        |
| <b>10</b> | <b>Summary and conclusions</b>                                                                                                                               | <b>205</b> |
| <b>A</b>  | <b>Custom boosted <math>W/Z</math> jet tagger for the large-<math>R</math> jet in-situ<br/>analysis</b>                                                      | <b>211</b> |
| <b>B</b>  | <b>Breakdown of the JMS and JMR uncertainties of the large-<math>R</math> jet<br/>in-situ analysis</b>                                                       | <b>215</b> |
| <b>C</b>  | <b>Alternative <math>t\bar{t}</math>+jet event reconstruction</b>                                                                                            | <b>217</b> |
| C.1       | $t\bar{t}$ +jet system reconstruction from the 7 and 8 TeV analyses . . . .                                                                                  | 217        |
| C.2       | $t\bar{t}$ +jet system reconstruction using the KLFITTER algorithm . . .                                                                                     | 220        |
| C.3       | Optimization of the $\ln L$ cut in the KLFITTER reconstruction . .                                                                                           | 222        |
| <b>D</b>  | <b>Complementary information and studies about the SPA-Net<br/>model used to reconstruct the <math>t\bar{t}</math> and <math>t\bar{t}</math>+jet systems</b> | <b>227</b> |
| D.1       | Architecture of the transformer encoder . . . . .                                                                                                            | 228        |
| D.2       | Hyper-parameters of the SPA-NET model . . . . .                                                                                                              | 229        |
| D.3       | Overtraining study for the SPA-NET model . . . . .                                                                                                           | 229        |
| D.4       | SPA-NET model matching efficiencies, $\rho_s$ resolution, and $M_{tb}$<br>resolution for all the signal and control regions in the analysis . . .            | 232        |

|          |                                                                                                                            |            |
|----------|----------------------------------------------------------------------------------------------------------------------------|------------|
| D.5      | Additional SPA-NET performance plots and distributions . . . . .                                                           | 235        |
| <b>E</b> | <b>Event yields and control plots after the final event selection</b>                                                      | <b>239</b> |
| <b>F</b> | <b>Complementary information about the profile likelihood fit</b>                                                          | <b>241</b> |
| F.1      | Efficiency factor, acceptance factor, and migration matrix for the<br>SRLjets5j1b region . . . . .                         | 241        |
| F.2      | Ranking plot for the $\gamma$ NPs in the profile maximum likelihood fit .                                                  | 243        |
| F.3      | Correlation matrix for the POI and NP in the profile maximum<br>likelihood fit . . . . .                                   | 245        |
| <b>G</b> | <b>Complementary studies about the top quark pole mass fit</b>                                                             | <b>247</b> |
| G.1      | Uncertainty arising from the parametrization of $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$ . | 247        |
| G.2      | Fit validation: Top quark MC mass extraction at parton level . . .                                                         | 249        |
| G.3      | Extraction of the top quark pole mass using various theory<br>predictions computed with different PDF sets . . . . .       | 254        |
| G.4      | Extraction of the top quark pole mass using alternative binnings<br>for the $\mathcal{R}$ observable . . . . .             | 258        |
|          | <b>Resum</b>                                                                                                               | <b>263</b> |
|          | <b>Acronyms</b>                                                                                                            | <b>281</b> |
|          | <b>List of Publications</b>                                                                                                | <b>285</b> |
|          | <b>Bibliography</b>                                                                                                        | <b>287</b> |



# Chapter 1

## The Standard Model of particle physics

The main goal of this thesis is the measurement of the top quark mass using events where a top-antitop quark pair is produced in association with an additional jet and then decays into a final state containing a lepton and at least five jets. To reach this goal, it is important to set the basics of the theoretical framework in which this analysis is performed, the Standard Model of particle physics.

The Standard Model of particle physics (SM) is the theory that describes the current knowledge about the elementary particles and their interactions. It is based on Quantum Field Theory (QFT), a mathematical framework that combines quantum mechanics and special relativity. In QFT, particles are described as excited states of quantum fields, and their interactions, as exchange of force carriers called *bosons*. The SM includes the strong, electromagnetic and weak interactions, three out of the four fundamental forces of nature. These forces are described under the symmetry group  $SU(3)_C \times SU(2)_L \times U(1)_Y$ , where the  $SU(3)_C$  component describes the strong interactions and the  $SU(2)_L \times U(1)_Y$  components described the unified electroweak interactions. The fourth force, gravity, is not included within the SM since a quantized gravitational field theory has not been successfully formulated yet.

An overview of the particle constituents of the SM and their interactions is given in Section 1.1. After that, the different components of the theories which make up the SM are described, starting with Quantum Electrodynamics (Section 1.2) and the electroweak theory (Section 1.3). The theory that describes

the strong interactions, Quantum Chromodynamics, is introduced in Section 1.4. At last, Section 1.5 describes some of the limitations of the SM by discussing some of the known properties of nature that cannot be explained by this model.

When working with relativistic and quantum mechanical systems, as in the case of elementary particle physics, it is useful to use natural units. In these units, the speed of light and the Planck constant are redefined to become:  $c = \hbar = 1$ . As a consequence, the mass and momentum are measured in electronvolts, the unit of energy,  $[E] = 1 \text{ eV}$ . The system of natural units is used throughout this thesis.

## 1.1 Elementary particles and their interactions

In the SM, particles are defined as local excitations of the quantum fields that are permeating space. Within the energy regime explored so far, the fundamental constituents of matter are elementary particles, which are defined as point-like objects that cannot be decomposed into other particles.

Particles are characterized by their spin, mass, and charge quantum numbers. According to their intrinsic angular momentum (spin), particles can be classified into *fermions*, particles with half-integer spin ( $s = 1/2, 3/2, \dots$ ), and *bosons*, particles with an integer spin ( $s = 0, 1, \dots$ ). Fermions, as particles with half-integer spin, have an anti-symmetric wave function hence they obey Fermi-Dirac statistics and follow the Pauli exclusion principle. The Pauli principle states that two identical fermions cannot occupy the same quantum state. Bosons, as particles with integer spin, have a symmetric wave function, hence they obey Bose-Einstein statistics and several bosons can share the same quantum state. In the SM, there are only elementary fermions and bosons with spin- $\frac{1}{2}$  and spin-0, 1, respectively. The charge quantum numbers of a particle determine in which interactions they partake.

A schematic view of the elementary particles of the SM is shown in Figure 1.1. In the following, a brief description of these particles is provided. This description is loosely based on the explanations in Reference [1].

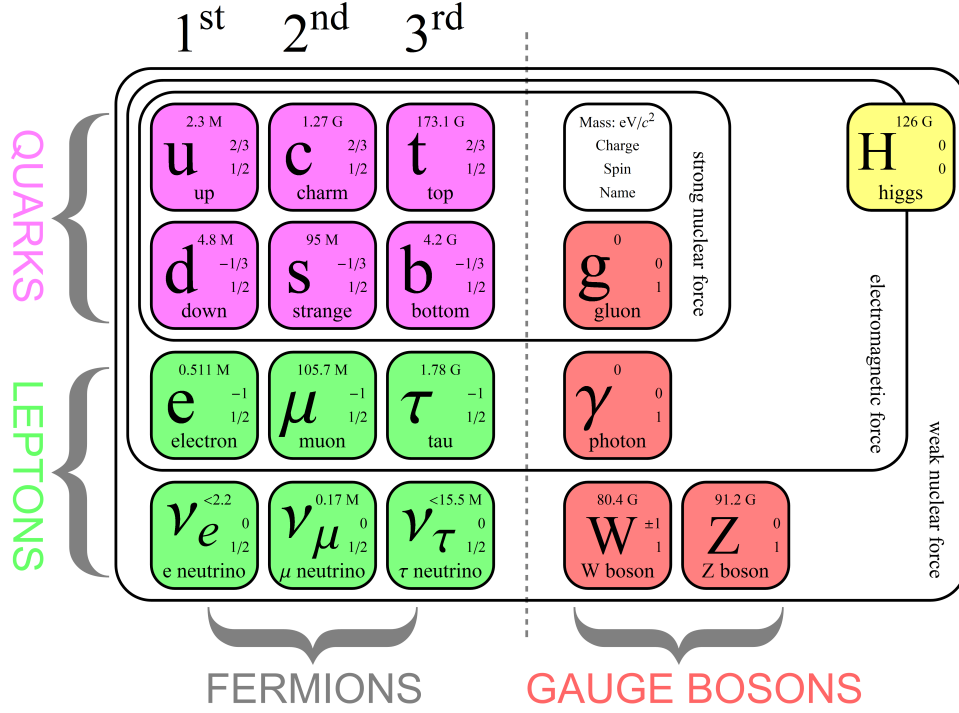


Figure 1.1: The elementary particles of the SM. The three first columns show the three generations of fermions (quarks and leptons), which are the constituents of the matter in the universe. The fourth and fifth columns show the gauge bosons, which act as the mediators of the electromagnetic, weak and strong forces. The sixth column includes the Higgs boson, which generates the masses of the particles. For each particle, its mass, electrical charge and spin are given [2].

### 1.1.1 Fermions: Matter constituents

According to the SM, the elementary particles of spin- $\frac{1}{2}$  called fermions are the building blocks of matter. This is because, as fermions obey the Pauli exclusion principle, they are allowed to form complex structures such as nuclei and atoms. Fermions are classified into two basic groups based on the interactions that they partake in: *leptons* and *quarks*.

The group of particles formed by the leptons contains the fermions that interact via the electroweak interaction, but not via the strong interaction. This group is composed of three electrically charged particles, the electron ( $e$ ), the muon ( $\mu$ ), the tau ( $\tau$ ), and their corresponding electrically neutral neutrinos, the electron neutrino ( $\nu_e$ ), the muon neutrino ( $\nu_\mu$ ), and the tau neutrino ( $\nu_\tau$ ). The electrical charge of the electron, muon, and tau is the same and equal to the negative value of the elementary charge<sup>1</sup>, whereas neutrinos do not carry any electrical charge.

<sup>1</sup>The charge of the electron with the sign changed is used to define the elementary unit of

Leptons also interact via the weak interaction, however, as discussed in Section 1.3, the weak force only couples with left-chiral particles<sup>2</sup> (also known as *left-handed* particles). This means that a distinction between left-handed and right-handed leptons has to be made. Left-handed leptons are grouped into three doublets (generations) formed by one charged lepton and its corresponding neutrino based on the weak isospin quantum number,  $T_3 = \pm \frac{1}{2}$ . Right-handed leptons form singlets, have  $T_3 = 0$ , and do not undergo weak interactions. Since only left-handed neutrinos have been observed in experiments [3], right-handed neutrinos are not included in the SM. Neutrinos are assumed to be massless in the SM because the mechanism that generates the masses of fermions, the Higgs mechanism (Section 1.3.2), requires the left and right-handed version of a particle. The electron, muon, and tau have sizeable masses of  $m_e \approx 0.511$  MeV,  $m_\mu \approx 105.7$  MeV, and  $m_\tau \approx 1777$  MeV, respectively. The properties of the leptons are summarized in Table 1.1.

Table 1.1: The leptons of the SM listed with their mass, electric charge, possible chiralities, and third component of the weak isospin. The numerical values for these properties are taken from Reference [4].

| Lepton (Symbol)               |                             |                             | $Q/ e $ | Chirality | $T_3$          |
|-------------------------------|-----------------------------|-----------------------------|---------|-----------|----------------|
| electron ( $e^-$ )            | muon ( $\mu^-$ )            | tau ( $\tau^-$ )            | -1      | left      | $-\frac{1}{2}$ |
| 0.51 MeV                      | 105.66 MeV                  | $1776.86 \pm 0.12$ MeV      |         | right     | 0              |
| electron neutrino ( $\nu_e$ ) | muon neutrino ( $\nu_\mu$ ) | tau neutrino ( $\nu_\tau$ ) | 0       | left      | $+\frac{1}{2}$ |
| < 1.1 eV                      | < 0.19 MeV                  | < 18.2 MeV                  |         |           |                |

The group of particles formed by the quarks contains the fermions that undergo the electroweak and the strong interactions. This group is composed of three *up-type* quarks, the up ( $u$ ), the charm ( $c$ ), the top ( $t$ ), and three *down-type* quarks, the down ( $d$ ), the strange ( $s$ ), and the bottom ( $b$ ). Unlike leptons, quarks carry a fractional value of the elementary unit of electrical charge. Up-type quarks carry an electrical charge of  $Q = +2/3$ , whereas down-type quarks carry a charge of  $Q = -1/3$ .

Quarks also interact via the weak force and, similarly to leptons, they are

---

charge,  $e$ . In the international system of units, it is equivalent to  $e \sim 1.60 \times 10^{-19}$  C.

<sup>2</sup>A phenomena is chiral if it is not identical to its mirror image. The origin of Chirality comes from the representation theory of the  $SO(3,1)$  Lorentz group, where Chiral projectors are used to decompose the particle fields into their right- and left-handed chiralities. In the massless limit, chirality is equivalent to helicity, which is the projection of the particle spin in the direction of it's linear momentum.



organized according to the third component of the weak isospin into three generations. Left-handed quarks are grouped into doublets formed by an up- and a down-type quark and have  $T_3 = \pm\frac{1}{2}$ . Right-handed quarks form singlets, have  $T_3 = 0$ , and do not undergo weak interactions.

In addition to the electroweak interactions, quarks contain a kind of charge named *color charge* that enables them to interact via the strong force. The color charge is classified into three kinds: *red*, *green*, and *blue*. In Section 1.4 a detailed description of Quantum Chromodynamics, the theory behind the strong interaction in the SM, is given. Because of the confinement property of the strong interaction, quarks cannot be observed as free particles, they are embedded into composite bound states called *hadrons*. Hadrons can be classified into *baryons* and *mesons* depending on whether they are made of three quarks (antiquarks), or out of a quark-antiquark pair, respectively. Other more exotic forms of hadrons such as pentaquarks, bound states composed of three quarks and a quark-antiquarks pair, and tetraquarks, composed of two quark-antiquark pairs, have also been observed by the experiments at the Large Hadron Collider [5, 6].

Nevertheless, the top quark, the heaviest particle in the SM, is so massive that its associated mean-lifetime is shorter than the hadronization time, hence bound states (hadrons) cannot be formed before its decay. As a consequence, the properties of the top quark can be reconstructed from their decay products allowing the unique possibility to study the properties of a quasi-free quark. The physics of the top quark is essential for the development of this thesis, so this is further discussed in Chapter 2. The masses of the quarks, as well as their other properties, are summarized in Table 1.2.

Table 1.2: The quarks of the SM listed with their mass, electric charge, possible chiralities and third component of the weak isospin. The numerical values for these properties are taken from Reference [4].

| Quarks (Symbol)            |                     |                           | $Q/ e $        | Chirality | $T_3$          |
|----------------------------|---------------------|---------------------------|----------------|-----------|----------------|
| up ( $u$ )                 | charm ( $c$ )       | top ( $t$ )               | $+\frac{2}{3}$ | left      | $+\frac{1}{2}$ |
| $2.16^{+0.49}_{-0.26}$ MeV | $1.27 \pm 0.02$ GeV | $172.4 \pm 0.7$ GeV       |                | right     | 0              |
| down ( $d$ )               | strange ( $s$ )     | bottom ( $b$ )            | $-\frac{1}{3}$ | left      | $-\frac{1}{2}$ |
| $4.67^{+0.48}_{-0.17}$ MeV | $93^{+11}_{-5}$ MeV | $4.18^{0.03}_{-0.02}$ MeV |                | right     | 0              |

It is important to note that, for each fermionic particle in the SM, an anti-

particle exists with the same mass, but with the opposite quantum numbers (electric charge, weak isospin, color charge, etc).

### 1.1.2 Gauge bosons: Force mediators

In the SM, the interactions between particles are mediated by elementary particles of spin-1 called *gauge bosons*. Bosons follow the Bose-Einstein statistics allowing an arbitrary amount of them to share the same quantum state. These mediators are connected to the symmetry groups that describe each of the three fundamental interactions included in the SM: the unified electromagnetic and weak interactions, described by the  $SU(2)_L \times U(1)_Y$  transformation group, and the strong interaction, described by the  $SU(3)_C$  group. A compilation of the associated force mediators with their associated mass and electric charge are shown in Table 1.3. The strength of each interaction is determined by their associated *coupling constant*.

Table 1.3: The bosons of the SM listed with their associated force, mass and electric charge. The numerical values for these properties are taken from Reference [4].

|                          | Force              | Field Particles | Mass (GeV) | $Q/ e $ |
|--------------------------|--------------------|-----------------|------------|---------|
| Gauge bosons<br>(spin-1) | electromagnetic    | $\gamma$        | 0          | 0       |
|                          | weak               | $W^\pm$         | 80.4       | $\pm 1$ |
|                          | weak               | $Z$             | 91.2       | 0       |
|                          | strong             | $g$             | 0          | 0       |
| Scalar boson<br>(spin-0) | Higgs<br>mechanism | $H$             | 125.3      | 0       |

The electromagnetic force is the physical interaction responsible for the molecular structure, chemical reactions, and all other electromagnetic phenomena. All electrically charged particles interact via this force. At energies below the electroweak unification scale ( $\simeq 246$  GeV), it is described by Quantum Electrodynamics (Section 1.2) and the mediating gauge boson is the photon ( $\gamma$ ). The photon is a massless particle with no electric charge that appears as a consequence of imposing the local  $U(1)_{\text{EM}}$  symmetry into the free Lagrangian of a fermionic field. As the photon is a chargeless and massless particle, the range of the electromagnetic force is, theoretically, infinite.

The weak force is the physical interaction responsible of the radioactive decay

of subatomic particles and the nuclear fusion reaction among other phenomena. In the SM, the weak force is unified with the electromagnetic force both originating from the  $SU(2)_L \times U(1)_Y$  transformation symmetry. Below the electroweak unification scale, the weak interaction is mediated by three massive gauge bosons, the electrically charged  $W^\pm$  bosons and the electrically neutral  $Z$  boson. A description of the electroweak unification is given in Section 1.3.1. Fermions couple to the weak bosons through the third component of the weak isospin,  $T_3$ . The large mass of the  $W^\pm$  and the  $Z$  bosons (80.4 and 91.2 GeV, respectively) limits the range of the weak interaction to subnuclear scales.

The strong force is the physical interaction responsible for the quarks and gluons forming protons, neutrons, and other hadrons. It is also responsible for the strong nuclear force, the interaction that holds the protons and neutrons of an atom together inside the nuclei through the exchange of pions. In the SM, the strong interaction is described by the theory of Quantum Chromodynamics (Section 1.4), a theory based on imposing the  $SU(3)_C$  symmetry to the Lagrangian. The gauge bosons mediating this interaction are an octet of gluons, which are electrically neutral and massless. Unlike photons, gluons carry themselves the charge and anti-charge of the force that they mediate, the color charge. This means that they do not only interact with colored-charged fermions (quarks) but also among themselves. The self-interaction of gluons leads to a strength of the interaction that is low at high energy, but high at low energy. As a consequence, color-charged particles are asymptotically free at high energies but cannot be observed in isolation (confinement).

### 1.1.3 The Higgs boson

The invariance of the SM Lagrangian under  $SU(2)_L \times U(1)_Y$  implies that all fermions, as well as the gauge bosons, have to be massless. This theoretical conclusion is in clear contradiction with the experimental observations [7, 8], therefore, a mechanism to introduce the masses of particles, without breaking the original gauge invariance, has to be added to the model. In the SM, the weak interaction gauge bosons and all the fermions (except the neutrinos) acquire their mass through the Higgs mechanism, which is based on the Spontaneous Electroweak Symmetry Breaking (EWSB) mechanism. The EWSB keeps the invariance of the model to the different symmetry groups, while making the vacuum state (the ground state of the system), no longer exhibit this invariance.

A detailed description of the EWSB process is given in Section 1.3.2.

The Higgs boson ( $H$ ) is the particle generated from the excitation of the Higgs field. It is a massive spin-0 boson that interacts with all massive particles, including itself. The strength of this interaction is proportional to the mass of the particle. It was observed for the first time in 2012 by the ATLAS [9] and CMS [10] collaborations being the last particle of the SM to be discovered. A summary of its properties can be found in Table 1.3.

## 1.2 Quantum Electrodynamics

In this section, the basics of a Quantum Field Theory are described by deriving, as an example, the formulation of electromagnetism using this mathematical framework. This formulation is known as Quantum Electrodynamics (QED) and it is valid at energies below the electroweak unification scale ( $\sim 246$  GeV). The derivation of the Electroweak Theory (Section 1.3) and Quantum Chromodynamics (Section 1.4) follow a similar methodology. For this reason, it is not repeated in detail in the corresponding sections to, instead, concentrate on the most important physical effects of each respective theory. The description of QED given in this section is based on the explanations in Reference [11].

### 1.2.1 Derivation of the QED Lagrangian

In a QFT, particles are described as quantum fields. As in classical field theory, the equations of motion for these fields are obtained from the Euler-Lagrange equations, which are derived from imposing the principle of stationary action to the Lagrangian density. For the case of a single field  $\phi(x)$ , the Euler-Lagrange equation takes the form shown in Equation 1.1, where  $\mathcal{L}$  represents the Lagrangian density of the theory and  $\partial_\mu$  is the four-gradient. From now on, the *Lagrangian density* will be referred to only as *Lagrangian* as it is commonly done in QFT.

$$\partial_\mu \left( \frac{\partial \mathcal{L}}{\partial (\partial_\mu \phi)} \right) - \frac{\partial \mathcal{L}}{\partial \phi} = 0 \quad (1.1)$$

Once the Lagrangian of the theory is known, the equations of motion of all the

fields in the theory can be derived and, as a consequence, the full phenomenology of the particles in the theory.

QED aims to give a description of the electrically charged particles and their interactions with the electromagnetic field. To derive the associated QED Lagrangian, it is natural to start from the equation of motion for a free, massive, charged particle of spin- $\frac{1}{2}$ . The equation of motion that describes this kind of particles is the Dirac equation:

$$(i\gamma^\mu \partial_\mu - m)\psi(x) = 0 \quad (1.2)$$

where  $\psi(x)$  is the quantum field associated with the particle,  $m$  is the mass associated with this field, and  $\gamma^\mu$  are the Dirac matrices for the four-dimensional Minkowski space. In Equation 1.2, the Einstein notation is used where the summation over index variables that appear twice is implied. This notation is used for all equations throughout this thesis.

The underlying Lagrangian for the Dirac theory, the one that leads to the Dirac equation of motion when applying the corresponding Euler-Lagrange equations for  $\psi(x)$  and for  $\bar{\psi}(x) = \psi^\dagger(x)\gamma^0$ , is:

$$\mathcal{L}_{\text{Dirac}} = \bar{\psi}(x)(i\gamma^\mu \partial_\mu)\psi(x) - m\bar{\psi}(x)\psi(x) \quad (1.3)$$

It can be noticed that this Lagrangian is not only Lorentz-invariant, but that it also has the following Abelian  $U(1)$  global symmetry:

$$\begin{aligned} \psi(x) &\rightarrow \exp(i\alpha)\psi(x) \\ \bar{\psi}(x) &\rightarrow \exp(-i\alpha)\bar{\psi}(x) \end{aligned} \quad (1.4)$$

If now the  $U(1)$  global symmetry of the Dirac Lagrangian is upgraded to a local  $U(1)$  symmetry<sup>3</sup>, then the Lagrangian is no longer local invariant because of the derivative term, the term with  $\partial_\mu\psi(x)$ . To recover the invariance, a spin-1 gauge field,  $A_\mu(x)$ , is introduced and the partial derivative is replaced by the

---

<sup>3</sup>This means that now the phase depends on the space-time location,  $\alpha \rightarrow \alpha(x)$ .

gauge covariant derivative of Equation 1.5. The  $A_\mu(x)$  field transforms under local  $U(1)$  transformations as shown in Equation 1.6.

$$\mathcal{D}_\mu \equiv \partial_\mu + iqA_\mu(x) \quad (1.5)$$

$$A_\mu(x) \rightarrow A_\mu(x) - \frac{1}{q}\partial_\mu\alpha(x) \quad (1.6)$$

Once the gauge covariant derivative and the  $A_\mu(x)$  vector-field are added to the Dirac Lagrangian, it takes the following form:

$$\begin{aligned} \mathcal{L} &= \bar{\psi}(i\gamma^\mu\mathcal{D}_\mu)\psi - m\bar{\psi}\psi \\ &= \bar{\psi}(i\gamma^\mu\partial_\mu)\psi - m\bar{\psi}\psi - qA_\mu\bar{\psi}\gamma^\mu\psi, \end{aligned} \quad (1.7)$$

Where the new  $-qA_\mu\bar{\psi}\gamma^\mu\psi$  term of the Lagrangian describes the interaction of two fermionic fields via the gauge field with the strength of the interaction being described by the coupling constant  $q$ .

The  $A_\mu(x)$  field in the Lagrangian of Equation 1.7 lacks a free propagation term. To derive the term that has to be added to the Lagrangian to describe the dynamics of the  $A_\mu(x)$  field, it is natural to start from the equation of motion for a free, massive, spin-1 particle. The equation of motion that describes this kind of particles is the Proca equation (Equation 1.8) and its associated Lagrangian is shown in Equation 1.9, where  $F^{\mu\nu} \equiv (\partial^\mu A^\nu - \partial^\nu A^\mu)$  is the strength field tensor.

$$(\partial_\mu\partial^\mu - m_A^2)A^\nu = 0 \quad (1.8)$$

$$\mathcal{L}_{\text{Proca}} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \frac{1}{2}m_A^2 A^\nu A_\nu \quad (1.9)$$

Note that the mass term in the Proca Lagrangian is not invariant under the local  $U(1)$  gauge transformation. By requiring the mass of the vector field to be 0,  $m_A = 0$ , the Proca Lagrangian becomes gauge invariant and it takes the form

of the covariant form of the Maxwell equations. In this form, the  $A_\mu$  gauge field can be identified as the photon field. At last, by adding the photon propagation term to Equation 1.7 the Lagrangian of QED is complete:

$$\begin{aligned}\mathcal{L}_{\text{QED}} &= \bar{\psi}(i\gamma^\mu \mathcal{D}_\mu)\psi - m\bar{\psi}\psi - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} \\ &= \bar{\psi}(i\gamma^\mu \partial_\mu)\psi - m\bar{\psi}\psi - q(\bar{\psi}\gamma^\mu\psi)A_\mu - \frac{1}{4}F^{\mu\nu}F_{\mu\nu}\end{aligned}\tag{1.10}$$

Noether's theorem states that, for each symmetry of the Lagrangian, there is a conserved quantity. In the case of the Abelian  $U(1)$  local symmetry of the QED Lagrangian, the conserved current derived from Noether's theorem is  $j^\mu = \bar{\psi}\gamma^\mu\psi$ , and it's associated conserved charge is  $q$ , the strength of the coupling between the two fermion fields and the photon field. This conserved charge is identified as the electric charge associated with the fermionic field.

To sum up, only by considering the equations of motions for massive spin- $\frac{1}{2}$  and spin-1 particles and the gauge invariant under the  $U(1)$  local symmetry, the Lagrangian of QED can be built and all the associated phenomenology can be derived.

The theory of QED was the first gauge QFT that successfully described one of the fundamental interactions of Nature. The theory of QED was developed in the 1940s by R. Feynman, J. Schwinger, and S.I. Tomonaga, independently of each other [12–14]. It has provided accurate predictions of quantities such as the Lamb shift of the energy levels of hydrogen [15], and the anomalous magnetic dipole moment of the electron [16]. The other QFTs that describe the Weak and the Strong interactions are based on the principles established by this highly successful theory.

### 1.2.2 Perturbation theory for QED and Feynman diagrams

Many of the models constructed within the QFT framework lead to unsolvable equations which means that, for now, it has not been possible to find exact analytical solutions for the predictions of the theory. The theory of QED and the whole SM are two of these models, so in order to calculate predictions that

can be compared with the experimental results, a solvable approximation of these equations is obtained through *perturbation theory*. Perturbation theory provides an approximation to the full solution by expanding around a small parameter of the model, which in the case of the SM, are the coupling constants. This approximation is valid as long as the couplings are small and the similarity between the perturbative calculation and the full unknown solution depends on the order of the expansion. If only the first order is considered, the calculation is said to be performed at *leading order* (LO), if the second order is also considered, the calculation is said to be performed at *next-to-leading order* (NLO), and so on.

All the terms which make up the perturbative calculations can be constructed from just three sets of building blocks: interaction vertices, particle propagators, and external lines. Interactions vertices describe the interaction between multiple particles, propagators describe the probability for a particle to propagate from one space-time point to another, and the external lines represent the incoming and outgoing particles. Each of these building blocks has an associated mathematical expression that is derived from the Lagrangian that describes the theory. The different contributions to each order in perturbation theory can be represented graphically in what is known as *Feynman diagrams*.

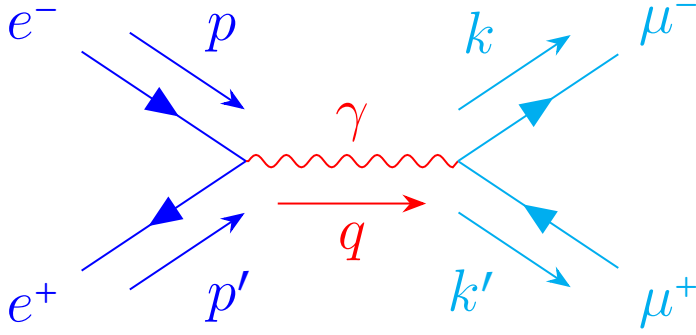
Using these diagrams, the Feynman Rules provide a recipe for the construction of the transition amplitude<sup>4</sup> between any incoming and outgoing particle state, allowing for the calculation of measurable quantities, such as cross sections and decay rates. As an example, the simplest process in QED, the annihilation of an electron and a positron into a pair of muons at LO, can be expressed with only the Feynman diagram in Figure 1.2, where the  $p$ ,  $p'$ ,  $q$ ,  $k$ , and  $k'$  represent the momenta of the incoming electron, the incoming positron, the virtual photon, the outgoing muon, and the outgoing antimuon, respectively. The term  $g_{\mu\nu}$  denotes the components of the spacetime metric tensor. Additionally, the  $u^s$  ( $\bar{u}^s$ ) terms represent the spinor<sup>5</sup> of an incoming (outgoing) fermion, whereas  $\nu^s$  ( $\bar{\nu}^s$ ) terms are the spinor for an incoming (outgoing) antifermion.

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<sup>4</sup>The transition amplitude is also known as the *scattering matrix element* or only *matrix element*.

<sup>5</sup>A spinor is a vector-like quantity with special transformation properties under rotations.





$$= \bar{\nu}^{s'}(p')(-ie\gamma^\mu)u^s(p)\left(\frac{-ig_{\mu\nu}}{q^2}\right)\bar{u}^r(k)(-ie\gamma^\nu)\nu^{r'}(k')$$

Figure 1.2: Feynman diagram for the scattering  $e^-e^+ \rightarrow \mu^-\mu^+$  at LO with the incoming particles, the intermediate virtual photon, and the outgoing particles painted in blue, red, and cyan, respectively. The associated matrix element obtained using the Feynman rules for each of the components is also shown.

## 1.3 Electroweak Theory

### 1.3.1 Electroweak Unification

In the SM, the electromagnetic and the weak interactions are unified and described by the Electroweak Theory (EW), developed by S. L. Glashow, A. Salam and J. C. Ward, and S. Weinberg in the decade of 1960 [17–19]. The symmetry group that characterizes this theory is  $SU(2)_L \times U(1)_Y$ , where the  $U(1)$  is the same symmetry group as in QED (Section 1.2), and  $SU(2)_L$  is the special unitary group of 2x2 matrices. The conserved quantities associated to  $U(1)_Y$  and  $SU(2)_L$  are the hypercharge ( $Y$ ) and the third component of the weak isospin ( $T_3$ ), respectively. The hypercharge and the third component of the weak isospin are related to the electromagnetic charge by the Gell–Mann–Nijijima formula [20]:

$$Q = T_3 + \frac{1}{2}Y \quad (1.11)$$

The  $L$  in  $SU(2)_L$  indicates that the gauge fields associated with this symmetry group only couple to left-handed fermions, which makes the EW theory left-chiral. The distinction between left and right-handed particles in the theory is introduced

to reflect the results from the Wu experiment [21]. In this experiment it was found that the weak interaction does not interact with right-handed particles, resulting in a maximal violation of the parity symmetry.

To manifest the chirality of the EW theory, first, the fermion fields ( $\psi$ ) are decomposed into a left- and right-handed component ( $\psi_L, \psi_R$ ) defined as:

$$\begin{aligned}\psi_L(x) &= \frac{1}{2}(1 - \gamma^5)\psi(x) \\ \psi_R(x) &= \frac{1}{2}(1 + \gamma^5)\psi(x)\end{aligned}\tag{1.12}$$

where  $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$  is the product of the four Dirac matrices.

In non-Abelian Yang-Mills gauge theories such as  $SU(2)_L$ , the symmetry imposed to the Lagrangian is described by the  $U(\theta)$  unitary transformation:

$$\psi(x) \rightarrow U(\theta)\psi(x)\tag{1.13}$$

$$U(\theta) = \exp(igT^a\theta_a)\tag{1.14}$$

where  $g$  is the gauge coupling strength,  $T^a$  are the group generators, and  $\theta_a$  are the parameters associated with the unitary transformation.

In the particular case of  $SU(2)_L$ , the generators of the group take the value of  $T^a = \frac{\sigma^a}{2}$ , when acting on left-handed fields ( $\psi_L$ ), and  $T^a \equiv 0$ , when acting on right-handed fields ( $\psi_R$ ), where  $\sigma^i$  represent the three Pauli matrices with  $i = 1, 2, 3$ . These generators have three associated gauge boson fields represented by  $W_i^\mu = W_1^\mu, W_2^\mu, W_3^\mu$ . The associated gauge coupling is indicated by  $g$ .

The gauge boson field associated with the  $U(1)_Y$  symmetry group is represented by  $B^\mu$ . As it is represented by the same  $U(1)$  symmetry as the photon field of QED (Section 1.2), its properties are described by the same group of equations. The conserved current associated with this interaction is the hypercharge ( $Y$ ) and the gauge coupling is indicated by  $g'$ .

The Lagrangian resulting from imposing the  $SU(2)_L \times U(1)_Y$  symmetries, without the mass terms, is:

$$\mathcal{L} = \bar{\psi}_L(i\gamma^\mu \mathcal{D}_\mu)\psi_L + \bar{\psi}_R(i\gamma^\mu \mathcal{D}_\mu)\psi_R - \frac{1}{4}W_{\mu\nu}^i W^{i,\mu\nu} - \frac{1}{4}B_{\mu\nu}^i B^{i,\mu\nu} \quad (1.15)$$

where  $\mathcal{D}_\mu\psi_L$  and  $\mathcal{D}_\mu\psi_R$  are the covariant derivatives acting on left- and right-handed fermion fields (Equation 1.16), and  $W_{\mu\nu}^i$  ( $i = 1, 2, 3$ ) and  $B^{\mu\nu}$  are the strength field tensors for each of the gauge bosons of the theory (Equation 1.17). As a result of  $SU(2)_L$  only affecting to left-handed particles, the covariant derivatives in Equation 1.16 act differently on each chirality state. The  $\epsilon^{ijk}$  symbol in Equation 1.17 is the Levi-Civita tensor. The mass terms for the fermion and vector fields are not included in the Lagrangian of Equation 1.15 because they would violate the  $SU(2)_L$  gauge invariance.

$$\begin{aligned} \mathcal{D}_\mu\psi_L &= \left( \partial_\mu - ig\frac{\sigma^i}{2}W_\mu^i - ig'\frac{Y}{2}B_\mu \right) \psi_L \\ \mathcal{D}_\mu\psi_R &= \left( \partial_\mu - ig'\frac{Y}{2}B_\mu \right) \psi_R \end{aligned} \quad (1.16)$$

$$\begin{aligned} B_{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu \\ W_{\mu\nu}^i &= \partial_\mu W_\nu^i - \partial_\nu W_\mu^i - g\epsilon^{ijk}W_\mu^j W_\nu^k \end{aligned} \quad (1.17)$$

The experimentally observed charged current interactions ( $W_\mu^\pm$ ) are derived from linear combination of the  $W_\mu^1$  and  $W_\mu^2$  fields:

$$W_\mu^\pm = \frac{1}{\sqrt{2}}(W_\mu^1 \mp iW_\mu^2) \quad (1.18)$$

while the photon field ( $A_\mu$ ) and the neutral current field of the weak interaction ( $Z_\mu$ ) are derived from a rotation of the remaining  $W_\mu^3$  and  $B_\mu$  fields:

$$\begin{pmatrix} A_\mu \\ Z_\mu \end{pmatrix} = \begin{pmatrix} \cos\theta_W & -\sin\theta_W \\ \sin\theta_W & \cos\theta_W \end{pmatrix} \begin{pmatrix} B_\mu \\ W_\mu^3 \end{pmatrix} \quad (1.19)$$

where  $\theta_W$  is the Weinberg mixing angle which, expressed in terms of the  $g$  and  $g'$  couplings, is defined as  $\cos \theta_W = \frac{g}{\sqrt{g^2+g'^2}}$  and  $\sin \theta_W = \frac{g'}{\sqrt{g^2+g'^2}}$ .

From the short range of the weak interaction, the predicted  $W^\pm$  and  $Z$  bosons are expected to be massive, but with the formulation of the theory shown so far, they are massless. In the next section, the Spontaneous Symmetry Breaking mechanism, the mechanism used to introduce the masses of the electroweak bosons and the fermions in the SM is described.

### 1.3.2 Electroweak Symmetry Breaking

The introduction of mass terms in the Lagrangian of the electroweak theory of Equation 1.15 would make it no longer gauge invariant under  $SU(2)_L \times U(1)_Y$  transformations. However, it is experimentally known that the fermions and the  $W^\pm$  and  $Z$  gauge bosons are massive. The conflict between the two opposite requirements is solved by the Higgs-Brout-Englert (HBE) mechanism, which generates the mass of the particles through the Spontaneous Symmetry Breaking (SSB) mechanism. This mechanism introduces a new complex scalar field,  $\phi$ , which is a doublet of the weak isospin  $SU(2)_L$  symmetry. The equations of motion of this field are described by the following Lagrangian:

$$\mathcal{L}_{\text{Higgs}} = (\mathcal{D}_\mu \phi)^\dagger (\mathcal{D}^\mu \phi) - V(\phi) \quad (1.20)$$

where  $\phi$  is the Higgs field and  $V(\phi)$  is the Higgs potential.

$$\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \phi_1 + i\phi_2 \\ \phi_3 + i\phi_4 \end{pmatrix} \quad (1.21)$$

$$V(\phi) = \mu^2 |\phi|^2 + \lambda |\phi|^4 \quad (1.22)$$

The Higgs field carries four degrees of freedom, the four real scalar fields  $\phi_{i=1,2,3,4}$ . The shape of the  $V(\phi)$  potential depends on the value of the real parameters  $\mu^2 < 0$  and  $\lambda > 0$ . The  $\lambda$  parameter is required to be greater than 0

to ensure that the potential is bounded from below, thus it has at least one ground state<sup>6</sup>. If the  $\mu^2$  parameter would be positive, the  $V(\phi)$  potential would have a unique absolute minimum,  $\phi_0$ , situated at  $\phi = 0$ , which does not allow for symmetry breaking. However, since  $\mu^2$  is negative, the zero particle state,  $\phi = 0$ , is an unstable local maximum of the potential, hence the minimum has  $\phi \neq 0$ . This means that there is a misalignment between the zero particle state and the vacuum state, thus the Higgs field ( $\phi$ ) has a non-zero vacuum expectation value (VEV),  $v$ .

$$\langle 0|\phi|0\rangle = \sqrt{-\frac{\mu^2}{2\lambda}} \equiv \frac{v}{2} \neq 0 \quad (1.23)$$

A schematic representation of the Higgs potential is shown in Figure 1.3. In the space formed by the real and imaginary components of the Higgs field, the potential is symmetric under rotations around the zero particle state (the origin). However, when the state of the field is placed at a minimum, the vacuum state does not share this symmetry with the Lagrangian.

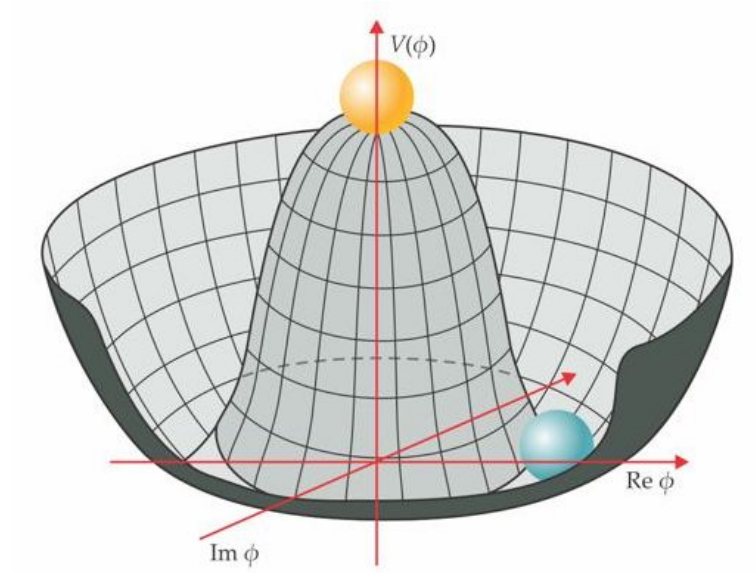


Figure 1.3: A schematic representation of the Higgs potential [22]. The yellow ball represents the symmetric solution for the potential, where the photon and  $W/Z$  bosons are massless. In contrast, the blue ball represents the post-symmetry breaking solution, where the  $W/Z$  bosons acquire mass.

<sup>6</sup>Theories where the potential is not bounded from below do not have an absolute minimum and are unstable

The ground state of the Higgs field doublet can be chosen to have a zero value of the charged component,  $\phi^+$ , while the neutral component has the VEV.

$$\phi_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v \end{pmatrix} \quad (1.24)$$

Small excitations of the scalar field doublet around the vacuum state in the direction of the zero particle state are parametrized as:

$$\phi = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + H \end{pmatrix} \quad (1.25)$$

where  $H$  is the *Higgs boson* and has a mass of  $m_H = \sqrt{-\mu^2}$ . The choice of a particular minimum breaks the  $SU(2)_L \times U(1)_Y$  symmetry of the Lagrangian in the vacuum state. The remaining three degrees of freedom introduced in the  $\phi$  complex scalar field doublet are *reabsorbed* by the  $Z$  and  $W^\pm$  bosons of the EW theory, becoming massive in the process. The associated mass terms in the Lagrangian arise from introducing the value of the  $\phi_0$  into the covariant derivative of the EW theory,  $\mathcal{D}(\phi)$  (Equation 1.16). This leads to the following mass terms:

$$\mathcal{L}_{\text{mass}} = \frac{g^2 v^2}{4} W_\mu^+ W^{-,\mu} + \frac{g^2 v^2}{\cos^2(\theta_W)} Z_\mu Z^\mu \quad (1.26)$$

Since the mass term associated with a vector field  $X_\mu$  has the form  $M_X^2 X_\mu X^\mu$ , the  $W^\pm$  and  $Z$  boson masses can be identified as:

$$M_W = \frac{gv}{2}, \quad M_Z = \frac{gv}{2 \cos(\theta_W)} = \frac{M_W}{\cos(\theta_W)} \quad (1.27)$$

where  $g$  is the gauge coupling of  $SU(2)_L$ , and  $\theta_W$  is the Weinberg mixing angle (Section 1.3.1). The SSB mechanism does not introduce any quadratic term for the  $A_\mu$  photon field, therefore, the photon remains massless.

### 1.3.3 Masses of fermions

The mass terms for the fermionic fields, as in the case of the weak gauge bosons, violate the  $SU(2)_L$  symmetry of the Lagrangian. To solve this problem, in the SM, the masses of fermions originate from their interaction with the Higgs field. This interaction is introduced by coupling the fermions with the Higgs field through the direct linear combination of the fields known as *Yukawa coupling*, which general form is described by the Lagrangian:

$$\mathcal{L}_Y = -g_Y \bar{\psi} \phi \psi \quad (1.28)$$

where  $g_Y$  is the coupling constant associated with the interaction.

For all the fermions of the SM, the total Yukawa Lagrangian, after considering the non-existence of right-handed neutrinos in the theory, take the following form:

$$\mathcal{L}_{\text{Yukawa}} = -y_l^{ij} l_{L,i}^\dagger e_{R,j} \phi - y_q^{ij} q_{L,i}^\dagger u_{R,j} i\sigma_2 \phi^* - y_q^{ij} q_{L,i}^\dagger d_{R,j} \quad (1.29)$$

where the index  $i$  ( $j$ ) references each of the three generations of leptons. The  $y_q^{ij}$  and  $y_l^{ij}$  matrices describe the Yukawa couplings between the Higgs field,  $\phi$ , and the quarks and charged leptons, respectively.  $e_{R,i}$  is the right-chiral weak-isospin lepton singlet, and  $u_{R,i}$  ( $d_{R,i}$ ) is the right-chiral weak isospin up- (down-) quark singlet for each of the  $i$ -th generations.  $l_{L,i}$  ( $q_{L,i}$ ) is the left-chiral weak-isospin lepton (quark) doublet field for the  $i$ -th generation.  $\sigma_2$  is the second Pauli matrix.

The Yukawa coupling matrices are non-diagonal, which indicates that the mass eigenstates of the fermions are a mixture of the EW flavor eigenstates of the EW theory. The description of the mixing between the three different families of quarks is given by the Cabibbo-Kobayashi-Maskawa (CKM) matrix [23, 24].

The introduction of the SSB and the VEV of the Higgs field (Equation 1.25) into the Lagrangian of Equation 1.29 generate quadratic terms for the fermionic fields. These terms can be identified as the mass terms of the fermion fields and the corresponding masses for each of the fermions take the following form:

$$m_f = y_f \frac{v}{\sqrt{2}}, \quad (1.30)$$

where  $y_f$  is the Yukawa coupling of the Higgs field with the corresponding fermion ( $f = e, u, d, \dots$ ). Equation 1.30 predicts that the mass of the fermions is proportional to the strength of their coupling with the Higgs boson, hence the more massive a particle is, the stronger is its coupling with the Higgs boson. This prediction of the SM has been studied by the ATLAS and CMS collaborations showing experimental results which are compatible with the theory (Figure 1.4). The top quark, due to its large mass, has the strongest coupling to the Higgs boson ( $y_t \sim 1$ ), which suggests that it may play a special role in the SSB mechanism.

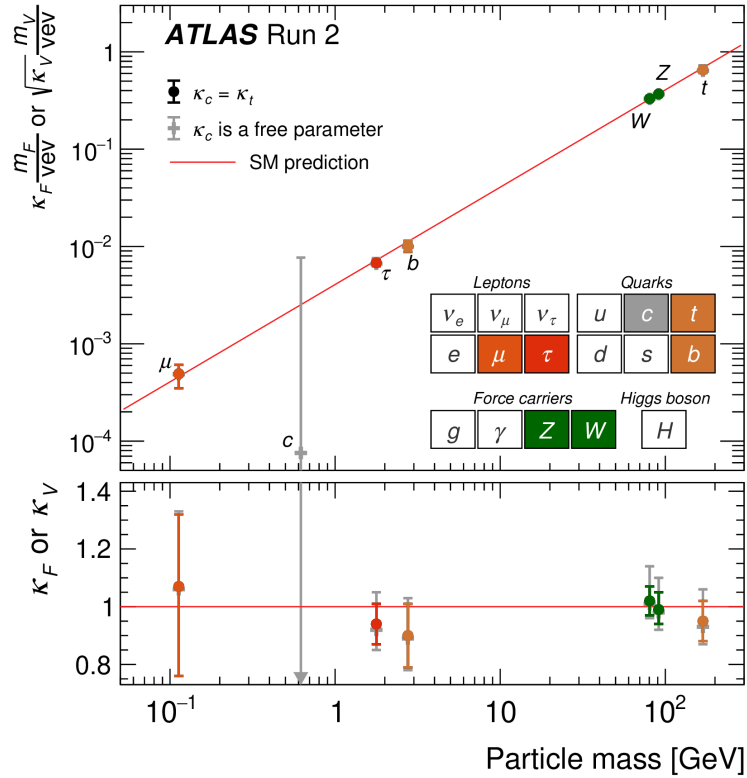


Figure 1.4: ATLAS measurements on the Higgs boson coupling strength with the fermions ( $t, b, \tau, \mu$ ) and the weak gauge bosons ( $W^\pm, Z$ ) respect to their mass. The compatibility between the SM predictions (dotted line) and the combined measurement is 84% [25].



## 1.4 Quantum Chromodynamics

### 1.4.1 Mathematical description and motivation

In the SM, the strong interaction is described by the theory of Quantum Chromodynamics (QCD), developed by H. Fritzsch, H. Leutwyler and Gell-Mann in the decade of 1970 [26]. The symmetry group that characterizes this theory is  $SU(3)_C$ , the special unitary group of 3x3 matrices. The conserved quantity associated with this theory, as the  $C$  subscript indicates, is the color charge. QCD has three different kinds of color charges, which are usually referred to as red, green and blue. Quarks are the only fermions that carry color charge and form triplets under the  $SU(3)_C$  symmetry group, whereas leptons are colorless and form singlets.

The existence of these three color quantum numbers was proposed to reconcile the baryon spectrum predicted from the quark model with the spin-statistics theorem. In particular, the observation of the  $\Delta^{++}(1232)$  baryon, a spin-3/2 particle with a charge of  $+2|e|$  and interpreted as a bound state composed of three up quarks ( $uuu$ ) with zero angular momentum and all three quarks with parallel spins, presented a conflict. As the  $\Delta^{++}$  particle is a fermion, its wave function has to be anti-symmetric and, at the same time, symmetric under the interchange of any of the quark pairs in space-, spin-, and flavor wave functions. This cannot be achieved with three identical up quarks, hence a new degree of freedom, the three color quantum numbers, is introduced. Since the Pauli exclusion principle only applies to identical particles and now each quark carries a different color charge, the problem vanishes.

As in the case of the  $SU(2)_L$  symmetry group of the EW interaction,  $SU(3)_C$  is a non-Abelian Yang-Mills gauge theory so the symmetry imposed to the Lagrangian is described by the same general  $U(\theta)$  unitary transformation in Equation 1.14. In the particular case of  $SU(3)_C$ , the generators of the group take the value of  $T^a = \frac{1}{2}\lambda^a$ , where  $\lambda^a$  are the Gell-Mann matrices which follow the commutation relation  $[\lambda^a, \lambda^b] = if^{abc}\lambda^c$ , with  $f^{abc}$  being the structure constants of the  $SU(3)$  group. These generators have eight associated gauge boson fields represented by  $G_\mu^a$  with  $a = 1, \dots, 8$  which represent the gluons.

The Lagrangian resulting from imposing the  $SU(3)_C$  is:

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}(i\gamma^\mu \mathcal{D}_\mu)\psi - m\bar{\psi}\psi - \frac{1}{4}G_a^{\mu\nu}G_{\mu\nu}^a + \text{h.c.} \quad (1.31)$$

where  $\mathcal{D}_\mu\psi$  is the covariant derivative of QCD over fermion fields and  $G_{\mu\nu}^a$  is the strong field tensor, described by Equation 1.32 and Equation 1.33, respectively. The first term of  $\mathcal{L}_{\text{QCD}}$  describes the free propagation of quarks and the interaction between quarks and gluons, the second term is the mass term for fermions, and the third term describes the free propagation of a gluon and their self-interactions. Analogously to the fine-structure constant of QED, the gauge coupling associated with the strong interaction ( $g_s$ ) is used to define the QCD coupling constant as  $\alpha_s = \frac{g_s^2}{4\pi}$ .

$$\mathcal{D}_\mu\psi = \left( \partial_\mu - ig_s \frac{\lambda^a}{2} G_\mu^a \right) \psi_L \quad (1.32)$$

$$G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a - g_s f^{abc} G_\mu^b G_\nu^c \quad (1.33)$$

Since gluons interact with each other (Figure 1.5), the gluon field between a pair of color charges such as two quarks forms a string with a constant energy density no matter the distance. When two color charges are pulled apart, it reaches a point where the energy of the field is large enough to produce a quark-antiquark pair. Each quark of this new pair forms a bound state with each of the original color charges. This phenomena is known as *color confinement* and makes it impossible to observe free color-charged particles. Nevertheless, the gluon self-interactions also make colored particles to be *asymptotically free* because the strength of the QCD coupling decreases at high energies.

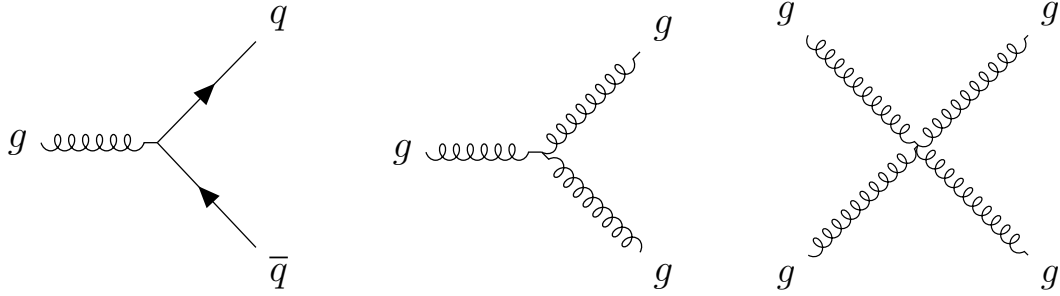


Figure 1.5: The three kinds of interaction vertices of QCD.

### 1.4.2 Ultraviolet divergencies, renormalization, and the running of the couplings and masses

When computing cross sections and other observables beyond LO in perturbation theory, contributions from virtual processes as the ones shown in Figure 1.6 start to play a role. In particular, these contributions lead to logarithmic divergencies when integrating over the momentum loop of the virtual particle,  $k$ . The divergencies arise in the high energy limit, when  $k \rightarrow \infty$ , hence they are known as *ultraviolet divergencies*.

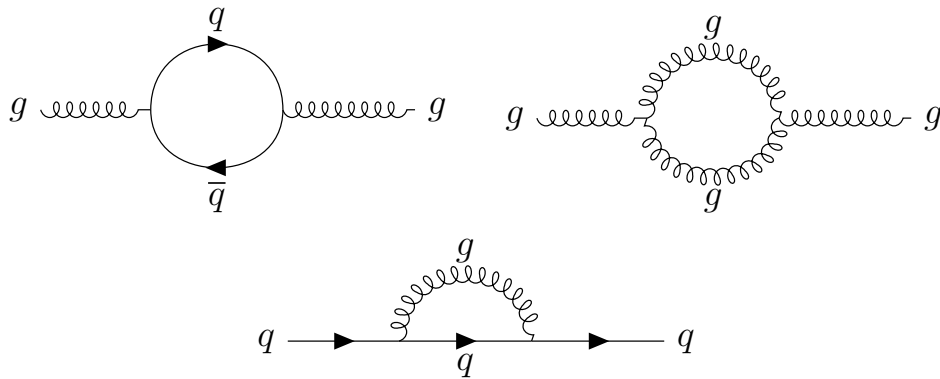


Figure 1.6: Beyond LO, the propagator of the gluon (upper) and the quark (lower) are corrected. In the  $\overline{MS}$  scheme, these corrections are absorbed into the strong coupling constant and the quark masses, respectively.

However, it has been experimentally measured that these observables have a finite value, therefore, a method that counters the infinities in the calculations is established to produce meaningful predictions. This method is called *renormalization* and it consists of subtracting and reabsorbing the divergent

behaviours into the definition of the bare parameters of the Lagrangian<sup>7</sup>. To do so, the unfixed parameters of the theory such as masses, couplings, and field normalizations are redefined in terms of arbitrary scale parameters, usually denoted as  $\mu$ . The new parameters are called *renormalized* (or *dressed*) parameters and they are written as the product between the bare parameters and some associated *renormalization counterterms*, which are functions selected to cancel the UV divergencies at a fixed order in perturbation theory.

The choice of the renormalization scheme used to reabsorb the divergencies is not unique, therefore, various definitions of the parameters are possible. The three most common choices of renormalization schemes are the *minimal subtraction scheme* ( $MS$ ), where the counterterms do not include any finite term, the *modified minimal subtraction scheme* ( $\overline{MS}$ ), a modified version of the  $MS$  scheme where a universal constant is also subtracted to simplify the calculations, and the *on-shell scheme*, where every parameter is fixed in order that the on-shell particles always have the masses which are measured by the experiments. However, as the choice of the renormalization scheme and the renormalization scale are unphysical, the observables must be independent of these choices. This fact leads to a set of differential equations known as the *renormalization group equations* (RGE) that relate the value of a renormalization constant at a new energy scale ( $\mu$ ) with its value at a given reference scale ( $\mu_0$ ). For example, at NLO in perturbative QCD, the strong coupling constant ( $\alpha_S$ ) and quark mass RGEs in the  $\overline{MS}$  scheme reads as:

$$\alpha_S(\mu^2) = \frac{\alpha_S(\mu_0^2)}{1 + \beta_0 \alpha_S(\mu_0^2) \ln(\mu^2/\mu_0^2)} \quad (1.34)$$

$$m(\mu) = m(\mu_0) \left[ 1 - c_0 \alpha_S(\mu) \ln\left(\frac{\mu^2}{\mu_0^2}\right) \right] \quad (1.35)$$

where the  $\beta_{n-1}$  and  $c_{n-1}$  coefficients contain the n-loop corrections to the propagators and vertices. In the particular case of Equations 1.34 and 1.35, the 1-loop correction coefficients are  $c_0 = 1/\pi$  and  $\beta_0 = (33 - 2n_f)/12\pi$ , where  $n_f$  is the number of active flavors, i.e., the number of quarks with masses below the

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<sup>7</sup>These parameters are also known as tree-level or unrenormalized parameters and they are regarded as unphysical quantities.

considered scale,  $\mu$ .

The evolution of the strong coupling as a function of the energy scale predicted by Equation 1.34 (also known as  $\alpha_s$ ) give rise to some of the main properties of QCD discussed in Section 1.4.1. In particular, as the energy scale of the process increases, the value of  $\alpha_s$  decreases loosening the strength of the interaction, which is the origin of the asymptotic freedom property of the theory. On the other hand, as the energy scale of the processes decreases, the value of  $\alpha_s$  increases making the strength of the interaction stronger, which is the origin of the confinement of colored particles. Another effect of the increase of  $\alpha_s$  at low energies is that, at energies around the QCD scale,  $\Lambda_{\text{QCD}} \sim 300$  MeV,  $\alpha_s(\Lambda_{\text{QCD}}) \sim 1$ , which invalidates the perturbative treatment of QCD. From a practical perspective, the perturbative treatment of QCD is only valid for energies above 1 GeV, hence other theories have to be used to describe the hadronic states and the hadronization process. A comparison between several  $\alpha_s$  measurements realized at different energy scales and the extrapolation of the  $\alpha_s(m_Z)$  measurement using the SM RGE equations is shown in Figure 1.7.

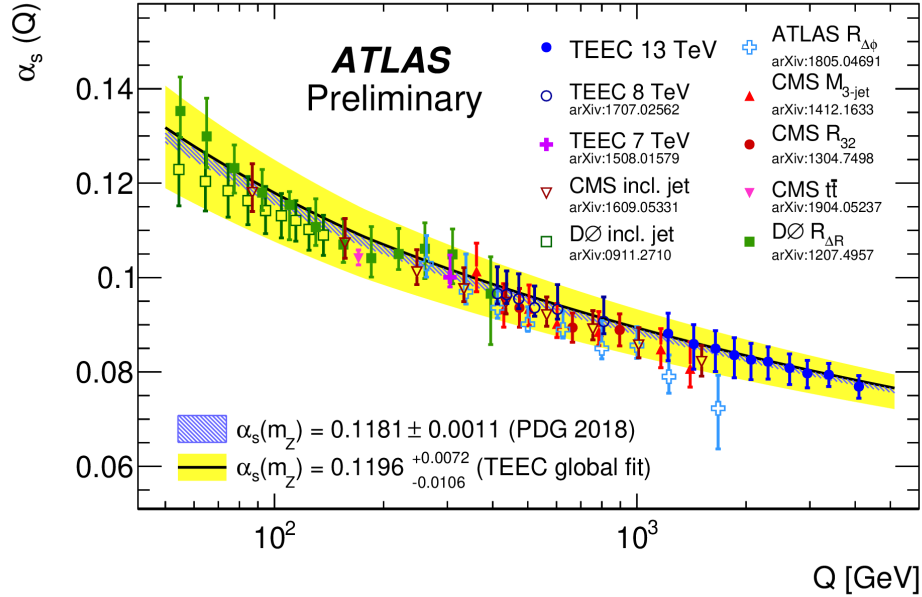


Figure 1.7: Comparison of the  $\alpha_s$  measurements as a function of the energy scale  $Q$ . The different measurements have been provided by several experiments using a wide variety of techniques [27].

In the main study of this thesis, the theoretical predictions used for the fit are calculated using the on-shell scheme, hence the definition of the top quark mass

that is being measured is the on-shell mass, also known as the top quark pole mass,  $m_t^{\text{pole}}$ .

## 1.5 Limitations of the Standard Model

The theory of the SM has been exhaustively tested through multiple experiments and, so far, it has been consistent with most of the measurements and searches. Indeed, it predicted the existence of many particles before they were discovered, such as the  $Z$  and  $W^\pm$  weak bosons and the Higgs boson. Despite the success of the SM, it cannot be the ultimate theory since there are many open questions and several fundamental physics phenomena that this theory cannot explain. Some of these questions and phenomena are listed below:

- **Neutrino masses:** Neutrinos in the SM are predicted to be massless. However, the observation of neutrino oscillations [28] implies that neutrinos are actually massive and that their flavor eigenstates do not coincide with their mass eigenstates. A possible extension to the SM that introduces neutrino masses and explains their smallness is the Seesaw mechanism [29]. Within this mechanism, neutrinos can be defined as Dirac or Majorana particles<sup>8</sup>. One of the possibilities to prove that neutrinos are Majorana is by looking for the existence of neutrinoless double-beta decay in nature. The search for this decay is being carried out by the NEXT experiment [30] at Canfranc, among others.
- **Matter-antimatter asymmetry:** In the SM, matter and antimatter are always created and annihilated in pairs, however, the universe we see today is composed of matter and not antimatter. The quark sector of the SM has some CP violation components, but they are not large enough to explain the observed asymmetry. Any possible theoretical model that solves this problem needs to fulfill the Sakharov conditions, which include baryon number violation, C and CP violation, and deviation from thermal equilibrium [31]. One of such models is the Grand Unification Theory (GUT) baryogenesis [32], which also predicts proton decay.

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<sup>8</sup>Majorana particles are those from which its particle and antiparticle are the same, whereas if the two are different, they are referred to as Dirac particles

- **Cosmological discrepancies:** A series of astrophysical and cosmological observations lead to the conclusion that the matter-energy content of the universe cannot be explained with the particles of the SM and Einsteins' general relativity [33].
  - To explain the mismatch between several gravitation effects and the amount of visible matter<sup>9</sup>, a new kind of matter that interact mainly gravitationally is proposed, the so called *dark matter*. It is called *dark* because it lacks the electromagnetic interaction and, therefore, it is invisible to light. The SM only provides one stable particle with these characteristics, the neutrino, but the observed properties of dark matter and its abundance indicate that it cannot be its main component.
  - To explain the accelerated expansion rate of the universe, a new kind of energy called *dark energy* is proposed. There is also no candidate for dark energy in the SM. Together, dark energy and dark matter are estimated to account for about 25% and 70% of the matter/energy content of the universe, whereas the SM particles account only for about 5%.
- **Gravity:** The gravitational interaction described by General Relativity (GR) is not included in the SM since a quantization of this theory has not been successfully formulated yet. There are several problems that arise during the quantization of GR, some of them are mild, such as the black hole information paradox [34], whereas others are more fundamental, such as the non-renormalizability of the resulting theories or the conflict between GR and the Heisenberg uncertainty principle at distances smaller than the Planck Length [35].

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<sup>9</sup>These effects include the rotation speed curves of spiral galaxies and the strength of the gravitational lensing of some systems among others





## Chapter 2

# The top quark and its mass

The top quark is a fundamental particle of spin- $\frac{1}{2}$  and charge  $Q = +\frac{2}{3}|e|$  predicted by the SM as the weak isospin partner of the bottom quark, both belonging to the third generation of fermions. The introduction of a third generation of quarks into the SM was proposed by Kobayashi and Maskawa in 1973 [24] in order to explain the CP-violations observed in the decay of neutral mesons, a phenomenon that was observed for the first time in the decay of the neutral K-meson [36]. At that time, the SM framework only included two generations of quarks, the mixing of which is described by a  $2 \times 2$  matrix and parametrized with a single free parameter, the Cabibbo angle. The addition of a third generation of quarks extended the mixing into a  $3 \times 3$  matrix parametrized with four free parameters, which include three angles and a complex phase that could explain the CP-violations. This matrix is called the Cabibbo-Kobayashi-Maskawa (CKM) matrix.

After the discovery of the bottom quark in 1977 by the E288 experiment at Fermilab [37], the search for the top quark intensified. However, its discovery did not happen for almost two decades due to the large value of its mass. During that time, the discovery of the  $W$  and  $Z$  weak bosons and the measurement of their masses [38–41] allowed to constrain the top quark mass in a range between  $113 < m_t < 212$  GeV, under the assumption of a Higgs boson mass of  $m_H = 100$  GeV [42]. The top quark was finally observed in 1995 at the Tevatron in Fermilab by the DØ and CDF collaborations using  $p\bar{p}$  collisions at a center-of-mass energy of 1.8 TeV [43, 44]. The first value they reported for its mass was:

$$\begin{aligned}
m_t &= 199_{-21}^{+19} \text{ (stat.)} \pm 22 \text{ (syst.) GeV} & (\text{D}\bar{\text{O}}), \\
m_t &= 176 \pm 8 \text{ (stat.)} \pm 10 \text{ (syst.) GeV} & (\text{CDF}),
\end{aligned}
\tag{2.1}$$

which makes the top quark the most massive particle in the SM.

In this chapter, a general overview of the physics of the top quark and its phenomenology at the LHC are discussed, with a particular emphasis on the methods used to measure its mass. The sections in this chapter are organized as follows: In Section 2.1, an introduction to the top quark physics is given, which includes a description of its properties (Section 2.1.1), as well as the production and decay modes of this particle (Section 2.1.2). The important role of the top quark mass in proving the consistency of the SM is described in Section 2.2. A comprehensive review of the methods employed to measure the top quark mass is presented in Section 2.3, including a detailed description of the method used in this thesis to measure the top quark pole mass.

## 2.1 The physics of the top quark

### 2.1.1 Top quark properties

#### Top quark mass

The top quark is the most massive elementary particle in the SM, with a mass of the order of  $\sim 170$  GeV. The top quark mass, together with the elements of the CKM mixing matrix, is the only free parameter of the top quark sector of the SM. Therefore, it cannot be calculated from first principles and has to be determined experimentally.

The top quark mass has been measured at the Tevatron and in the LHC experiments using several direct and indirect methods. A detailed discussion of these measurements can be found in Section 2.3. The value of the top quark mass from direct measurements ( $m_t^{\text{MC}}$ ), as extracted from the LHC Run 1 combination of direct measurements [45], is shown in Equation 2.2, while the combined value of the top quark mass from indirect measurements ( $m_t^{\text{pole}}$ ), as reported in Ref. [4], is shown in Equation 2.3.

$$m_t^{\text{MC}} = 172.52 \pm 0.33 \text{ GeV} \quad (\text{direct measurements}) \quad (2.2)$$

$$m_t^{\text{pole}} = 172.5 \pm 0.7 \text{ GeV} \quad (\text{indirect measurements}) \quad (2.3)$$

Due to its large mass, the top quark has the strongest coupling to the Higgs field ( $y_t \sim 1$ ), which makes the study of its properties essential to the understanding of the electroweak sector and to the search of physics beyond the SM (BSM).

### Top quark width

The decay width ( $\Gamma$ ) of a particle encodes the probability of a heavy particle to decay into multiple other lighter particles. At LO in perturbation theory, the top quark can decay via the electroweak interaction into a  $W$  boson and a down-type quark (more details in Section 2.1.2). The total decay width of the top quark ( $\Gamma_t$ ) is obtained by adding the partial decay widths of all possible decay channels of this particle:

$$\Gamma_t = \sum_q \Gamma(t \rightarrow Wq), \quad q = d, s, b. \quad (2.4)$$

Each partial decay width can be computed in the SM at LO, assuming  $m_q = 0$  for  $q = d, s, b$ , using the following equation [46]:

$$\Gamma(t \rightarrow Wq) = \frac{G_F}{8\pi\sqrt{2}} m_t^3 |V_{tq}|^2 \left( 1 - 3 \left( \frac{m_W}{m_t} \right)^4 + 2 \left( \frac{m_W}{m_t} \right)^6 \right), \quad (2.5)$$

where  $G_F$  is the Fermi constant. Equation 2.5 shows that the partial decay width is proportional to the squared value of the corresponding CKM mixing matrix element,  $|V_{tq}|^2$ , and the total decay width is proportional to the third power of the top quark mass,  $m_t^3$ . As the top quark has an extremely high mass, its associated decay width is expected to be also relatively large.

The value of the total top quark width, as reported by the CMS collaboration in Ref. [47], is:

$$\Gamma_t = 1.36 \pm 0.02 \text{ (stat.)}_{-0.11}^{+0.14} \text{ (syst.) GeV} \quad (2.6)$$

Since the lifetime of an unstable particle is given by the inverse of its total decay width, the top quark has an extremely short lifetime of  $\tau_t = 1/\Gamma_t \sim 0.5 \times 10^{-24}$  s, which is smaller than the hadronization time-scale ( $\tau_{\text{QCD}} \sim 1/\Lambda_{\text{QCD}} \sim 10^{-23} - 10^{-24}$  s). This short lifetime inhibits the formation of bound states involving top quarks, as they decay before undergoing the hadronization process, granting the unique opportunity to study the properties of a quark free of confinement effects, a quasi-free (bare) quark. One of the properties that can be measured thanks to this unique property is the top quark polarization, since the spin information of the top quark is carried by its decay products without being diluted by the hadronization process.

### Top quark charge

The electric charge of the top quark is predicted by the SM to be  $Q_t = +\frac{2}{3}|e|$ . However, there are some theoretical models that predict the existence of *exotic* quarks with charge  $-\frac{4}{3}|e|$  [48]. To ensure that the particle that is identified today as the SM top quark is not, indeed, one of these exotic particles, the value of the top quark charge has to be determined. The charge of this particle can be determined experimentally by studying the  $t - \gamma$  interaction vertex or the charge of top quark decay products.

To evaluate the strength of the  $t - \gamma$  interaction vertex, which is proportional to the top quark charge ( $Q_t$ ), one can study the cross sections of processes such as  $t\bar{t}\gamma$  and  $t\gamma q$ . Although these cross sections have been measured at the LHC [49–51], no attempt has been made to interpret the results in terms of the  $t - \gamma$  vertex. This is because the photon in the final state can originate from other electrically charged particles besides the top quark, which complicates the analysis and its interpretation.

Alternatively,  $Q_t$  can be determined from the study of the decay products of the top quark. In the leptonic decay of this particle ( $t \rightarrow Wb \rightarrow l\nu b$ ), the charge of the lepton can be determined easily, but the charge of the b quark can not be measured directly due to the confinement property of QCD. Instead, the charge of this quark is estimated from the correlation that exists between the charges of

the hadrons inside a jet, and the charge of the quark which originated it. The value of the top quark charge obtained by the ATLAS collaboration using this method is [52]:

$$Q_t = 0.64 \pm 0.02 \text{ (stat.)} \pm 0.08 \text{ (syst.)} , \quad (2.7)$$

which is compatible with the SM prediction of  $Q = +\frac{2}{3}|e|$  and excludes the possibility of this particle being an exotic quark with charge  $\pm\frac{4}{3}|e|$ .

### Top quark spin

Since the top quark decays via the weak interaction before hadronizing, its spin information is carried by its decay products. Therefore, the SM assumption that the top quark is a spin- $\frac{1}{2}$  particle can be proven by studying the angular distributions between its decay products.

In the SM, the  $W$  boson originated from the top quark decay is always produced in one of the three possible polarization states: longitudinal, left-handed, or right-handed. The fractions of  $W$  bosons produced in each state<sup>1</sup> are denoted as  $F_0$ ,  $F_L$ , and  $F_R$ , respectively. These fractions are predicted in the SM at NNLO as [53]:

$$F_0 = 0.687 \pm 0.005, \quad F_L = 0.311 \pm 0.005, \quad F_R = 0.0017 \pm 0.0001, \quad (2.8)$$

and can also be determined experimentally from the distribution of the  $\theta^*$  angle, the angle between the charged lepton in the  $W$  boson rest frame, and the  $W$  boson in the top quark rest frame [54]. The observable that is typically used to measure the helicity fractions is the differential normalized cross section as a function of  $\cos \theta^*$ , which can be written in terms of the helicity fractions as [55]:

$$\frac{1}{\sigma} \frac{d\sigma}{d\cos \theta^*} = \frac{3}{4}(1 - \cos^2 \theta^*)F_0 + \frac{3}{8}(1 - \cos \theta^*)^2 F_L + \frac{3}{8}(1 + \cos \theta^*)^2 F_R, \quad (2.9)$$

---

<sup>1</sup>Also known as *helicity fractions*

Alternatively, the helicity fractions can be computed indirectly from their relation with the angular asymmetries  $A_{\pm}$  (see Ref [56]), which are defined as:

$$A_{\pm} = \frac{N(\cos \theta^* > z) - N(\cos \theta^* < z)}{N(\cos \theta^* > z) + N(\cos \theta^* < z)}, \quad (2.10)$$

where  $z = \pm(1 - 2^{2/3})$  for  $A_{\pm}$ . The definition of the asymmetry in terms of  $z$  allows for the cancellation of the  $F_L$  and  $F_R$  dependence in  $A_+$  and  $A_-$ , respectively.

A summary of the ATLAS measurements regarding the  $W$  helicity can be found in Figure 2.1. The experimental measurements are in agreement with the SM prediction, supporting the hypothesis that the top quark is, indeed, a spin- $\frac{1}{2}$  particle, as it is assumed in the SM.

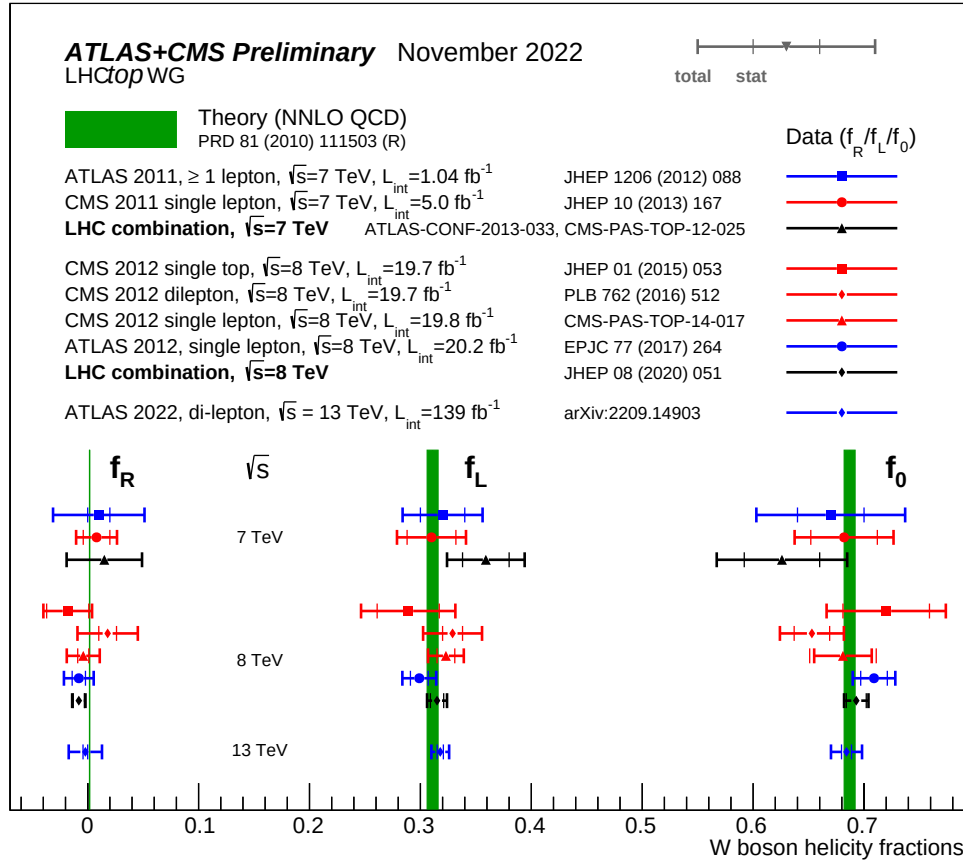


Figure 2.1: Overview of the ATLAS measurements of the  $W$  boson helicity fractions compared with the SM prediction [57].

### 2.1.2 Top quark production and decay

#### Top quark production

At the LHC, top quarks are produced predominantly in quark-antiquark pairs ( $t\bar{t}$  production) via the strong interaction, or as single top quarks (single- $t$  production) via the electroweak interaction. Combinations of these processes such as three- and four-top production are also possible within the SM. Indeed, the four-top production was observed for the first time in 2023 by the ATLAS and CMS collaborations [58, 59]. Additionally,  $t\bar{t}$  pairs and single-top quarks can be produced in association with other particles such as a  $W$ ,  $Z$ , or Higgs boson, or a photon.

In the case of top-pair production ( $p\bar{p} \rightarrow t\bar{t}$ ), there are two processes that contribute at leading order (LO) in QCD, the gluon fusion ( $gg \rightarrow t\bar{t}$ ) and the quark-antiquark annihilation ( $q\bar{q} \rightarrow t\bar{t}$ ), which are represented by the Feynman diagrams shown in Figure 2.2.

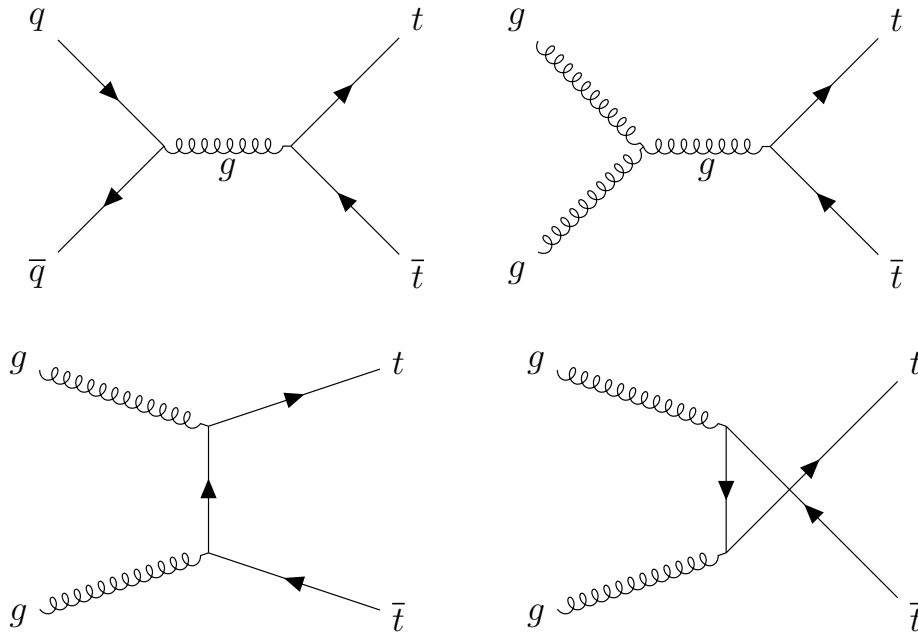


Figure 2.2: Leading order Feynman diagrams for the top quark pair production at the LHC via quark-antiquark annihilation and gluon fusion.

The relative contribution of each process to the total  $t\bar{t}$  cross section depends on the colliding objects and on their energy. In  $pp$  collisions at a center-of-mass energy of  $\sqrt{s} = 13$  TeV, due to the composition of the Parton Density Functions

(PDFs) at this energy, the gluon fusion accounts for approximately 90% of the events, while the  $q\bar{q}$  accounts for approximately 10% of the events.

The most precise theoretical calculations of the  $t\bar{t}$  inclusive and differential cross sections to date are computed at next-to-next-to-leading order (NNLO) in QCD, including the next-to-next-to-leading resummation of the logarithmic soft-gluon terms (NNLL) using the TOP++2.0 program [60–66], and assuming a top quark mass of 172.5 GeV. Fully differential QCD predictions for the top quark pair production have been calculated at NNLO in QCD [67] and implemented in the **Matrix** framework [68]. The uncertainties associated with these calculations originate from the variation of the factorization and renormalization scales ( $\mu_F$  and  $\mu_R$ ), the uncertainty associated with the proton parton density function (PDFs), and the value of the strong coupling constant ( $\alpha_S$ ). The inclusive  $t\bar{t}$  cross sections measured at the LHC and Tevatron are found to be compatible with the theoretical predictions, as shown in Figure 2.3.

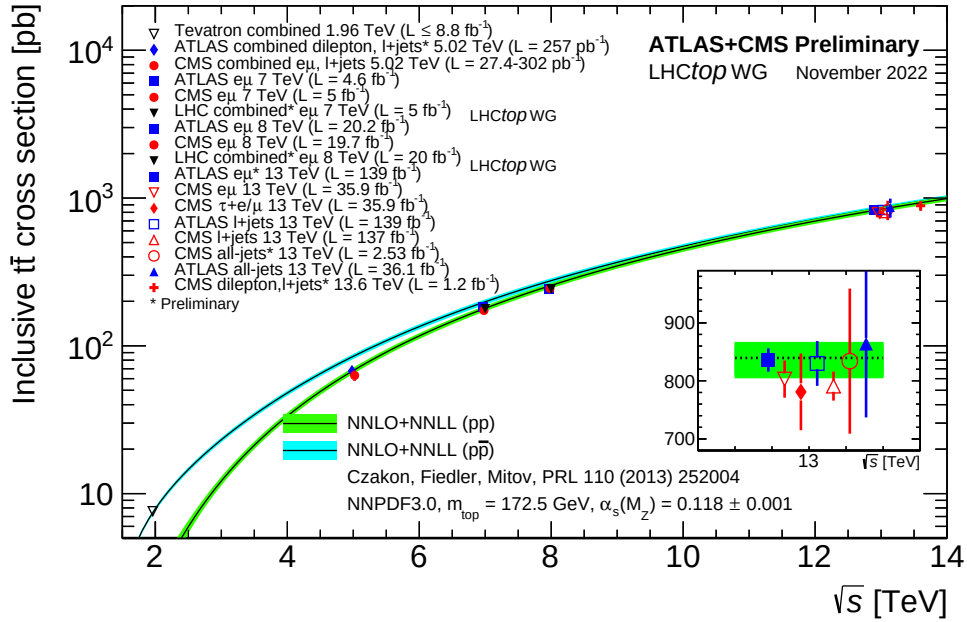


Figure 2.3: Summary of the LHC and Tevatron measurements for the top quark pair production cross section as a function of the center-of-mass energy of the system. The results are compared with the theoretical predictions computed using the TOP++2.0 program. The figure is taken from [57].



## Top quark decay

Due to its extremely short mean lifetime, the top quark can only be experimentally observed via its decay products. In the SM, top quarks decay via the weak interaction into a  $W$  boson and a down-type quark,  $t \rightarrow W^+q$  ( $\bar{t} \rightarrow W^-\bar{q}$ ), with  $q = d, s, b$ . The branching ratio for the different flavors of the produced quarks are governed by the  $V_{td}$ ,  $V_{ts}$ ,  $V_{tb}$  elements of the CKM matrix ( $V_{CKM}$ ). The magnitude of the parameters of the CKM matrix are obtained from a global fit to all available measurements, assuming the existence of only three quark generations and the unitarity of the matrix [69]:

$$V_{CKM} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \approx \begin{pmatrix} 0.974 & 0.227 & 0.004 \\ 0.226 & 0.973 & 0.041 \\ 0.009 & 0.040 & 0.999 \end{pmatrix}. \quad (2.11)$$

The branching ratio of each of the top quark decay channels in the SM can be calculated from the partial decay widths in Equation 2.5, following the equation:

$$BR(t \rightarrow Wq) = \frac{\Gamma(t \rightarrow Wq)}{\Gamma_t} = \frac{|V_{tq}|^2}{|V_{td}|^2 + |V_{ts}|^2 + |V_{tb}|^2}, \text{ with } q = d, s, b. \quad (2.12)$$

The  $W$  boson has a global measured decay width of  $\Gamma_W = 2.046 \pm 0.049$  GeV [70], so it can only be studied via its decay products. At LO, the  $W$  boson can decay leptonically into a charged lepton and its corresponding neutrino, or hadronically into a quark and an antiquark pair of different types (up-/down-), which produce two jets in the detector. The corresponding branching ratios are  $BR(W \rightarrow q\bar{q}') \approx 67.4\%$ , and  $BR(W^\pm \rightarrow l^\pm \nu) \approx 32.6\%$ , respectively [4], reflect the distribution of available decay modes for each type..

Based on the decays of the  $W$  bosons originated from the individual top (anti)quark, the experimental signature expected from top quark pair events can be classified into three channels:

- **Full-hadronic** channel: Both  $W$  bosons originated from the  $t\bar{t}$  system decay hadronically into quarks,  $t\bar{t} \rightarrow W^+bW^-\bar{b} \rightarrow b\bar{b}q\bar{q}'q''\bar{q}'''$ . The experimental

signature produced by the events in this channel consists of four jets originated from the light quarks from the  $W$  bosons, and two jets originated from the  $b$  quarks. While this decay channel has the highest branching ratio ( $BR(t\bar{t} \rightarrow \text{jets}) \approx 46\%$ ), its signal is not easily distinguishable from the large QCD multijet background, leading to a lower signal-to-background ratio when compared to the other channels. Moreover, since jets have a lower energy resolution than charged leptons and this decay channel has more jets in the final state than the others, the observables constructed in this channel such as invariant masses are affected by poor resolution and large systematic uncertainties. Additionally, matching the reconstructed jets to the partons from the  $t\bar{t}$  decay from which they originated is a challenging task due to the combinatorial complexity of the problem.

- **Dileptonic** channel: Both  $W$  bosons decay leptonically into a charged lepton and its corresponding neutrino,  $t\bar{t} \rightarrow W^+bW^-\bar{b} \rightarrow b\bar{b}l^+\nu_l l'^-\bar{\nu}_{l'}$ . The typical experimental signature of these events consists of two jets that originate from the  $b$  quarks, two high  $p_T$  leptons with opposite charges, and a considerable amount of missing transverse energy due to the non-detected neutrinos. While this channel has the lowest branching ratio ( $BR(t\bar{t} \rightarrow \text{dilepton}) \approx 9\%$ ), it has a very distinguishable signal, leading to the highest signal-to-background ratio among the  $t\bar{t}$  decay channels. Since the events in this channel have only two jets, the observables constructed in this channel have a reduced uncertainty originating from the jet kinematics reconstruction. Nevertheless, this channel presents a limited reconstruction efficiency since the system with two undetected neutrinos leads to an under-constrained equation system in the reconstruction of the  $t\bar{t}$  kinematics, unless a value of the top quark mass is assumed.
- **Semileptonic** channel: One of the  $W$  bosons decays hadronically into quarks, while the other decays leptonically into a charged lepton and its corresponding neutrino,  $t\bar{t} \rightarrow W^+bW^-\bar{b} \rightarrow bq\bar{q}'b l\nu_l$ . The typical experimental signature of these events consists of two jets originated from the light quarks from the hadronically decaying  $W$  boson, two jets originated from the  $b$  quarks, one high  $p_T$  lepton, and a considerable amount of missing transverse energy due to the undetected neutrino. This channel has a branching ratio larger than the one of the dileptonic channel ( $BR(t\bar{t} \rightarrow l + \text{jets}) \approx 45\%$ ), while having a higher signal-to-background ratio than the full-hadronic

channel, which provides a balance between signal-to-background ratio and large statistics. As the amount of collected data by the LHC increases, the large branching ratio of the semileptonic channel with respect to the dileptonic channel becomes less relevant. Nevertheless, as the final state in the semileptonic channel only contains one neutrino, the reconstruction of the  $t\bar{t}$  kinematics is usually better than in the dileptonic channel.

The  $t\bar{t}$  decay rates are graphically represented in Figure 2.4. In the final states of both the semileptonic and dileptonic channels, the charged leptons produced can be tau leptons, which have a lifetime of  $\tau_\tau \sim 2.9 \times 10^{-13}$  s, hence they decay before interacting with the detector and can only be observed via their decay products. Each tau lepton can decay into a tau neutrino and one or more hadrons, or into two neutrinos and either an electron or a muon, with branching ratios of  $BR(\tau \rightarrow \nu_\tau + \text{hadrons}) \approx 66\%$ ,  $BR(\tau \rightarrow e\nu_e\nu_\tau) \approx 17\%$ , and  $BR(\tau \rightarrow \mu\nu_\mu\nu_\tau) \approx 17\%$ , respectively. The identification of tau leptons in the detector is rather complex, so typically only electrons and muons are considered in the analyses. However, these particles can also originate from the leptonic decays of tau leptons if they satisfy the required selection criteria.

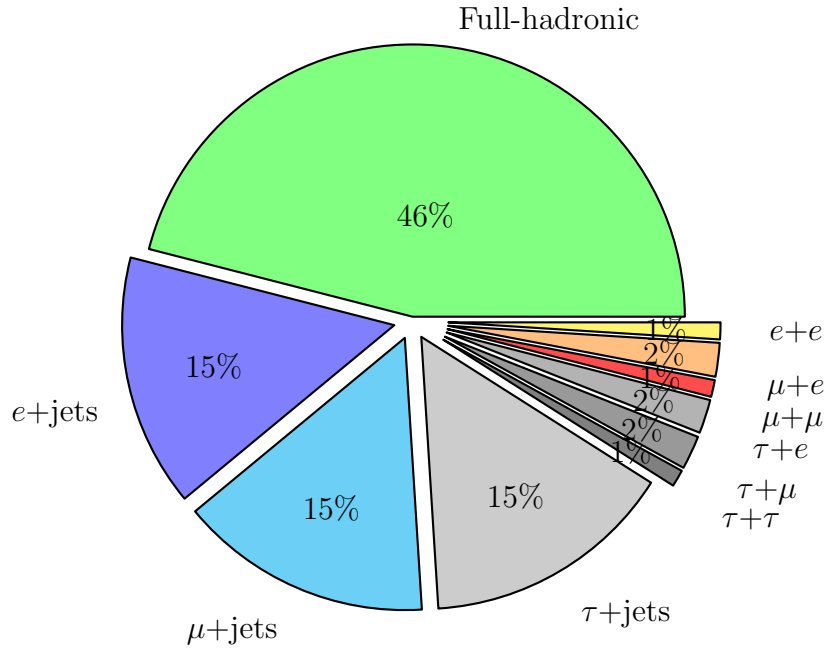


Figure 2.4: Graphical representation of the top quark pair branching ratios depending on the  $W$  bosons decay channels. The final states containing  $\tau$  leptons are shown in different grey tonalities to indicate that they are rarely used in analyses.

## 2.2 Testing the Standard Model consistency using the top quark mass

The top quark, due to its associated Yukawa coupling being close to unity ( $y_t \sim 1$ ), plays a special role in the SM, as well as in several new BSM scenarios. In particular, the SM makes a series of predictions that relate the top quark mass with other parameters of the theory allowing for the realization of several consistency tests of the theory.

### Stability of the Standard Model electroweak vacuum

Beyond LO in perturbation theory, the Higgs boson propagator is affected by large corrections due to the top quark mass. These corrections enter through loop diagrams like the one shown in Figure 2.5, which depends quadratically on the top quark Yukawa coupling, and consequently, on  $m_t$ .

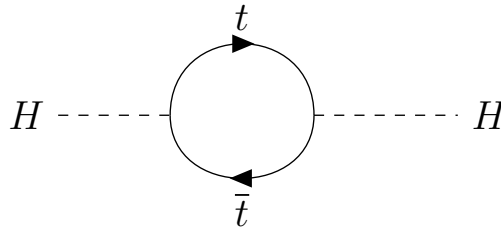


Figure 2.5: Feynman diagram for the one-loop correction to the Higgs boson propagator containing top quarks.

These kind of contributions modify the value of the Higgs mass, and therefore also modify the value of the  $\mu^2$  parameter of the Higgs potential. The other parameter that determines the structure of this potential,  $\lambda$ , is also modified by similar loop corrections that also involve top quarks. As a consequence, the shape of the Higgs potential depends on the top quark mass, as well as on the strong coupling constant ( $\alpha_S$ ), and the Higgs mass ( $M_h$ ), resulting in three possible stability scenarios for the SM electroweak vacuum state: stable, meta-stable, or unstable. These scenarios are schematically represented in Figure 2.6 and can be defined as follows:

- **Stable:** The electroweak vacuum is the absolute minimum of the potential.

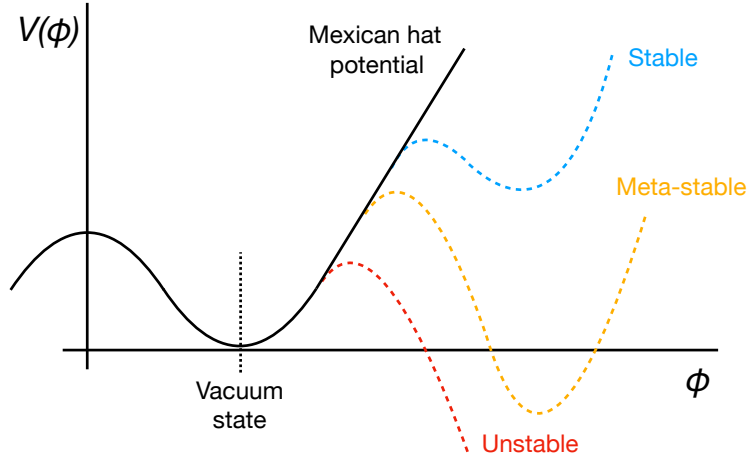


Figure 2.6: Schematic representation of the Higgs potential with the classical *Mexican hat* configuration. Beyond LO in perturbation theory, the higher-order corrections deform the shape of this potential leading to a potential that can be stable, meta-stable, or unstable with respect to the original vacuum state of the system. These three states are represented by the blue, orange, and red dashed lines, respectively.

- Meta-stable: The electroweak vacuum is not the absolute minimum of the potential, but its lifetime is longer than the age of the Universe.
- Unstable: The electroweak vacuum is not the absolute minimum of the potential and its lifetime is shorter than the age of the Universe. Alternatively, the  $\lambda$  parameter of the Higgs potential can be negative leading to a potential with no absolute minimum.

In Figure 2.7, the running of the quadratic coupling parameter ( $\lambda$ ) of the Higgs potential as a function of the energy scale is shown. At high energy scales, the sign of the  $\lambda$  parameter (which is responsible of the stability of the EW vacuum) depends greatly on the value of the top quark mass.

Figure 2.8 displays the phase diagram of the electroweak vacuum in terms of the values of the top quark mass ( $m_t$ ) and the Higgs boson mass ( $M_h$ ). The current  $m_t$  and  $M_h$  measurements lie in the meta-stable region of the diagram, however, with the current precision in the determination of these parameters, only the unstable vacuum hypothesis can be excluded. To confidently distinguish between the stability and meta-stability hypothesis, a more precise determination of the top quark mass is needed.

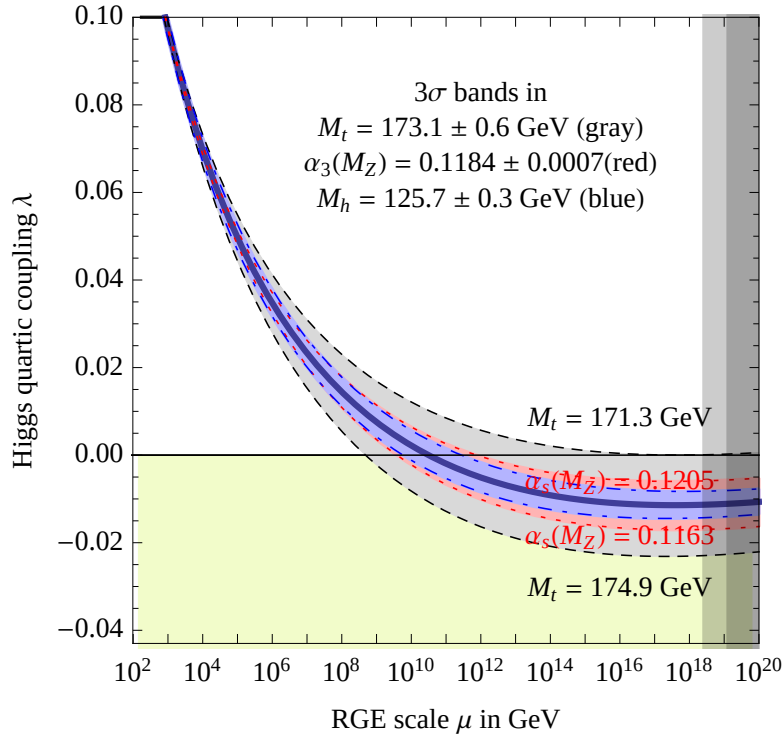


Figure 2.7: Evolution of the quadratic coupling  $\lambda$  as a function of the scale  $\mu$ . The red and blue dashed lines cover the three standard variation contours associated with the  $m_t$  and  $\alpha_s$  values, respectively. Figure taken from [71].

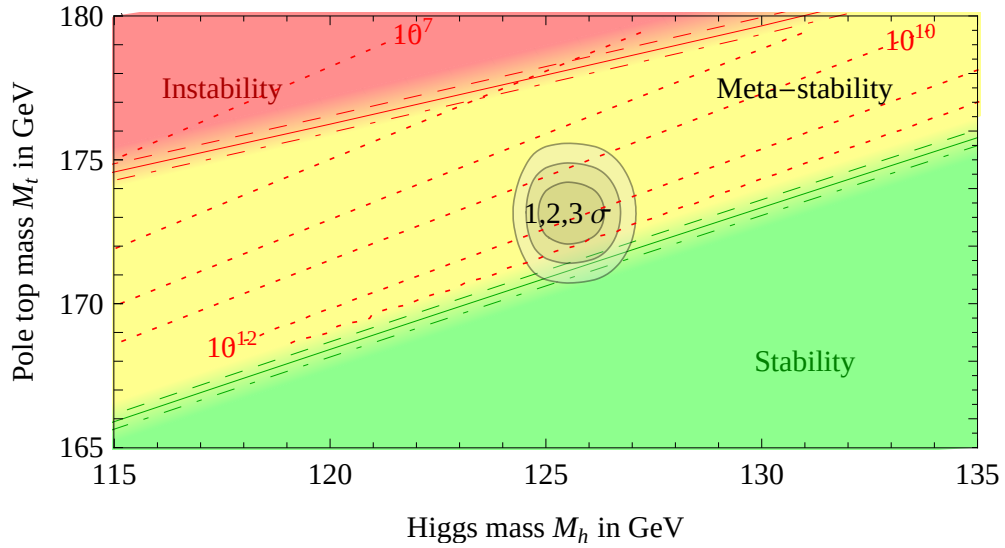


Figure 2.8: Phase diagram of the EW vacuum stability as a function of the top quark and Higgs boson masses. Figure taken from [71].

### Electroweak global fit and the compatibility of the top, Higgs, and $W$ boson mass measurements

The radiative corrections introduced through loop diagrams do not only establish a relation between the Higgs boson mass and the top quark mass, but also establish relations between many other free parameters of the SM.

The use of the relations predicted by these radiative corrections, in combination with precise measurements of many parameters in the electroweak theory, can be used to evaluate the value of unmeasured or poorly measured parameters of the model in what is known as a *global electroweak fit*. Additionally, if all the parameters are measured with a good level of precision, the global electroweak fit can be used to check the self-consistency of the model by comparing the predicted value of a parameter, considering all other measurements in the theory, with the experimentally measured value of the parameter.

Some representative Feynman diagrams involving top and Higgs boson loops that contribute to the radiative corrections to the  $W$  boson propagator are illustrated in Figure 2.9. After the  $Z$  boson mass and the value of the  $\theta_W$  angle are fixed to their very precisely measured values, the global electroweak fit predicts a direct dependence between the masses of the top quark, Higgs boson, and  $W$  boson.

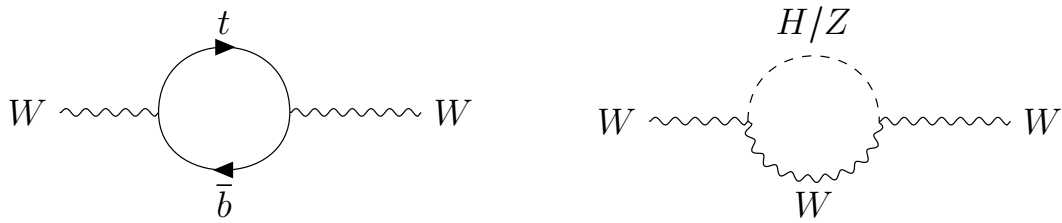


Figure 2.9: Feynman diagrams exemplifying one-loop radiative corrections to the  $W$  boson propagator involving top quarks and Higgs bosons.

Before the discovery of the Higgs boson by the ATLAS and CMS collaborations, the relation between the Higgs, top, and  $W$  masses predicted by the electroweak global fit was used to provide constraints on the possible values of the Higgs boson mass. After the discovery of the Higgs, the relation predicted by this fit is used to test the self-consistency of theory [72], as shown in Figure 2.10.

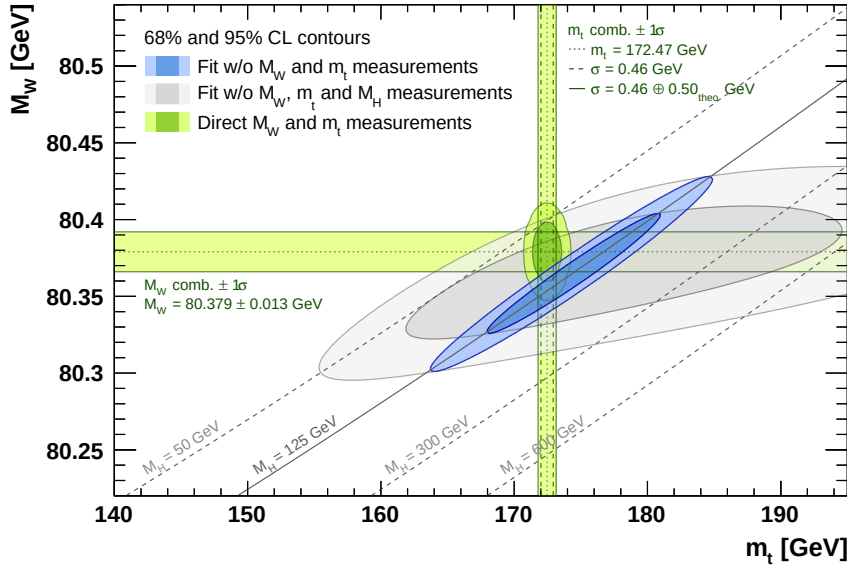


Figure 2.10: Electroweak global fit scan of the  $W$  boson mass ( $M_W$ ) as a function of the top quark mass ( $m_t$ ), displayed with the associated 68 and 95% confidence level contours. The blue (grey) region shows the fit results when the Higgs mass measurement is included (excluded) from the fit. For comparison, the direct measurements of  $m_t$  and  $M_W$ , which are not included in the global fit, are shown in the vertical and horizontal green bars, respectively. Figure from Ref [73].

With the experimental measurements for the top quark and  $W$  boson masses plotted in Figure 2.10, the SM is self-consistent. However, in April 2022, the CDF collaboration reported an extremely precise  $W$  boson mass measurement of  $M_W = 80433.5 \pm 9.4 \text{ MeV}$  [8]. If confirmed by other experiments, this would indicate a failure in the SM consistency test, suggesting the existence of BSM physics.

This hint of physics BSM has led to an ongoing discussion within the particle physics community [74, 75] as the CDF measurement disagrees with previous measurements on the  $W$  boson mass from the DØ and ATLAS experiments [76, 77]. Moreover, in March 2023, the ATLAS collaboration published an improved version of the  $W$  boson mass measurement in Ref. [77], resulting in a value of  $M_W = 80360 \pm 16 \text{ MeV}$  [78], which is consistent with the SM expectation. This latest result has eased the tension caused by the CDF measurement, but further theoretical studies and experimental measurements are required to resolve this issue.



## 2.3 Top quark mass measurements

Physics analyses that seek to determine the top quark mass can be classified into two categories, depending on the strategy adopted to measure this parameter. These two categories are known as *direct measurements* and *indirect measurements*, and they are described in the following sections.

### 2.3.1 Direct measurements

Direct measurements of the top quark mass are based on the reconstruction of the kinematic properties of the final-state decay products of the top quark, from which observables sensitive to the top quark mass are derived. The value of the top quark mass is then extracted from data by comparing the reconstructed distributions of these observables with the distributions predicted by multipurpose Monte Carlo event generators [79, 80], with varied input values of the top quark mass parameter in the generator [81]. Since the parameter extracted from the fit to data is the top quark mass parameter in the MC generator, the resulting mass is commonly referred to as the top quark Monte Carlo mass parameter ( $m_t^{\text{MC}}$ ).

The MC generators used to produce the predictions are not purely based on perturbative QCD. While the NLO Matrix Element implemented in the generator adopts the pole mass scheme, these generators also rely on parton shower models and heuristic models to describe the non-perturbative QCD effects, such as the parton shower, the underlying event, the hadronization process, and the Color Reconnection<sup>2</sup>. These effects may alter the mass definition in subtle ways, complicating the identification of the MC mass parameter with the pole mass. In particular, the parton-shower cut-off scale has been shown to modify the mass definition in around 0.5 GeV [83]. Several other studies have also investigated this relation [84–88], suggesting that the top quark mass parameter in the simulation can be related with the top quark pole mass parameter with an additional uncertainty of the order of  $\sim 0.5\text{--}1$  GeV, depending on the observable under study. This additional theoretical uncertainty is not usually reported in the direct top quark mass measurements.

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<sup>2</sup>The Color Reconnection (CR) defines how the color strings form between the final partons before the hadronization process occurs. This process produces flow-like patterns that connect the partons produced during the collision, including the ones originated from multiple parton interactions as well as the beam remnants. However, the CR phenomena is not well-defined, therefore, several models have been developed to describe it [82].

A summary of the ATLAS and CMS direct measurements of the top quark mass is presented in Figure 2.11. The world average for  $m_t^{\text{MC}}$ , as well as some individual measurements, have achieved an astonishing level of precision of  $\sim 0.4$  GeV. This degree of precision corresponds to a 0.2% relative precision, which makes the top quark mass the most precisely known parameter in the QCD sector of the SM.

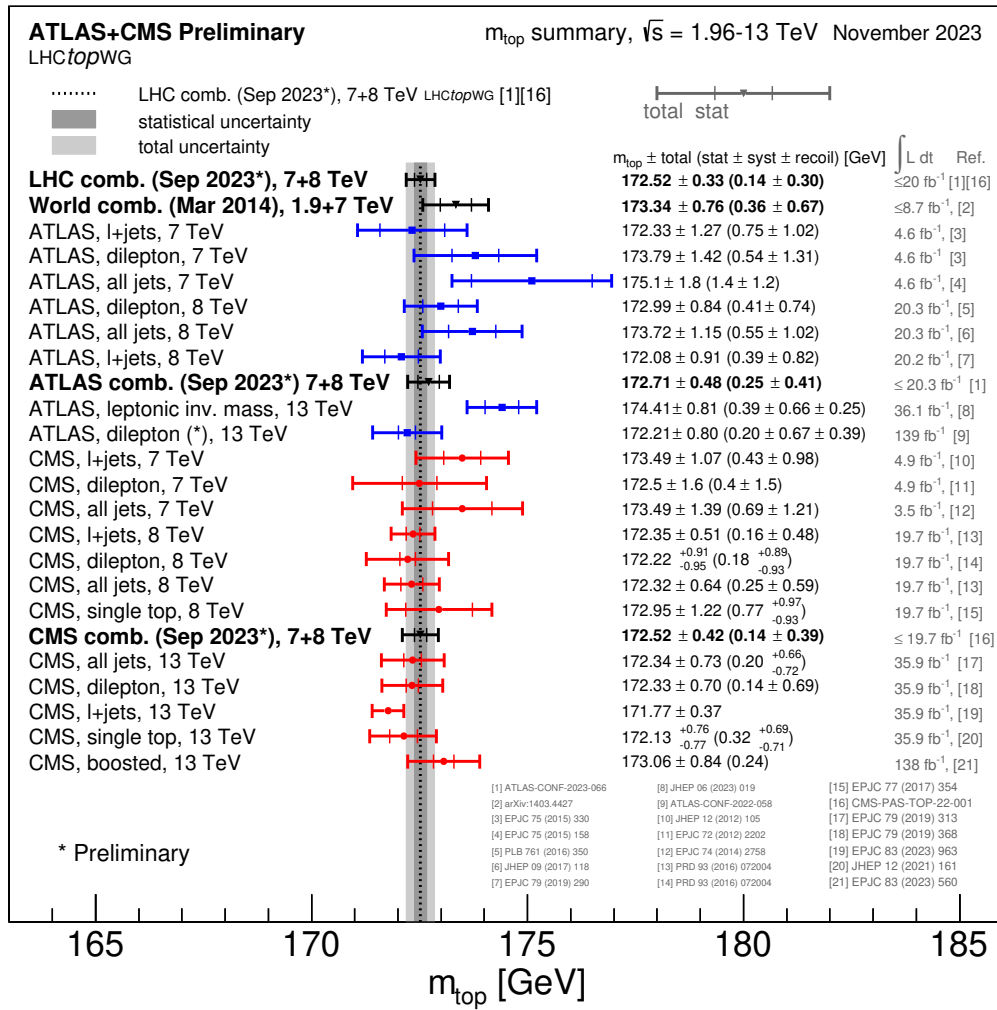


Figure 2.11: Summary of the direct top quark mass measurements published by the ATLAS and CMS collaborations. The results are compared with the 2014 world combination, which included all available Tevatron and LHC measurements at that time. The figure is taken from [57].

The measurements of Figure 2.11 have been performed in various event topologies, which include: the three decay channels of the  $t\bar{t}$  system, the boosted<sup>3</sup>

<sup>3</sup>A particle is considered *boosted* when it has a high momentum compared to its mass.

regime of the top quark decay in semileptonic  $t\bar{t}$  decays, and single-top event topologies. Depending on the topologies of the events being studied, different observables sensitive to the top quark mass can be reconstructed and used to measure  $m_t^{\text{MC}}$ . Some of these observables are described here below, with a particular emphasis on the  $M_{lb}$  observable, as it is the one used in this thesis to constrain and measure  $m_t^{\text{MC}}$  in the control regions of the analysis introduced in Chapter 5.

In the scope of this thesis, the top quark MC mass parameter is determined in the semileptonic decay channel of the  $t\bar{t}$  system by reconstructing, in several control regions of the analysis, the invariant mass of the lepton and the  $b$ -jet associated with the semileptonically decaying top quark, the  $M_{lb}$  observable. This observable is commonly used in the direct top quark mass measurements in the semileptonic and dileptonic decay channels of the  $t\bar{t}$  system because it has a high sensitivity to the top quark mass, without relying on the reconstruction of the four-momenta of the undetected neutrino. Figure 2.12 shows an example of the distribution of the  $M_{lb}$  observable in dileptonic  $t\bar{t}$  events, clearly demonstrating the high sensitivity of the observable to the top quark mass.

### 2.3.2 Indirect measurements: top quark mass determination from inclusive and differential cross sections

Indirect measurements of the top quark mass are based on observables that are sensitive to the top quark mass, but for which it is possible to calculate the associated distributions in a well-defined renormalization scheme, such as the pole or  $\overline{MS}$  scheme. To extract the top quark mass, the fixed-order theoretical predictions are computed for these observables across various values of the top quark mass and then compared with the corresponding data from the measurements. Inclusive and differential cross sections are typically used for these measurements, as they can be directly calculated using perturbative QCD. As these distributions are computed from first principles, the interpretation of the top quark mass as the associated parameter in the SM Lagrangian is more clear.

A summary of the ATLAS and CMS measurements based on cross section in the pole mass renormalization scheme is presented in Figure 2.13. The world average, as well as some individual measurements, have achieved a precision under

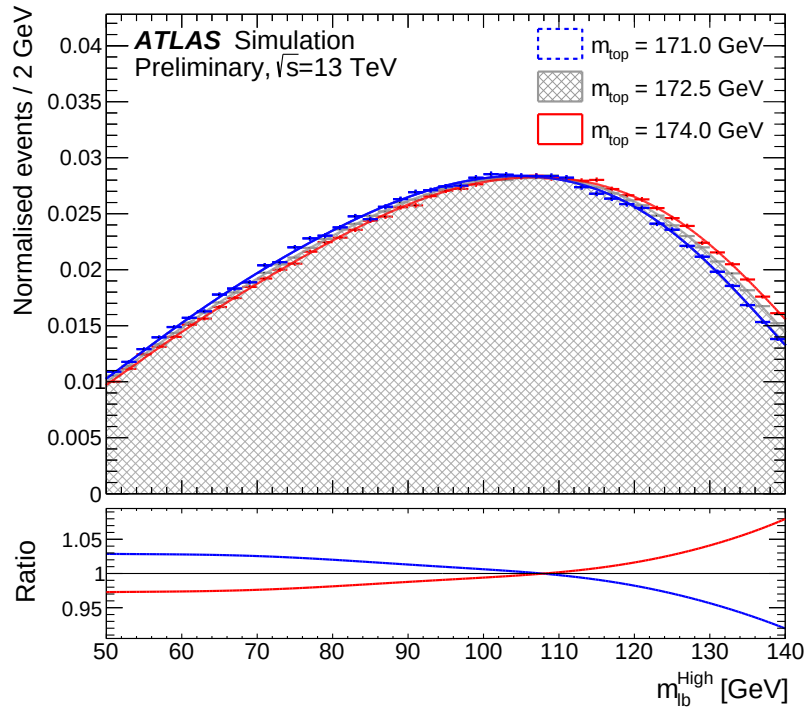


Figure 2.12: Simulated distributions of the  $m_{lb}^{\text{High}}$  observable for three different top quark mass values. These simulations are produced reproducing the conditions of the data collected by the ATLAS detector at 13 TeV. As this observable is reconstructed in the dileptonic decay channel, only the  $m_{lb}$  with the highest  $b$ -tagged jet  $p_T$  is used ( $m_{lb}^{\text{High}}$ ). Figure taken from Ref. [81].

1 GeV. The uncertainty associated with these measurements is, in general, larger than those associated with direct measurements.

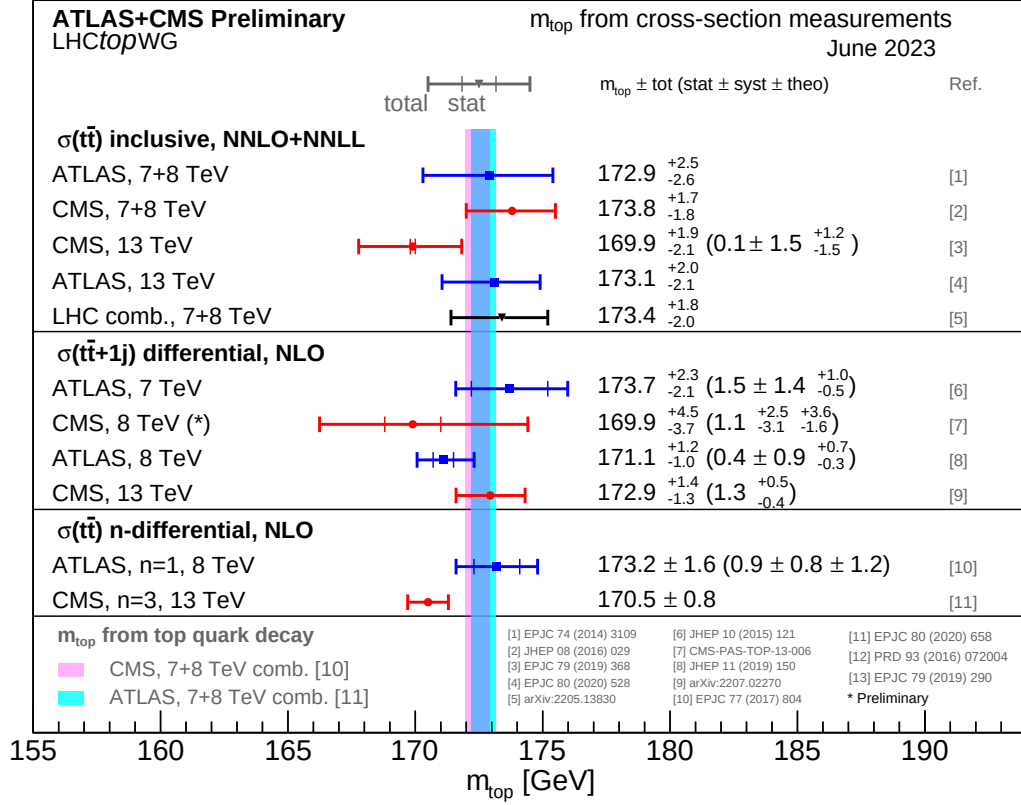


Figure 2.13: Summary of the top quark pole mass measurements published by the ATLAS and CMS collaborations. These values have been determined by fitting cross section measurements to various QCD theoretical predictions. The figure is taken from [57].

The results of the measurements shown in Figure 2.13 were obtained using several different observables that are sensitive to the top quark mass, which include the inclusive cross section of a top-pair,  $\sigma_{t\bar{t}}$ , the n-differential cross section of this production, and the differential cross section of top quark pair produced in association with at least one energetic jet,  $t\bar{t} + \text{jet}$ . Since this last method is the one used in this thesis to measure the top quark pole mass using the 13 TeV data collected by the ATLAS detector, it is described in more detail in the following Section 2.3.3.

### 2.3.3 Top quark pole mass measurements from $t\bar{t}$ +jet topologies

The method used to extract the top quark pole mass in this thesis was proposed for the first time in Ref. [89]. This method exploits the sensitivity to the top quark mass of the differential cross section of the  $t\bar{t}$  production in association with at least one energetic jet ( $\sigma_{t\bar{t}+\text{jet}}$ ) [90, 91]. In the Born approximation, the partonic reactions that lead to the  $t\bar{t}$  +jet final state are:

$$gg \rightarrow t\bar{t}g, \quad q\bar{q} \rightarrow t\bar{t}g, \quad qg \rightarrow t\bar{t}q, \quad \bar{q}g \rightarrow t\bar{t}\bar{q}, \quad (2.13)$$

where the last three are related by crossing symmetries, reducing the number of matrix elements that need to be computed. In Figure 2.14, a set of representative LO Feynman diagrams for the  $t\bar{t}$  +jet production via gluon fusion and quark-antiquark annihilation are depicted. There are a total of 16 LO diagrams for the generic matrix elements  $0 \rightarrow t\bar{t}ggg$  and 5 for the  $0 \rightarrow t\bar{t}q\bar{q}g$  [92].

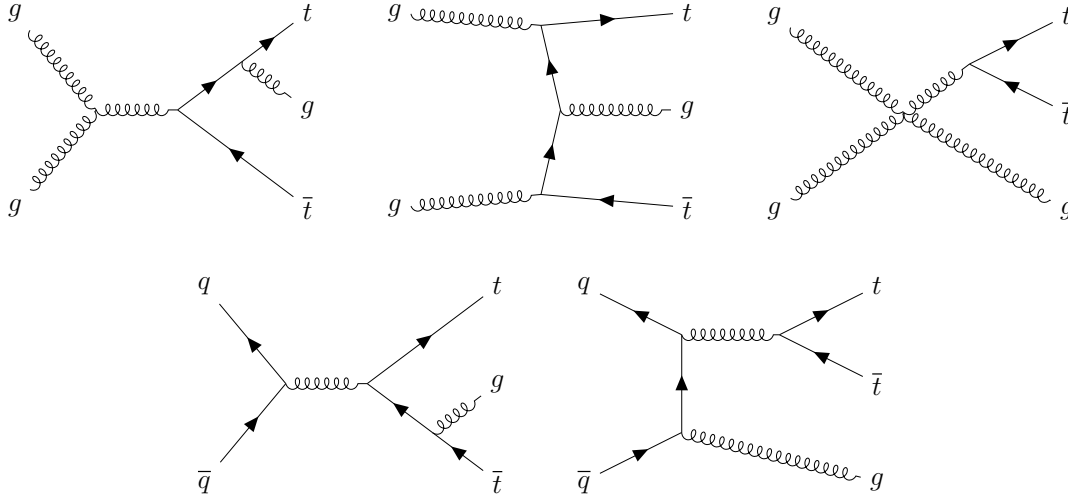


Figure 2.14: Representative LO Feynman diagrams for the  $t\bar{t}$  +jet production at the LHC via gluon fusion (top) and quark-antiquark annihilation (bottom).

Utilizing  $t\bar{t}$  +jet event topologies, the authors of Ref. [89] introduced the following observable, which is defined as the normalized differential cross section of  $t\bar{t}$  +jet events, as a function of the  $\rho_s$  variable:

$$\mathcal{R}(m_t^{\text{pole}}, \rho_s) = \frac{1}{\sigma_{t\bar{t}+\text{jet}}} \frac{d\sigma_{t\bar{t}+\text{jet}}}{d\rho_s}(m_t^{\text{pole}}, \rho_s), \quad (2.14)$$

with  $\rho_s$  defined as:

$$\rho_s = \frac{2m_0}{\sqrt{s_{t\bar{t}+\text{jet}}}}, \quad (2.15)$$

where  $m_0$  is an arbitrary scaling constant that is typically chosen to be of the order of the top quark mass, and  $\sqrt{s_{t\bar{t}+\text{jet}}}$  is the invariant mass of the  $t\bar{t}$  +jet system,  $\sqrt{s_{t\bar{t}+\text{jet}}} = m_{t\bar{t}+\text{jet}}$ . In [7, 93, 94] and in the analysis presented in this thesis, the  $m_0$  constant is set to  $m_0 = 170$  GeV, which has the effect of bounding the values of  $\rho_s$  in the range between 0 and 1.

The definition of the  $\mathcal{R}$  observable includes a normalization term,  $1/\sigma_{t\bar{t}+\text{jet}}$ , which is added into the definition of the observable since it leads to the total or partial cancellation of many experimental and theoretical uncertainties, such as the luminosity uncertainty in the recorded data, or the  $\alpha_s$  variations included in the *parton density functions* (PDFs) uncertainties.

The  $\sigma_{t\bar{t}+\text{jet}}$  cross section is measured differentially as a function of the  $\rho_s$  variable rather than inclusively because differential cross sections contain more information about the underlying physics processes, which allows for a more detailed analysis of the physical phenomena involved. The  $\rho_s$  variable is chosen because, as it is inversely proportional to the invariant mass of the  $t\bar{t}$  +jet system, it is able to isolate the phase space region where an enhanced sensitivity to the top quark mass is expected, the region close to the production threshold, where  $\rho_s \rightarrow 1$ .

The main features of the  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  observable are shown in Figure 2.15, where the  $\mathcal{R}$  distribution is calculated at NLO in  $pp$  collisions at a center of mass energy of 13 TeV. The distribution is plotted for three varied values of the  $m_t^{\text{pole}}$ , showing that variations in this parameter result in significant changes in the shape of the  $\mathcal{R}$  observable.

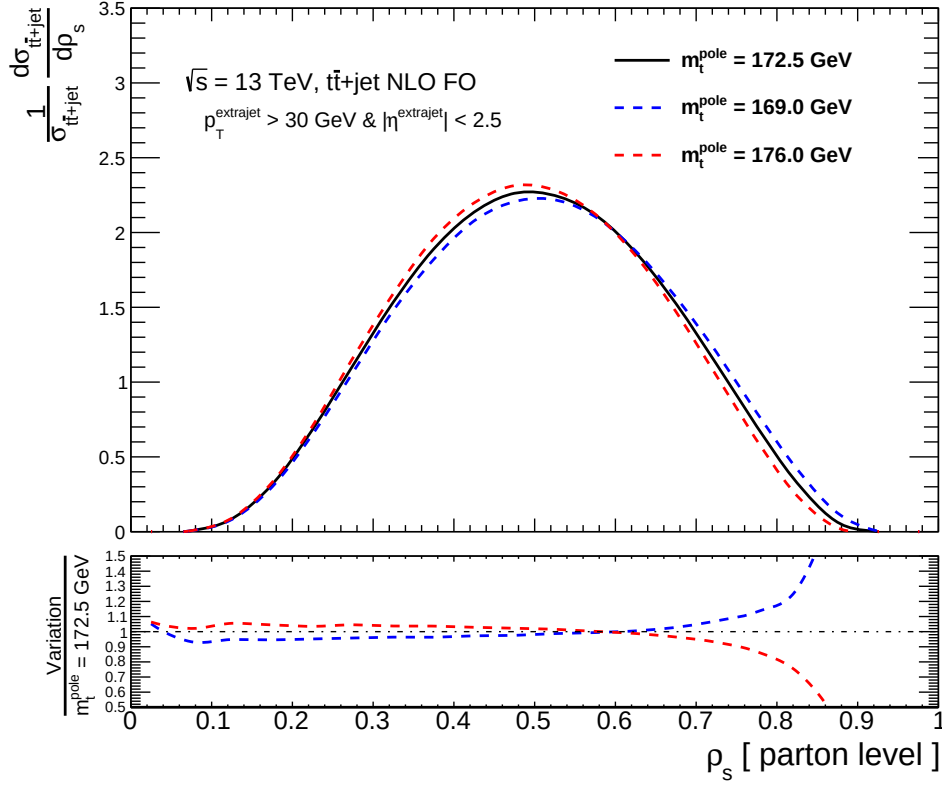


Figure 2.15: Predictions of the normalized differential cross section of the  $t\bar{t}$  +jet system as a function of  $\rho_s$  at parton level. Several curves are displayed for three different assumptions of the top quark pole mass:  $m_t^{\text{pole}} = 167, 172.5$ , and  $178$  GeV. These theory predictions are computed at  $t\bar{t}$  +jet NLO fixed-order using the Powheg-Box-v2  $ttJ$  process [95].

In the FO calculations of the  $\mathcal{R}$  observable depicted in Figure 2.15, the differential cross sections are calculated using on-shell stable top (anti-)quarks. The additional jet is defined using anti- $k_t$  clustering with distance parameter  $R = 0.4$ , with the selection requirements of  $p_T^{\text{extrajet}} > 30$  GeV and  $|\eta^{\text{extrajet}}| < 2.5$ . The selection requirements on the extrajet are optimized in this analysis taking into account the precision of the differential cross-section obtained in the unfolding, the systematic uncertainties originating from the choice of the renormalization and factorization scales in the FO calculations, and the PDF uncertainties.

As expected from the definition of the  $\mathcal{R}$  observable, the sensitivity to the top quark mass is large in the phase space region with high values of  $\rho_s$  (low  $s_{t\bar{t}+\text{jet}}$ ) and small in the region with low values of  $\rho_s$  (high  $s_{t\bar{t}+\text{jet}}$ ). Since the distributions are normalized to the same value, the curves cross, which occurs around  $\rho_s \sim 0.6$ .



In the region surrounding this value, the distribution loses its sensitivity to the top quark mass. To numerically evaluate the sensitivity of the observable in Equation 2.14 to the top quark mass, the following sensitivity metric is defined:

$$\mathcal{S}(\rho_s) = \sum_{\Delta=\pm\delta \text{ GeV}} \frac{|\mathcal{R}(m_t^{\text{pole}} + \Delta, \rho_s) - \mathcal{R}(m_t^{\text{pole}}, \rho_s)|}{2|\Delta|\mathcal{R}(m_t^{\text{pole}}, \rho_s)}, \quad (2.16)$$

where  $\delta$  is the difference between top mass value set in the nominal calculation and the alternative calculations of the  $\mathcal{R}$  observable. The sensitivity  $\mathcal{S}$  is almost independent of the chosen value of  $\delta$  because the dependence of the observable to the top mass is almost linear [89].

In Figure 2.16, the sensitivity to the top quark mass of the  $\mathcal{R}$  observable is shown, together with the sensitivity of a similar observable defined in  $t\bar{t}$  event topologies, where  $s_{t\bar{t}+\text{jet}}$  in the definition of  $\rho_s$  is replaced with  $s_{t\bar{t}}$ ,  $\rho_s = 2m_0/\sqrt{s_{t\bar{t}}}$ .

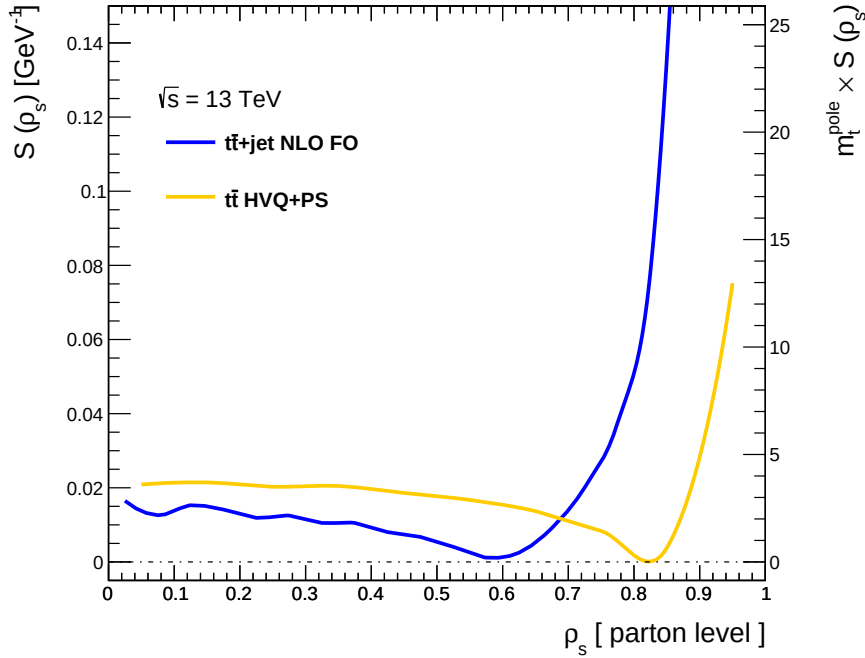


Figure 2.16: The sensitivity of  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  to the top quark mass, as defined in Equation 2.16 (blue curve). This sensitivity is compared with the sensitivity of a similar observable defined in  $t\bar{t}$  topologies (orange curve).

The sensitivity metric shows that the  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  observable defined in  $t\bar{t} + \text{jet}$

topologies is more sensitive to the top quark mass than the similar observable defined in  $t\bar{t}$  events. The rightmost  $y$ -axis in Figure 2.16 show the product of  $m_t^{\text{pole}} \times \mathcal{S}(\rho_s)$ , as it relates the relative change in the observable with that of the top quark pole mass:

$$\left| \frac{\Delta \mathcal{R}}{\mathcal{R}} \right| \approx (m_t^{\text{pole}} \mathcal{S}) \times \left| \frac{\Delta m_t^{\text{pole}}}{m_t^{\text{pole}}} \right|. \quad (2.17)$$

This means that, for example, a variation of 1% in  $m_t^{\text{pole}}$  results in a 20% variation on the  $\mathcal{R}$  observable in the regions with  $\rho_s \sim 0.8$ , showing the high sensitivity of this observable to the top quark pole mass.

The sensitivity to the top quark mass of the normalized  $t\bar{t}$  +jet differential cross section as a function of  $\rho_s$  was exploited by several analyses of the ATLAS and CMS collaborations to measure the top quark mass in the pole and also the  $\overline{MS}$  renormalization schemes.

The first measurement of the top quark mass using the  $\mathcal{R}$  observable was performed by the ATLAS collaboration using  $pp$  collision data provided by the LHC at a center of mass energy of 7 TeV [93]. This analysis was performed in the semileptonic decay channel of the  $t\bar{t}$  system, using a total integrated luminosity of  $4.6\text{fb}^{-1}$ . The result reported for the top quark pole mass was:

$$m_t^{\text{pole}} = 173.7 \pm 1.5 \text{ (stat.)} \pm 1.4 \text{ (syst.)}_{-0.5}^{+1.0} \text{ (theo.) GeV}. \quad (2.18)$$

After the publication of this result, a reinterpretation of the measured unfolded data distribution using theoretical predictions calculated in the  $\overline{MS}$  renormalization scheme was performed [96], yielding the following results:

$$m_t(m_t) = 165.9 \pm 1.4 \text{ (stat.)} \pm 1.3 \text{ (syst.)}_{-0.6}^{+1.5} \text{ (theo.) GeV}. \quad (2.19)$$

Utilizing  $pp$  collision data provided by the LHC at a center of mass energy of 8 TeV, the ATLAS collaboration performed an analysis following a similar methodology to the one at 7 TeV. This analysis was also carried out in the

semileptonic decay channel of the  $t\bar{t}$  system, but with a total integrated luminosity of  $20.2\text{fb}^{-1}$ . The results reported by the collaboration for the top quark mass in both, the pole and the  $\overline{MS}$  renormalization schemes were [7]:

$$m_t^{\text{pole}} = 171.1 \pm 0.4 \text{ (stat.)} \pm 0.9 \text{ (syst.)}_{-0.3}^{+0.7} \text{ (theo.) GeV} \quad (2.20)$$

and

$$m_t(m_t) = 162.9 \pm 0.5 \text{ (stat.)} \pm 1.0 \text{ (syst.)}_{-1.2}^{+2.1} \text{ (theo.) GeV} . \quad (2.21)$$

Compared with the results at 7 TeV, the statistical and systematic uncertainties were reduced by more than a factor of two. The reasons for these reductions were the increase in the integrated luminosity by more than a factor four, and the improvement in the knowledge of the detector response. The result of the top quark mass in the  $\overline{MS}$  scheme is affected by a larger theoretical uncertainty when compared with the top quark pole mass result. This is because the top quark mass in the  $\overline{MS}$  scheme suffers from logarithmic contributions which dominate in the threshold region, and which heavily depend on the renormalization and factorization scales [97].

The CMS collaboration also exploited the sensitivity to the top quark mass of the  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  observable to extract this value using the  $pp$  collision data provided by the LHC at a center of mass energy of 13 TeV [94]. In contrast to the ATLAS 7 and 8 TeV measurements, the CMS measurement was performed in the dileptonic decay channel of the  $t\bar{t}$  system, using a total integrated luminosity of  $36.3\text{fb}^{-1}$  (13 TeV 2018 dataset). To reconstruct the  $\rho_s$  variable in the dileptonic channel without assuming a constrain in the top quark mass, the authors of this paper utilized a fully connected neural network to regress the value of this variable. Additionally, the detector level  $\rho_s$  distribution was corrected to parton level using the profile likelihood unfolding method [98]. The result reported for the top quark pole mass in this measurement was:

$$m_t^{\text{pole}} = 172.94 \pm 1.27 \text{ (fit)}_{-0.43}^{+0.51} \text{ (scale) GeV} , \quad (2.22)$$

---

where the *fit* uncertainty accounts for the statistical, systematic, and PDF uncertainties. This approach is adopted because all these uncertainties are incorporated within the covariance matrix used to fit the corrected data distribution to the theoretical predictions. Therefore, the resulting uncertainty is reported all together, allowing for a proper consideration of the correlations among the different sources of uncertainties.

# Chapter 3

## The LHC and the ATLAS experiment

Since top quarks are exceptionally heavy, they can only be produced and thus studied in high-energy experiments. This chapter provides a description of one of the few experiments that have been able to study the physics of the top quark, the ATLAS experiment, which is located along the LHC ring at CERN. This chapter is divided into two sections. In Section 3.1, the LHC acceleration complex is introduced, together with a brief description of the various steps of the acceleration process and the experiments placed in the LHC ring. In Section 3.2, a comprehensive description of the systems of subdetectors that compose the ATLAS experiment is provided.

### 3.1 The LHC acceleration complex

The Large Hadron Collider (LHC) [99] is a superconducting hadron accelerator and collider located at the CERN laboratories near Geneva. It is placed  $\sim 100$  m underground in the 26.7 km ring previously used for the Large Electron Positron (LEP) collider [100]. Having achieved collisions between proton beams at a center-of-mass energy of  $\sqrt{s} = 13.6$  TeV, and heavy ions (Pb) collisions at  $\sqrt{s_{NN}} = 5.36$  TeV/nucleon, the LHC is the most powerful particle collider ever built. To reach these energies, the particle beams are accelerated using radiofrequency cavities. Superconductive dipole magnets are used to bend the trajectories of the particles around the LHC ring, while quadrupole and octupole

magnets are used to squeeze and focus the bunches of particles.

Protons cannot be accelerated in the LHC until they reach a velocity close to the speed of light. Therefore, a series of intermediate particle pre-accelerators at the CERN accelerator complex, depicted in Figure 3.1, are used to increase their speed and energy in sequential stages. The colliding protons are extracted from a bottle of hydrogen gas, thanks to an electric field that strip the electrons from the Hydrogen atoms. Then they are inserted into the first linear accelerator, LINAC2, which accelerates them to an energy of 50 MeV. After this first stage, the protons are passed to the first circular accelerator, the proton synchrotron booster (PSB), where they acquire an energy of 1.4 GeV. Then the beam enters a second circular accelerator, the Proton Synchrotron (PS), where it is accelerated up to 25 GeV. The last circular accelerator before the LHC is the Super Proton Synchrotron (SPS), where the protons increase their energy up to 450 GeV. Finally, the protons are injected into the two beam pipes of the LHC, where they travel in opposite directions and are accelerated using radiofrequency cavities until the proton beams reach the target energy. In the successive runs of the LHC, the target energy of the beams has been increased from 3.5 and 4 TeV in Run 1, to 6.5 TeV in Run 2, and further to 6.8 TeV in Run 3. The LHC can also be used to accelerate heavy ions by replacing the initial source of particles and first linear accelerator by LINAC3.

Collisions between the proton bunches that form each proton beam happen every 25 ns at the four interaction points where the main LHC experiments are located. The ATLAS experiment is described in detail in Section 3.2. The other three main experiments are:

- **CMS:** The Compact Muon Solenoid (CMS) experiment [102], together with ATLAS, are the two multi-purpose detectors at the LHC. The CMS experiment is a detector that consists of a superconducting solenoid magnet and several subdetectors built in a cylindrical shape. These subdetectors are a silicon pixel and strip tracker, a lead tungsten crystal electromagnetic calorimeter (ECAL), a brass and scintillator hadron calorimeter (HCAL), and multiple gas-ionization muon chambers. Using all these systems, the CMS detector has sensitivity to a wide variety of final-state objects and topologies, which are used to study the SM interactions and possible signatures of BSM physics.
- **LHCb:** The Large Hadron Collider beauty (LHCb) experiment [103] is a

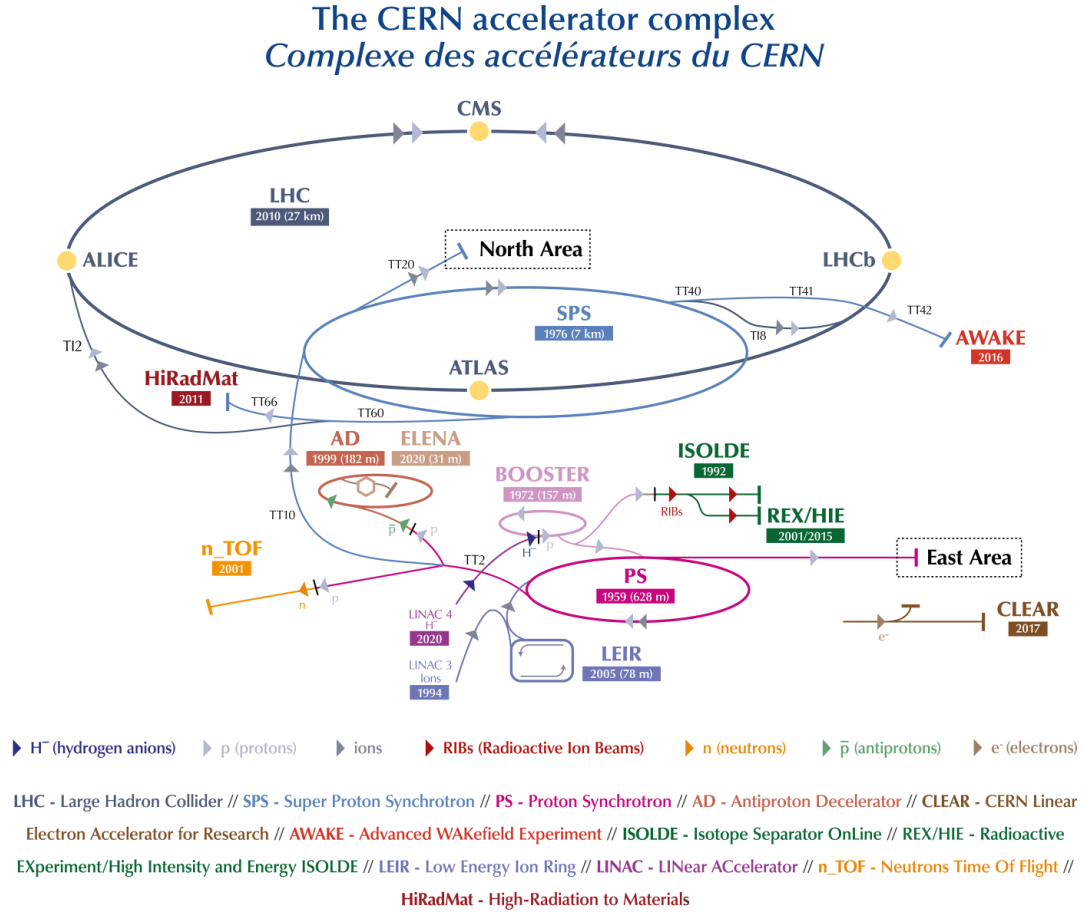


Figure 3.1: A schematic view of accelerator complex at CERN. The location of the four main experiments placed at the LHC ring is also displayed [101].

one-sided forward detector that focuses mainly on  $b$  quark flavor physics to study CP-violating processes. The LHCb experiment is designed with a forward geometry to cover the phase-space region where most B-hadrons are expected to be produced in the boosted regime, the forward region. Since B-hadrons have a lifetime of about 1.5 ps, boosted B-hadrons travel a significant distance in the LHCb detector, enabling the detailed study of their decay channels.

- **ALICE:** A Large Ion Collider Experiment (ALICE) [104] focuses on the study of heavy ion collisions. On these collisions, the very high temperatures and pressures experienced by the strongly interacting matter create a new phase of matter, the quark-gluon plasma, the state of matter that existed in the early universe. The distinguishing feature of ALICE lies in the

high granularity of its detectors, which facilitate the reconstruction and identification of charged particle tracks in the high multiplicity environment encountered in heavy ion collisions.

Besides the four main experiments at the LHC, there are four smaller experiments with special purposes. These include:

- **LHCf:** The LHC forward (LHCf) experiment [105] consists of two detectors placed at 140 m from the ATLAS interaction point in the beam direction. It studies very forward photons and neutral pions to imitate ultra-high energy cosmic rays in laboratory conditions.
- **TOTEM:** The TOTal cross section, Elastic scattering and diffraction dissociation Measurement (TOTEM) experiment [106] is a forward detector located close to CMS. It is dedicated to the precise measurement of the total  $pp$  cross section and the study of the proton structure using the protons that emerge from collisions at small angles.
- **MoEDAL:** The Monopole and Exotics Detector at the LHC (MoEDAL) [107] is located in the same interaction point as LHCb but on the opposite side. It specializes in the search for magnetic monopoles and other hypothetical high ionizing (pseudo-) stable massive particles.
- **FASER:** The Forward Search Experiment (FASER) [108] is located 480 m downstream of the ATLAS detector. It is positioned to look for light and extremely weakly interacting new particles and neutrinos.

In addition to all the experiments described in this section, some of the protons that are accelerated in the PS and the SPS pre-accelerators are used in other CERN experiments.

## 3.2 The ATLAS experiment

The ATLAS (A Toroidal LHC ApparatuS) experiment [109] is a multi-purpose particle detector operating at CERN and built around one of the four collision points of the LHC. It is composed of systems of sub-detectors, each of them



designed to measure the signals produced by specific types of particles. The combination of the signals measured by each sub-detector makes the experiment sensitive to a large variety of final-state particles and topologies. To cover almost the full  $4\pi$  solid angle around the interaction point, the ATLAS detector is split into a barrel consisting of cylindrical sub-detector layers around the beam axis, and two end-caps where the sub-detector layers are placed in planes perpendicular to the beam pipe. An illustrative representation of the detector is shown in Figure 3.2.

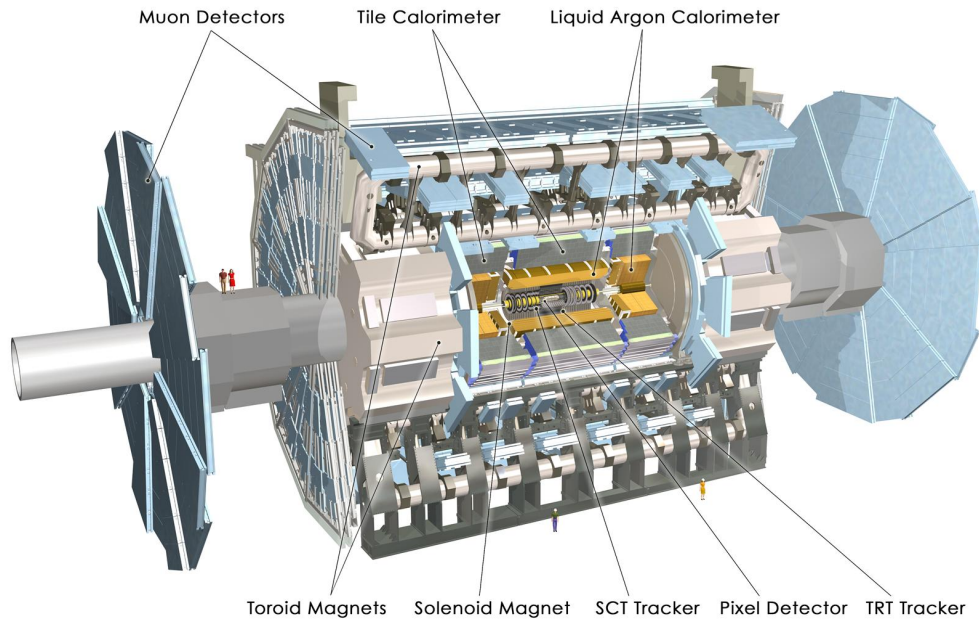


Figure 3.2: A schematic representation of the ATLAS detector and its components [110].

The innermost system of sub-detectors corresponds to the Inner Detector (ID), composed of the Pixel detector, the Semiconductor Tracker, and the Transition Radiation Tracker. This system is designed to reconstruct the trajectories of the charged particles that traverse it. The next layer corresponds to the LAr electromagnetic calorimeter, which measures the energy of electrons and photons. After this layer, the Tile hadronic calorimeter, which measures the energy of strongly interacting particles, is placed. The last layers correspond to the Muon Chambers, which are designed to reconstruct the trajectories of muons. The only particles that can escape the detector without being detected are the neutrinos. In addition to all the sub-detector systems, ATLAS has a system of superconducting magnets to measure the charge and momentum of charged particles. This system

is composed of a central solenoid magnet at the core of the experiment that provides a magnetic field of 2 T in the inner detector and a series of toroidal magnets that provide a magnetic field of up to 3.5 T to measure the momentum of muons. In the following section, a description of the individual sub-systems and the data-taking process in ATLAS is provided.

### 3.2.1 Coordinate system

The coordinate system adopted by ATLAS is briefly explained in this section since it is the convention used throughout this thesis. In Cartesian coordinates ( $x$ ,  $y$ ,  $z$ ), the origin of this system is placed at the nominal collision point inside the detector. The  $x$ -axis points inward into the center of the LHC ring, the  $y$ -axis points upwards, in the direction of the sky, and the  $z$ -axis is perpendicular to the  $x$ - $y$  plane and goes along the direction of the beam pipe.

However, instead of using a Cartesian coordinate system, it is more common to express the position of a component of the detector or a particle in terms of polar coordinates ( $r$ ,  $\phi$ ,  $\theta$ ). The  $r$  coordinate expresses the distance from the interaction point, the azimuthal angle,  $\phi$ , determines the angular distance in the  $x$ – $y$  plane, and the polar angle,  $\theta$ , determines the angular distance with respect to the  $z$ -axis. The angle  $\phi = 0$  corresponds to a vector pointing along the  $+x$  coordinate, and the angle  $\theta = 0$  corresponds to a vector pointing along the  $+z$  coordinate.

In hadron collider experiments, instead of  $\theta$ , the pseudorapidity  $\eta \equiv -\ln[\tan(\theta/2)]$  is frequently used. A value of  $\eta = 0$  corresponds to a vector in the  $x$ – $y$  plane, perpendicular to the beam pipe, while a value of  $\eta = \infty$  coincides with the  $z$ -axis, the direction of the beam pipe. For a particle of total momentum  $p$  and momentum in the direction of the  $z$ -axis,  $p_z$ , the pseudorapidity can be written as in Equation 3.1. The pseudorapidity is an approximation of the rapidity at high energies, when the mass of the particle is negligible with respect to its momentum.

$$\eta = \frac{1}{2} \ln \left( \frac{p + p_z}{p - p_z} \right) \quad (3.1)$$

Finally, it is useful to introduce and define two more magnitudes, the transverse momentum of a particle,  $p_T$ , as the projection of its momentum into the  $x$ – $y$  plane (Equation 3.2) and, the angular separation of two objects,  $\Delta R$ , as their separation

in the  $\eta - \phi$  plane (Equation 3.3).

$$p_T \equiv \sqrt{p_x^2 + p_y^2} \quad (3.2)$$

$$\Delta R \equiv \sqrt{(\eta_2 - \eta_1)^2 + (\phi_2 - \phi_1)^2} \quad (3.3)$$

### 3.2.2 Tracking system

The ATLAS tracking system is commonly referred to as the Inner Detector (ID) [111, 112] as it is the closest system to the interaction point, placed surrounding the beam pipe. Its main purpose is to measure the trajectories of charged particles traversing it, also known as *tracks*, and, with this information, calculate the impact parameters of the particles, their charges and momentum, and reconstruct the primary and the secondary vertices of the event (see Section 4.1). To measure the charge and momentum of charged particles, their trajectories are bent by immersing the ID in a 2 T magnetic field produced using the superconducting solenoid described in Section 3.2.5.

The ID has a coverage up to  $|\eta| < 2.5$  and it is composed of three main sub-systems. From closest to farthest from the interaction point, these sub-detectors are the Pixel Detector (PIX), the Semiconductor Tracker (SCT), and the Transition Radiation Tracker (TRT). A schematic view of the ID is shown in Figure 3.3, while Table 3.1 summarises the intrinsic resolution of each subdetector.

Table 3.1: Intrinsic resolutions of the ID subdetectors. The IBL, Pixel, and SCT resolutions are expressed in the  $r - \phi$  plane and  $z$ -axis, while the TRT resolution is only expressed along the  $z$ -axis.

| Subdetector                                                       | IBL           | Pixel           | SCT             | TRT |
|-------------------------------------------------------------------|---------------|-----------------|-----------------|-----|
| Intrinsic resolution<br>( $r - \phi \times z$ ) [ $\mu\text{m}$ ] | $8 \times 40$ | $10 \times 115$ | $17 \times 580$ | 130 |

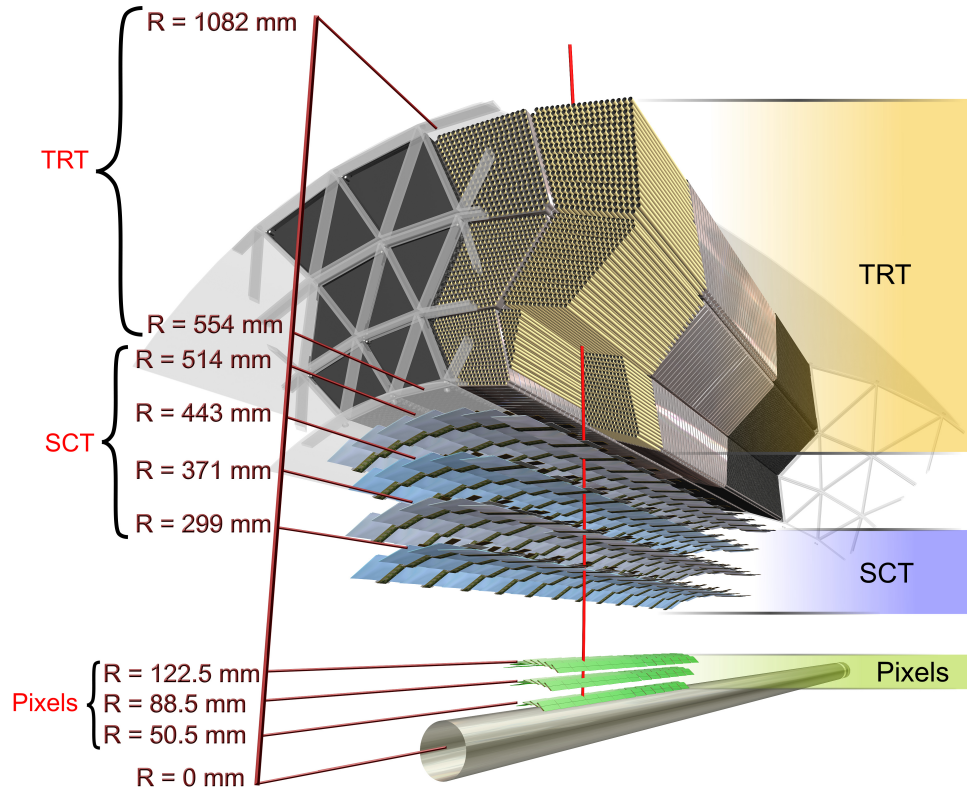


Figure 3.3: A layout of the ATLAS Inner Detector and its sub-components, Pixel, SCT, and TRT. This picture is missing the IBL, which is placed between the pipeline and the Pixel detector [113].

The **Pixel Detector** (PIX) is a high-resolution silicon detector composed of 80 million pixels organized in 1774 modular units and arranged in three layers around the beam pipe and three disks in each end-cap. The three layers are called the B-layer, Layer-1, and Layer-2 and are placed at 5.05, 8.85, and 12.25 cm of the beam pipe, respectively. In order to protect the Pixel detector from the higher radiation levels encountered during the LHC Run 2, as compared to Run 1, and to improve the identification of heavy-flavor jets (Section 4.5), this system is complemented with a fourth layer, the **Insertable B-Layer** (IBL), which is placed at only at 33.5 mm from the beam and was installed at the start of the Run 2. The whole system is cooled down to around  $-10\text{ }^{\circ}\text{C}$  to minimize radiation damage and reduce the thermal noise. As the innermost system, the pixel detector is crucial for the reconstruction of the primary and secondary vertices (Section 4.1). The accurate reconstruction of secondary vertices by this detector is essential for the reliable identification of B-hadrons.

The **Semiconductor Tracker** (SCT) is a silicon micro-strip detector placed outside the Pixel detector. It is composed of micro-strip modules arranged in four layers around the beam pipe and nine disks in each end-cap. As the Pixel detector, the system is cooled down to around  $-10\text{ }^{\circ}\text{C}$ . The micro-strip technology allows the system to cover a wider area than the Pixel detector with an acceptable drop in the resolution, as the SCT detector is located further away from the interaction point.

The **Transition Radiation Tracker** (TRT) is a gas detector placed in the outermost part of the Inner Detector. It is composed of 350848 thin-walled proportional drift tubes (straws) arranged in a barrel, where the straws are positioned in parallel to the beam pipe, and in two end-caps, where the straws are placed radially. Each tube has a diameter of 4 mm and is filled with a gas mixture of 70% xenon, 27% carbon dioxide, and 3% oxygen. When a charged particle traverses a straw, it ionizes the gas molecules. The negative charges are then collected by an anode wire situated at the center of the tube and this signal is registered as a hit. The geometry of the TRT detector covers the  $|\eta| < 2$  range, and it is guaranteed that any particle traversing the system will cross between 35 and 40 straws, which provides a continuous track at a radius between 0.55 and 1.08 m from the beam pipe. This system extends the tracker coverage up to the boundary of the calorimeter.

### 3.2.3 Calorimeter system

The ATLAS calorimeter system [114, 115] is located outside the superconducting solenoid magnet that surrounds the Inner Detector. It is a system designed to stop and measure the energy of most of the particles coming from the interaction point. To reach this goal, the ATLAS calorimeters consist of alternating layers made from a high-density material used to degrade the energy of the incoming particles (passive material), and a lower-density material that provides the detectable signals used to perform the energy measurement (active material). When an outgoing particle interacts with a layer of the passive material, it produces a *shower* of particles with lower energy. This shower can originate from the electromagnetic interactions, through the generation of bremsstrahlung photons and photons that produce electron-positron pairs, or from strong interactions, where the quarks and gluons within the penetrating hadron undergo successive branching and interactions, resulting in a cascade of secondary partons that

subsequently hadronize. Then, the particles conforming this shower traverse the layer of active material where they create a signal based on ionization, excitations, or Cherenkov radiation that is then collected and measured. The process repeats in each subsequent pair of layers until the energy of the particles is so low that they cannot produce any more *showers* and are eventually absorbed in the material. From the detectable signals collected in each of the layers of active material, the energy of the incoming particle is estimated. These kinds of calorimeters are known as sampling calorimeters, as they extrapolate the total energy of the incoming particle by sampling only a part of it.

Each of the components of the ATLAS calorimeter system is specialized in the measurement of the energy of different types of particles. There are two main components: the Lead-liquid Argon electromagnetic calorimeter (LAr), designed to measure the energy of particles that interact via the electromagnetic force (able to fully stop electrons and absorb photons), and the Tile hadronic calorimeter (TileCal), designed to stop and measure the energy of particles that interact via the strong force (hadrons). The only SM particles that are able to go through the ATLAS calorimeters without stopping are the muons and neutrinos. The energy of the muons is measured in the muon spectrometer (Section 3.2.4). The energy of the neutrinos can be estimated from the missing transverse energy (MET) (Section 4.6). The wide  $\eta$  range that the calorimeter system covers is crucial for a proper reconstruction of the MET. A schematic view of the calorimeter system is shown in Figure 3.4.

The **Lead-liquid Argon electromagnetic calorimeter** (LAr) is placed surrounding the superconducting solenoid magnet and it consists of an electromagnetic barrel (EMB) and end-caps (EMEC). These components use liquid argon as active material (scintillator) and lead plates arranged in an accordion-like structure as passive material. The EMB covers the  $|\eta| < 1.475$  range and the EMEC covers the  $1.375 < |\eta| < 3.2$  range. This means that there is a gap in the electromagnetic calorimeter where this system does not take any measurements. To keep the argon in a liquid state, the LAr calorimeter is kept in three cryostats at  $-184^\circ\text{C}$ .

The **Tile hadronic Calorimeter** (TileCal) is placed just outside the LAr calorimeter and it consists of a central barrel and two extensions on the end-caps covering the  $|\eta| < 1.7$  range. The TileCal uses iron plates as passive material and plastic tiles as active material (scintillators).



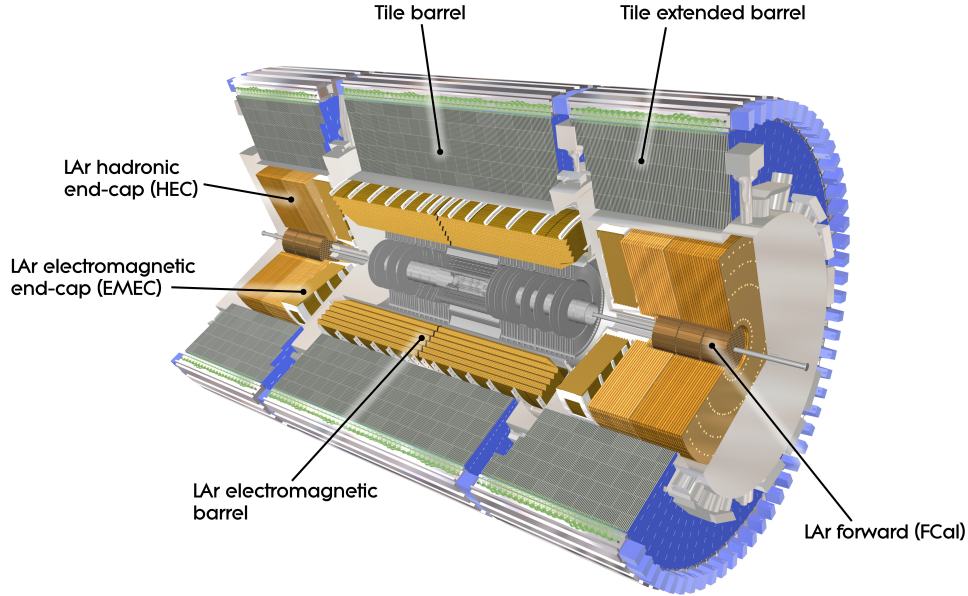


Figure 3.4: A layout of the ATLAS electromagnetic and hadronic calorimeters [116].

The **Hadronic End-Cap (HEC)** is placed behind the EMEC, inside the end-cap cryostat, and it covers the  $1.5 < |\eta| < 3.2$  range. This system uses liquid argon as active material and two wheels of copper plates as passive material.

The **Forward Calorimeters (FCal)** are placed inside the end-cap cryostat together with the EMEC and the HEC and they cover the very forward region in  $3.1 < |\eta| < 4.9$ . FCal is composed of three layers that use the liquid argon as active material. The first layer is designed for electromagnetic calorimetry and it uses copper as passive material. The second and third layers are designed for hadronic calorimetry and use tungsten as passive material. After the third layer, there is a passive layer made of brass that absorbs any hadronic shower remnants. This last layer is needed because of the high energy and density of particles in this region.

### 3.2.4 Muon spectrometers

The Muon Spectrometers (MS) [117] are the outermost system of sub-detectors of the ATLAS experiment. They are located from a distance to the beam pipe of  $\sim 4.25$  m and extend up to a distance  $\sim 11$  m. The MS are designed to detect and determine the trajectory of muons, the only charged particles that

escape the calorimeters. Some components of the MS are interspersed with the superconducting toroids of the magnet system (Section 3.2.5). These toroids create a magnetic field of up to 3.5 T which bends the trajectory of muons and enable measurement of their momentum. As muons only leave a small signal in the calorimeter, the measurement of their momentum/energy relies on the ID and the MS measurements. The MS consist of four different sub-systems of gas ionization chambers constructed with four different types of technologies and they cover the full azimuthal angle and the  $|\eta| < 2.7$  range. Two of these sub-components, the Muon Drift Tubes (MDTs) and the Cathode Strip Chambers (CSCs) are used for the high-precision reconstruction of the tracks whereas the other two, the Resistive Plate Chambers (RPCs) and the Thin Gap Chambers (TGCs), are used for triggering as they are faster detectors, but with a lower spatial accuracy. A schematic view of the ME is shown in Figure 3.5.

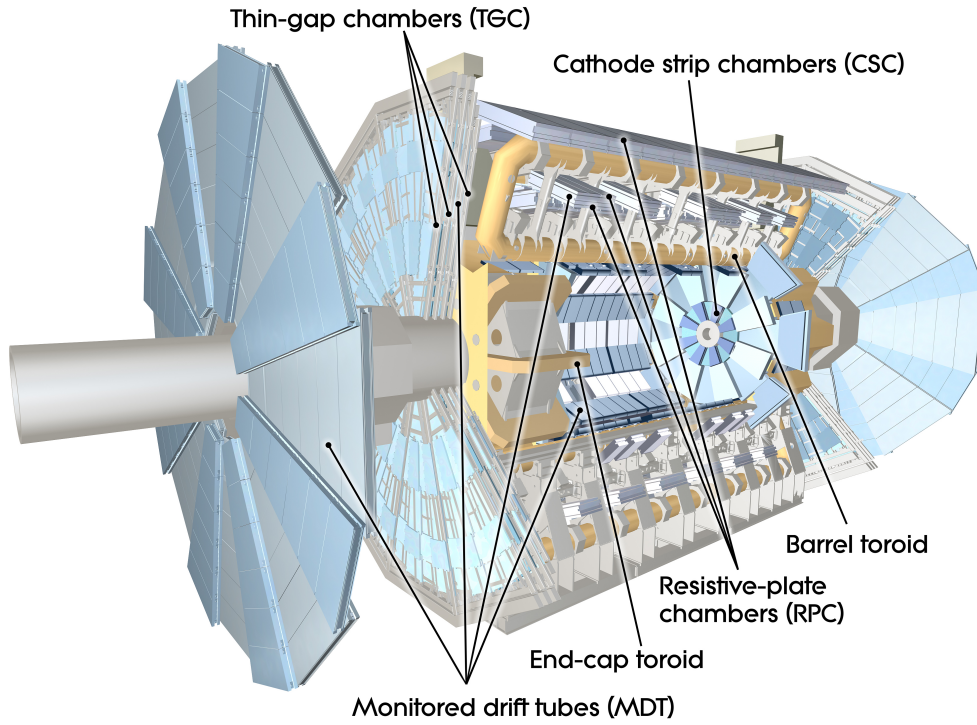


Figure 3.5: A layout of the ATLAS muon spectrometers, its sub-components, and the toroid magnets around them [118].

The **Muon Drift Tubes** (MDTs) are similar to the TRT of the ID (Section 3.2.2) as they are made of drift tubes. However, in this case, they are filled with a gas mixture of 93% argon and 7% carbon dioxide. The MDTs are arranged in three coaxial cylindrical layers in the barrel and six end-cap disks on



each side of the detector, covering the  $|\eta| < 2$  range.

The **Cathode Strip Chambers** (CSCs) are made of multi-wire proportional chambers filled with a gas mixture of 80% argon and 20% carbon dioxide. Positioned in the innermost layer of the barrel, they cover the forward region of the detector,  $2 < |\eta| < 2.7$ . Due to the high track density in this region, CSCs are built with a higher granularity than MDTs.

The **Resistive Plate Chambers** (RPCs) are arranged in three coaxial cylindrical doublet layers in the barrel covering the  $|\eta| < 1.05$  range. Each RPCs doublet layer is made of two RPCs filled with a gas mixture of 94.7% tetrafluoromethane, 5.0% isobutane, and 0.3% sulfur hexafluoride and separated with plastic spacers. The RPCs system has a space-time resolution of around  $2\text{cm} \times 2\text{ns}$ . With such a good time resolution, the RPCs are able to identify the bunch crossing window that originated the traversing muon and hence, they are used for triggering.

The **Thin Gap Chambers** (TGCs) are multi-wire proportional chambers used for triggering in the end-caps. The TGCs are arranged in three layers covering the  $1 < |\eta| < 2.7$  region. With a time resolution of 4 ns, the TGCs are able to identify the 25 ns bunch crossing window when the collision happened.

In ATLAS, the combination of the MS and ID information using the algorithms described in Section 4.3 allow for the reconstruction of the muon  $p_T$  with a resolution of about 2% for momenta up to 250 GeV.

### 3.2.5 Magnet system

The magnet system of ATLAS is composed of four sub-systems designed to provide a magnetic field in the ID and in the MS. A schematic view of its location in the detector is shown in Figure 3.6.

In the ID, a 2 T axial magnetic field is created by a superconducting solenoid magnet located surrounding the ID, just before the LAr calorimeter. The wires that compose the solenoid magnet are made of an alloy of niobium-titanium, which has to be cooled down to a temperature below 10 K to achieve the superconductive state. To reach this temperature, the solenoid is placed in the same cryostat as the LAr calorimeters, which serve as an external thermal shield. Subsequently, the internal thermal shield surrounding the solenoid material is cooled down

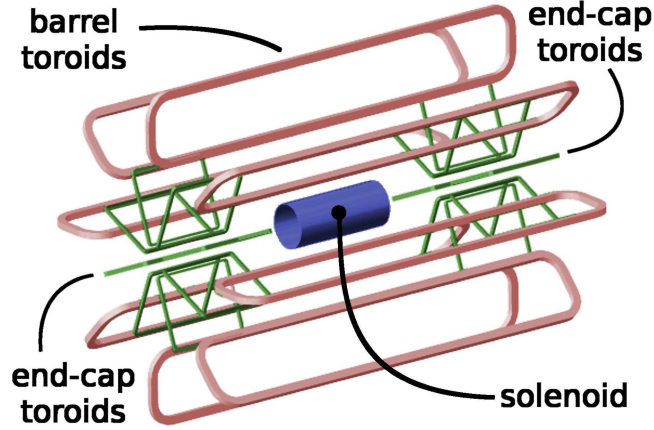


Figure 3.6: The layout of the ATLAS superconducting magnet system [119].

to a temperature between 40 K and 80 K using a liquid nitrogen/helium heat exchanger. Finally, the solenoid cold mass is further cooled down to its target temperature of 4.5 K using supercritical helium.

In the MS, the magnetic field is created by three systems of toroidal conductor magnets. The barrel toroid magnets system comprises eight toroid magnets placed outside the calorimeters, surrounding some of the MDTs and RPCs of the MS systems. The end-caps toroid magnet systems are composed of eight toroid magnets each. They are placed surrounding several of the components of the MDTs, CSCs, and TGCs of the end-caps region. The magnetic fields created by the toroid magnets reach up to 3.9 T for the barrel and 4.1 T for the end-caps. The magnetic field generated by the magnet system is used to bend the path of charged particles in the regions where the tracks are reconstructed to enable the measurement of the particle's charge and momentum.

### 3.2.6 Luminosity measurement and forward detectors

The number of events per unit of time (event rate) for a particular process  $x$  can be expressed in terms of the instantaneous luminosity ( $\mathcal{L}$ ) and the process cross section ( $\sigma_x$ ) as:

$$\frac{dN_x}{dt} = \mathcal{L}\sigma_x \quad . \quad (3.4)$$

In a  $pp$  circular collider as the LHC, the instantaneous luminosity can be

written in terms of the beam parameters using the following equation:

$$\mathcal{L} = f_c \frac{N_1 N_2 N_b}{4\pi\sigma_x\sigma_y} \quad , \quad (3.5)$$

where  $f_c$  represents the crossing frequency of the bunches,  $N_1$  and  $N_2$  the number of protons in each colliding bunch,  $N_b$  the number of bunches in each beam, and  $\sigma_x$  ( $\sigma_y$ ) the horizontal (vertical) profile width of the beam. The total integrated luminosity ( $L$ ) is calculated by integrating the instantaneous luminosity over the running time of the collider,  $L = \int \mathcal{L} dt$ .

In the ATLAS experiment, the main system that measures the luminosity is an evolution of the Luminosity Cherenkov Integrating Detector (LUCID) system used during Run 1, the LUCID-2 system [120]. The LUCID-2 system is composed of two modules located in the forward regions ( $|\eta| \simeq 5.8$ ) at 17 m of the interaction point. Each module consists of 16 photomultipliers connected to tubes filled with a gas mixture with a low threshold for Cherenkov radiation emission. The LUCID-2 system is used to measure the forward, inelastic  $pp$  scattering to calculate the instantaneous luminosity in the detector.

LUCID-2 is the main but not the only system that provides a measurement of the beam conditions and the luminosity in the ATLAS experiment. Other specific systems, such as ALFA (Absolute Luminosity For ATLAS), are also used to calculate and compare the luminosity. In addition to the specific systems, other detector systems can also provide a luminosity measurement. For example, the luminosity can also be deduced from the activity in the Tile calorimeter, the Tile and EMEC, and the number of tracks counted in the ID. The combination of the results of all these luminosity measurements using several algorithms leads to the result shown in Figure 3.7 where the total accumulated luminosity delivered by the LHC and recorded by ATLAS during the full Run 2 is shown. This figure also shows the mean number of interactions per bunch crossing,  $\mu$ , which is of key importance when evaluating and correcting the pile-up effects on the recorded data (see Section 4). The total integrated luminosity for the full Run 2 recorded by the ATLAS experiment, after detector and data quality requirements (Section 3.2.8), is  $140.1 \text{ fb}^{-1}$  with a 0.83% uncertainty [121].

At last, two forward detectors of the ATLAS experiment that have not been mentioned in this chapter yet are the Zero Degree Calorimeter (ZDC) and the

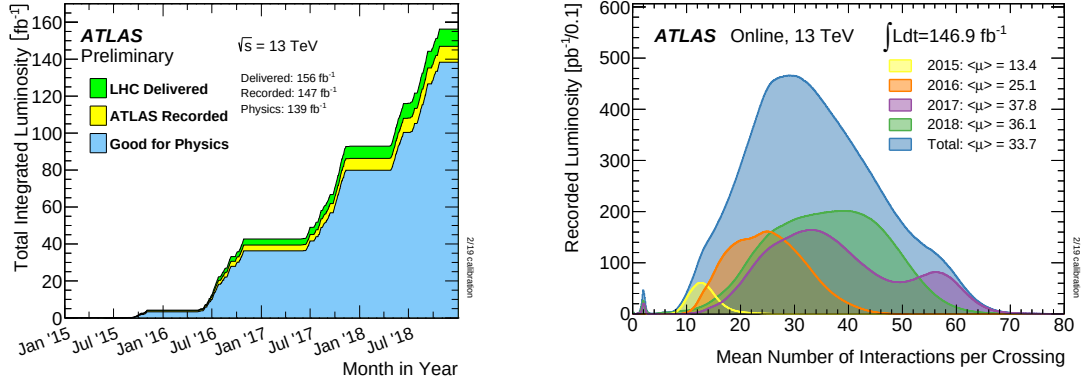


Figure 3.7: Left: Total integrated luminosity versus time delivered by the LHC (green), recorded by the ATLAS detector (yellow) and good for physics (blue) during the Run 2  $pp$  collisions. Right: Mean number of interactions per bunch crossing during the Run 2  $pp$  collisions [122].

ATLAS Forward Protons (AFP). The ZDC is designed to detect forward neutrons and protons in the  $|\eta| > 8.3$  range and its main purpose is to determine the centrality of heavy ions collisions. The AFP detector is located a distance of 220 m from the interaction point and it is equipped with high precision detectors that enable it to detect intact protons scattered at small angles and with low momentum losses.

### 3.2.7 Trigger system and data storage

The LHC is designed to collide proton bunches every 25 ns, corresponding to a collision rate of 40 MHz and an event rate in the ATLAS detector of about 1 GHz. At a size of about 1 MB per recorded event, this corresponds to around 1 PB of data per second. It is unfeasible to process and store such a huge amount of data with the current computing and storage technologies hence, a trigger system is needed to quickly identify, process, and store only the potentially interesting events. The ATLAS trigger system is divided into two levels of increasing complexity, the Level-1 Trigger (L1) and the High Level Trigger (HLT) [123].

The ATLAS **Level-1 Trigger** (L1) is the first step in the event selection at the ATLAS experiment. It is designed to reduce the accepted rate of events from up to 40 MHz, the bunch crossing rate, to a maximum of 100 kHz. The L1 trigger is a hardware-based trigger that is primarily derived from the information of the RPCs and TGCs muon spectrometers (Section 3.2.4) and the hadronic and electromagnetic calorimeters (Section 3.2.3). With this information, L1

identifies event features such as muons, electrons, photons, and jets candidates or a significant amount of missing transverse energy in the event. Then, L1 applies different algorithms to decide if the event should be rejected or if its information should be passed to the HLT. The L1 system is very fast, with a latency of just  $2.5 \mu s$ . This tight time constraint poses a strict limit, as the data from all sub-detectors must be stored during this short interval.

The ATLAS **High Level Trigger** (HLT) is a software-based trigger that refines the event reconstruction performed at L1 and applies a series of algorithms to select the events that will be stored for offline analysis. It further reduces the 100 kHz approximate event rate from L1 down to around 1 kHz. The algorithms used to reconstruct and select the events in the HLT are versions of the algorithms used in offline analysis but adapted to the timing constraints required at this level. The events that are not selected by the L1 and the HLT triggers are irreversibly lost and cannot be recovered.

### 3.2.8 Data quality

Before the data collected by the ATLAS detector can be used for physics analysis, it is important to ensure that it is clean of any software or hardware-related issues that could render it unusable. To ensure this, the recorded data quality is evaluated by monitoring different detector-level quantities as well as the characteristics of the reconstructed collision events. Problems may arise from different sources, such as noise, malfunctioning of the detector hardware, or misconfiguration of the electronics of one or more of the sub-systems. The data quality assessment is evaluated through a chain of steps represented in the Data Quality (DQ) operational workflow shown in Figure 3.8.

The first stage of this workflow consists of the monitoring of the data in real time to make a preliminary evaluation of the data quality. This preliminary evaluation aims to reduce the data losses during data-taking by performing a prompt identification and solving of any potential issue that could make the data unusable for physics analyses. To reach this goal, the data and the sub-detector systems are monitored using tools such as the *Data Quality Monitor Display*, the *Online History Plotter*, and the *Atlantis* event display [122]. During this stage, promptly fully reconstructed sub-samples of the data from the so called *express* and *calibration* streams are used. If any issue is found during this assessment,

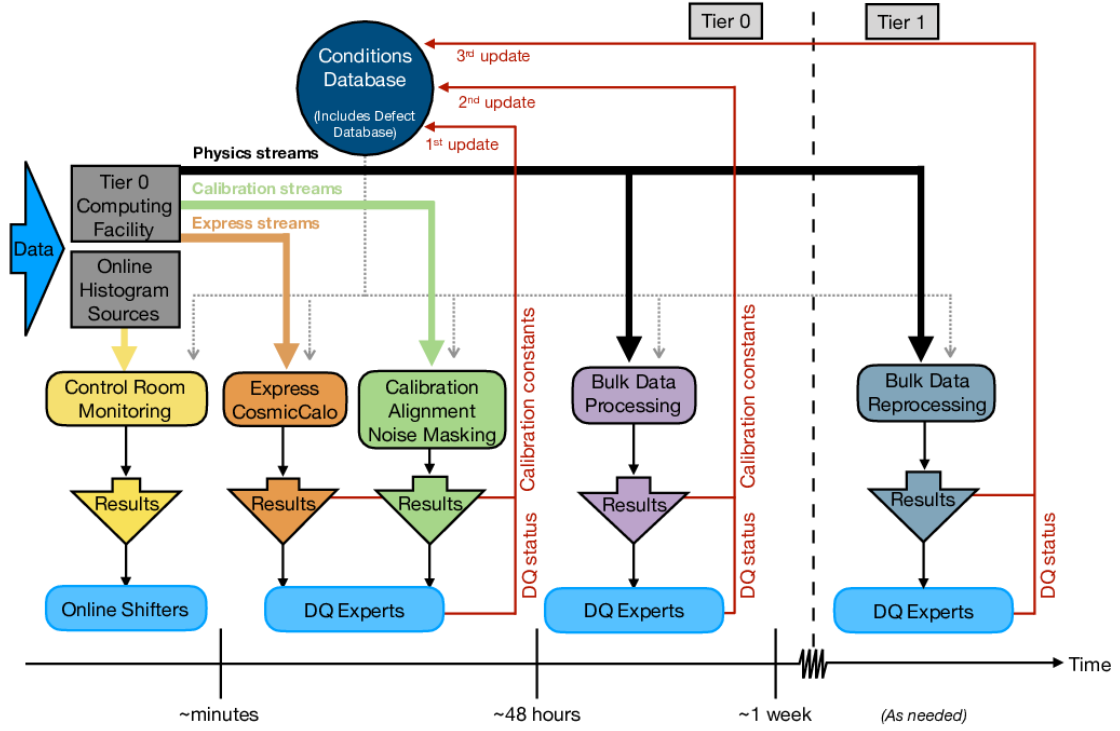


Figure 3.8: Schematic representation of the DQ assessment chain during the Run 2 data taking of the ATLAS detector [122].

the problem is communicated to the corresponding DQ expert responsible for the affected system for an in-depth analysis.

After the first iteration of checks has been performed, the so called *physics stream*<sup>1</sup> is reconstructed taking advantage of the information gathered from the first stage of the DQ workflow. This first reconstruction of the full data may include, for example, correcting residual noise, non-negligible losses in the detector coverage, or updating some calibration constants.

At last, the quality of the corrected data is assessed by an expert per system and combined performance area. The final result of the DQ workflow is the so called Good Run Lists (GRL), a set of files that contain all the data periods that are certified as *good-for-physics* data and, as so, can be used for physics analysis across the collaboration.

The author of this thesis has contributed to the early stages of the workflow

<sup>1</sup>The *physics stream* contains the full data statistics from the run.

in Figure 3.8 in the role of the *online shifter* in the ATLAS control room during the Run 3 data-taking period. The main difference between the Run 2 and the Run 3 periods is that, in the latter, the protons are collided at a center of mass energy of 13.6 TeV instead of 13 TeV. In Figure 3.9, the *Atlantis* event display of the first collision delivered by the LHC in ATLAS during the Run 3 is shown.

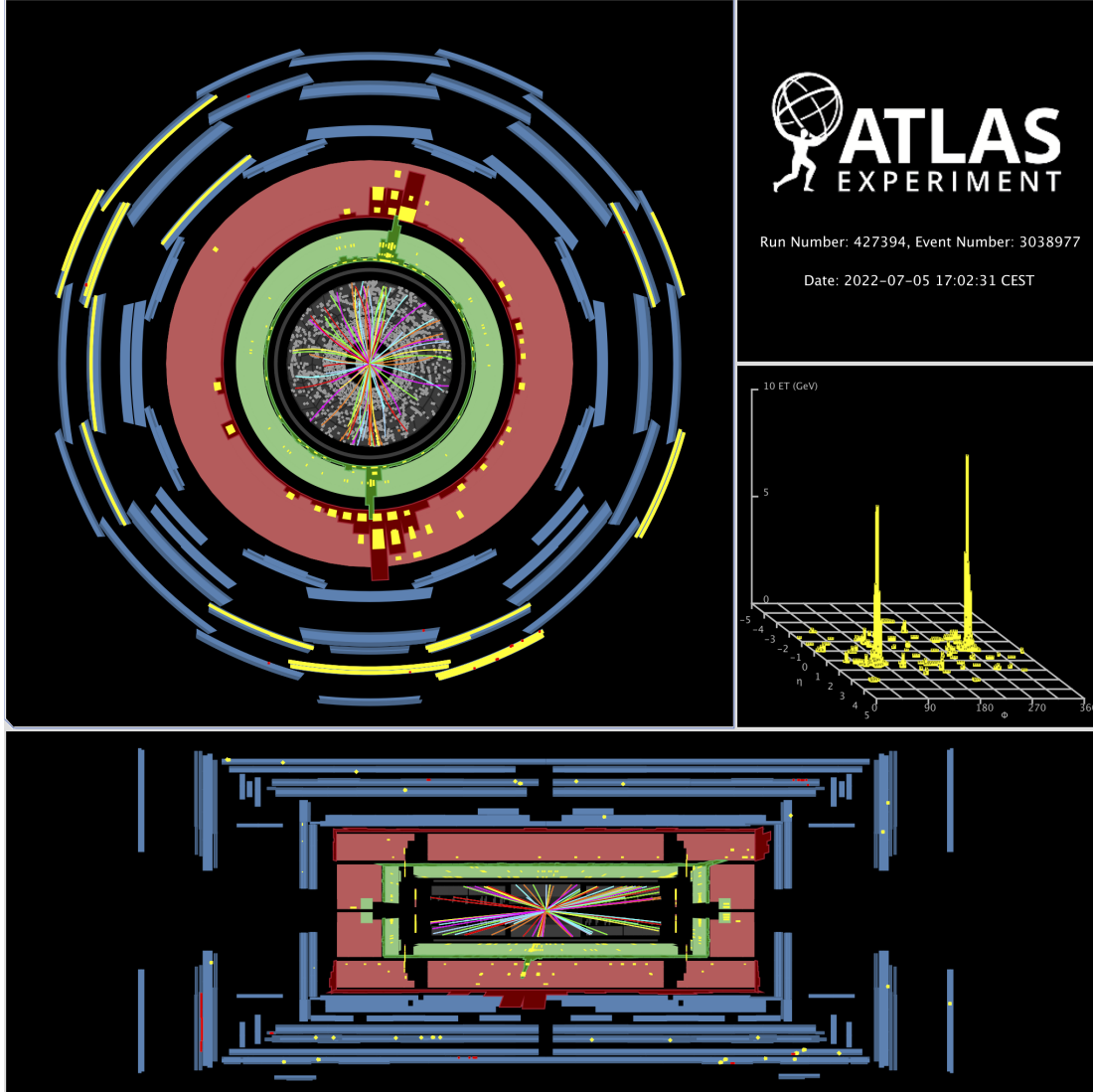


Figure 3.9: First collision delivered by the LHC in ATLAS during the Run 3 [124].





## Chapter 4

# Objects definition and event reconstruction in ATLAS

The *raw data* of an event selected and recorded by the trigger system consist of the electrical signals produced by the interaction of the particles coming from the collision with the material of the sub-detectors described in Chapter 3.2. This event data is then processed to identify and reconstruct the physical objects that created the signals. The identification of the different physics objects and the measurement of their kinematic properties are based on the combination of all the information gathered by the ATLAS sub-systems. An illustration representing the characteristic signatures provided by different types of particles in each of the ATLAS sub-detectors is shown in Figure 4.1.

Following the illustration in Figure 4.1, the trajectories of charged particles such as muons, protons, and electrons are reconstructed with the tracking system. This system is placed inside a magnetic field, which bends the trajectory of these particles allowing for the reconstruction of the sign of their charge and their momentum. Once the tracks are reconstructed, the origin of the particles can be traced back to different interacting points, which are called *vertices*. In the electromagnetic calorimeter, electrons are absorbed and their energy is measured. Photons are also absorbed in the electromagnetic calorimeter, but as they are neutral particles, they do not leave tracks in the tracking system. In the hadronic calorimeter, protons are absorbed and their energy is measured. Neutrons are also absorbed in the hadronic calorimeter, but since they are neutral particles, they do not leave tracks in the tracking system. The energy of all other hadrons is also measured in the hadronic calorimeter. Muons are detected and their

momentum is also measured in the muon spectrometers, which are placed inside a magnetic field. Neutrinos do not interact with the ATLAS detector and they escape undetected. However, their presence can be inferred from an imbalance in the transverse momentum of the full reconstructed event.

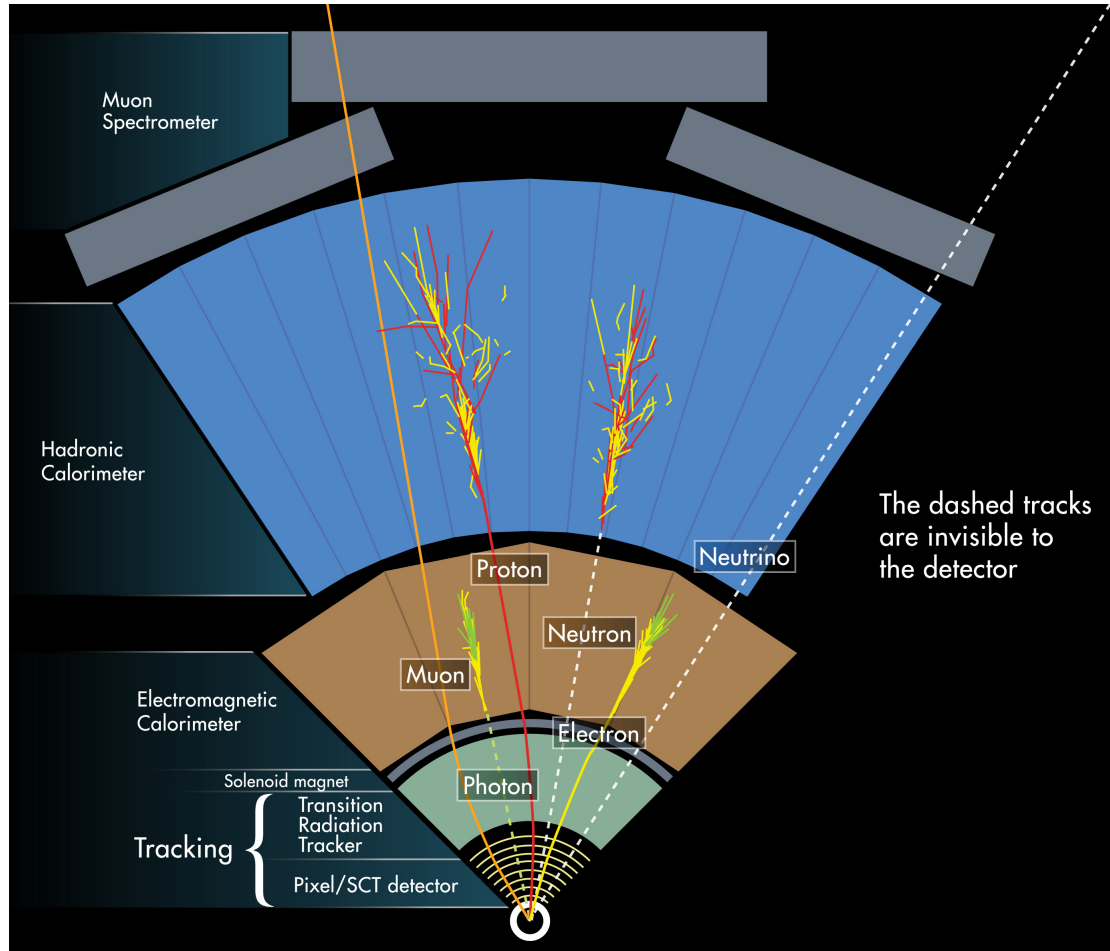


Figure 4.1: Simplified illustration of the signatures provided by different types of particles in each of the ATLAS sub-detectors [125].

This chapter summarises the definition of the physics objects and the reconstruction algorithms used in the ATLAS experiment, with an emphasis on the most relevant aspects for this thesis. The reconstruction of charged tracks and interaction vertices is described in Section 4.1. The identification criteria and the object definition of electrons, muons, and jets are described in Sections 4.2, 4.3, and 4.4, respectively. In Section 4.5, the identification of jets originating from  $b$  quarks is discussed. Section 4.6 describes the calculation of the missing transverse energy in an event. The criterion followed to deal with overlapping reconstructed objects is described in Section 4.7. At last, Section 4.8 contains an overview of

the calibration procedure for large- $R$  jets.

## 4.1 Tracks and vertices

The trajectories associated with charged particles (tracks) are reconstructed mainly from the three-dimensional space coordinates derived from the hits in the Pixel, SCT, and TRT detectors. These detectors are placed within a superconducting solenoid that produces a 2 T magnetic field aligned with the  $z$  axis. The trajectories of the charged particles traversing this field are curved. The curvature of the track enables the determination of the particle charge sign (negative or positive) and its momentum.

Several approaches exist for finding and connecting the space hit points to reconstruct a candidate track. The main pattern recognition algorithm used to reconstruct the tracks follows an inside-out sequence [126], which starts with the Pixel and SCT hits to create a seed and performs hit finding towards the outer part of the ID. This algorithm is complemented by a consecutive outside-in algorithm [127] to reduce the fraction of *fake tracks*<sup>1</sup>.

The locations from where particle tracks originate are called *vertices*. In collider experiments, these tracks can originate from  $pp$  collisions (*primary vertices*) or from the in-flight decay of particles (*secondary vertices*). The vertices reconstruction is performed using vertexing algorithms [128]. For primary vertices, these algorithms start performing a track-to-vertex association (vertex finding) and then they optimize the final position using an iterative fit to minimize the distance between the tracks and the reconstructed vertex. For the search of secondary vertices, which are crucial for identifying jets containing  $b$ -hadrons ( $b$ -jets, Section 4.5), a secondary vertex finder (SVF) algorithm is used [129]. This algorithm is similar to the one used for primary vertices, but it only considers tracks inside a given jet cone (Section 4.4).

Proton bunches at the LHC have a high number of protons, so it is typical to have several  $pp$  collisions during a single bunch crossing. The average number of interactions per bunch crossing for the ATLAS detector during Run 2 is  $\langle\mu\rangle \approx 33.7$  (Figure 3.7 of Section 3.2.6). Given that the bunch width is  $\sim 16\ \mu\text{m}$  in both the

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<sup>1</sup>Fake tracks are reconstructed tracks that do not correspond to any truth level objects' trajectory. They originate from detector noise and/or mismatched hits from multiple different charged particles.

$x$  and  $y$  directions, and  $\sim 75$  mm (0.25 ns) in the  $z$  direction, the secondary  $pp$  collisions inside the same bunch are spread along the  $z$  direction. Usually, only the most energetic  $pp$  collision in an interaction is analyzed, while the other collisions are referred to as *pile-up*. It is also common to only call *primary vertex* the vertex associated with the most energetic collision in the event and to call *pile-up vertices* the vertices associated with all other less energetic collisions. In Figure 4.2, the event display of a  $Z \rightarrow \mu^+\mu^-$  candidate together with 24 additionally reconstructed pile-up vertices is shown.

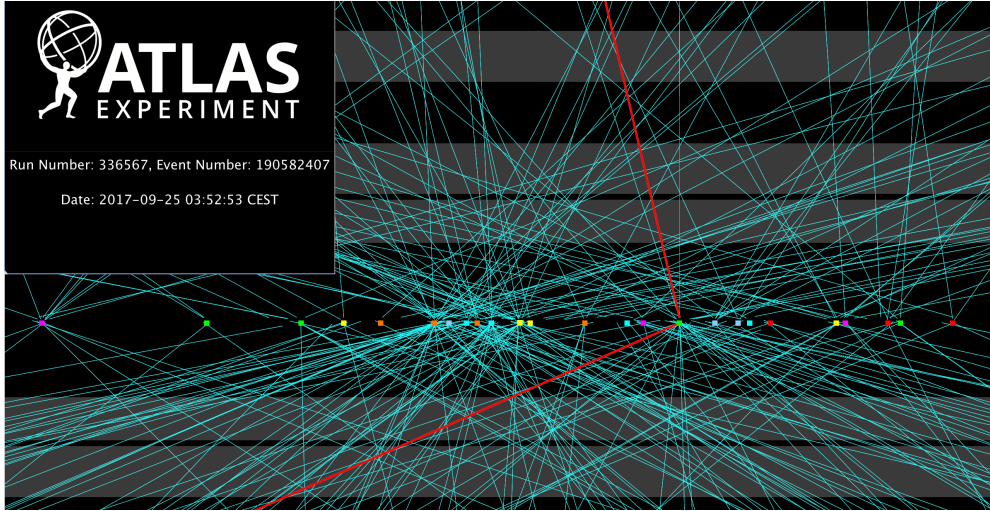


Figure 4.2: Event display of a  $Z \rightarrow \mu^+\mu^-$  candidate reconstructed together with 24 additional pile-up vertices. [130]

The compatibility of a track-to-vertex association is evaluated using two variables called *impact parameters*. The longitudinal and transverse impact parameters ( $z_0$  and  $d_0$ ) are defined as the closest point of approach between a track and a primary vertex in the longitudinal direction (along the  $z$  direction) and in the transverse plane, respectively. The secondary vertices inside a jet are identified using tracks with high impact parameters values (displaced tracks). The reconstruction of secondary vertices plays a key role in the identification of  $b$ -tagged jets and it is further discussed in Section 4.5. An illustration of the track parameters, including the impact parameters, is shown in Figure 4.5.

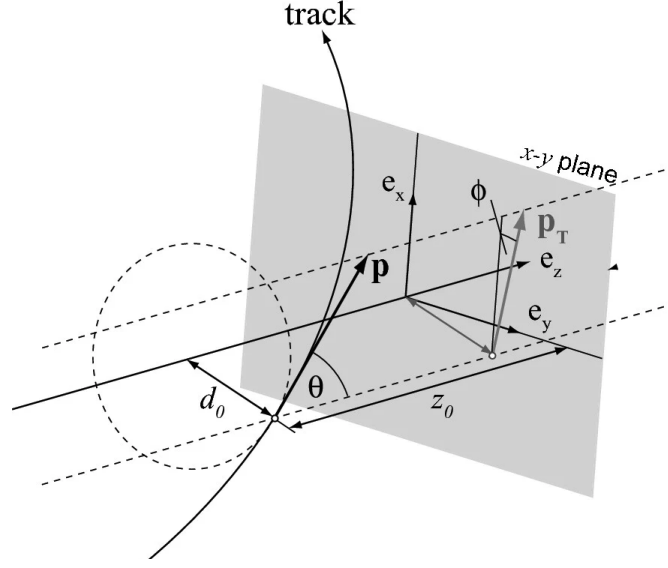


Figure 4.3: Schematic representation of the track parameters, which include the  $p_T$ ,  $\phi$ ,  $\theta$ , and the impact parameters  $z_0$  and  $d_0$  [131].

## 4.2 Electrons

Electron candidates are reconstructed by identifying deposits of energy in the electromagnetic calorimeters (ECal) matched with a track in the ID. The energy deposits of the ECal are clustered into cells with a granularity of  $\eta \times \phi = 0.025 \times 0.025$ . The cells with a transverse energy deposition above 2.5 GeV are used as *seeds* for the clustering algorithm [132]. This algorithm forms the energy clusters by grouping the energy deposits around these seed cells and by merging any pair of close clusters into *superclusters*. The resulting topologically connected cells are referred to as *topo-clusters* and are then matched to the tracks in the ID of at least  $p_T = 0.5$  GeV. If a topocluster in the ECal is not connected to any track, the object is identified and reconstructed as a photon. Only electrons in the central region of the detector ( $|\eta| < 2.47$ ) are considered, excluding the transition region between the barrel and the end-caps of the electromagnetic calorimeter ( $1.37 < |\eta| < 1.52$ ).

Depending on the true origin of an electron candidate reconstructed in the detector, it can be classified into three categories: *prompt electrons*, *non-prompt electrons*, or *fake electrons*. Prompt electrons originate from the hard scattering event and include electrons coming from the decay of  $W$ ,  $Z$ , or  $H$  bosons. Non-prompt electrons originate from the decay product of a secondary particle with a

relatively long lifetime, such as the decay of a  $b$ -hadron or the early conversion of a photon into an electron and a positron. Fake electrons are non-electron objects such as jets or photons that are identified by the algorithm as an electron. The algorithm that is used to distinguish between prompt electrons and the other two categories uses a likelihood-based quality criterion derived from the tracks and energy depositions [133]. The resulting discriminant provides three identification working points labeled as *tight*, *medium*, and *loose*, from most stringent to most relaxed. The events that pass a more stringent working point are a subset of those that pass a more relaxed working point.

To further separate the prompt electrons from non-prompt and fake electrons, an isolation criterion is also defined using the information from the calorimeter and the tracker independently. The calorimeter-based isolation imposes a cut on the energy deposited in the calorimeter cells inside a radius of  $\Delta R = 0.2$  around the electron. The track-based isolation imposes a cut on the transverse momentum of the tracks around a cone of  $\Delta R = 0.3$  around the electron. The calorimeter-based and the track-based isolation criteria are combined into an isolation criterion with three different working points tagged as *tight*, *medium*, and *loose*, following the same logic as in the case of the identification criteria.

To ensure the compatibility of the electron with originating from the event primary vertex, a cut on the impact parameters of  $d_0/\sigma(d_0) < 5$  and  $|z_0 \sin \theta| < 0.5$  mm is recommended for many Run 2 analyses.

At last, the energy of the reconstructed electrons is further calibrated to account for residual differences between the MC simulations and the data response. The uncertainties associated with the calibration of electrons are propagated throughout the analysis.

### 4.3 Muons

Muons experience minimal energy loss through electromagnetic radiation while traversing the ATLAS detector<sup>2</sup>, so they behave as minimum ionizing particles. As a consequence, muons are not stopped in the calorimeters and reach the muon spectrometers. The reconstruction of muon candidates is primarily based on the tracking information from the ID and the MS. However, the calorimeters

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<sup>2</sup>This is due to their mass being  $\sim 200$  times greater than that of electrons

information is also used to account for the energy loss in the calorimeters and for tagging the ID tracks as muon candidates without using the MS data.

Depending on the sub-detector's information used and the algorithm followed to reconstruct the tracks, various muon types are defined in ATLAS. These types are: combined muons, inside-out combined muons, muon-spectrometer extrapolated muons, segmented tagged muons, and calorimeter-tagged muons [134]. A brief description of the reconstruction process for each of these classes is given in the following:

- Combined muons (CB) are identified by matching the tracks reconstructed in the MS to the tracks reconstructed in the ID. Then, a combined track fit is performed using the hits in the ID, the hits in the MS, and considering the energy loss in the calorimeters. This reconstruction is used for muons in the precision region of the ID ( $|\eta| < 2.5$ ). For the region outside the TRT coverage,  $|\eta| > 2.5$ , the only hits in the ID that can be used are the ones in the Pixel and SCT detectors. The subset of combined muons that only use the ID hits in the Pixel and SCT detectors are called the *silicon-associated forward muons*.
- Inside-out combined muons (IO) use a complementary approach to the *combined muons*. In this definition, muons are reconstructed by extrapolating the ID tracks to the MS and searching for at least three loosely aligned hits in the MS. This algorithm does not require a fully independent reconstructed track in the MS. Hence it is able to increase the global muon reconstruction efficiency.
- Muon-spectrometer extrapolated muons are reconstructed when a track in the MS cannot be matched with any of the ID tracks. In this definition, the MS track is extrapolated to the beamline and the muon parameters are obtained directly from the MS track fit.
- Segmented tagged muons (ST) are reconstructed by extrapolating the ID tracks to the MS and searching for at least one local segment in the MS that fulfills a tight angular matching requirement with an ID track. This definition increases the acceptance of muons which only crossed one layer in the MS. The muon parameters are directly obtained from the ID track fit.
- Calorimeter-tagged muons (CT) are reconstructed by extrapolating the ID



tracks through the calorimeters. If the extrapolated energy deposits are compatible with being produced by a minimum ionizing particle, the track is tagged as a muon. As in the case of the *segmented tagged muons*, the muon parameters are directly obtained from the ID track fit. This definition increases the acceptance in the regions where the MS is only partially instrumented.

In a similar manner as for electrons, to distinguish between prompt and non-prompt/fake muons, a series of cut-based selection requirements are used to evaluate the *quality* of the reconstructed muon candidate. This cut-based algorithm is derived from variables that test the compatibility between the measurements performed by the ID and the MS, the number of hits in each of the sub-detectors modules, and the track fit properties. The cuts in this algorithm are chosen to construct three different *working points* labeled, in decreasing level of stringency, as *tight*, *medium*, and *loose*. To further separate prompt from non-prompt/fake muons, an isolation criteria for the ID and the MS tracks is also defined. To ensure the compatibility of the muon originating from the event primary vertex, a cut on the impact parameters of  $d_0/\sigma(d_0) < 3$  and  $|z_0 \sin \theta| < 0.5$  mm is recommended for many Run 2 analyses.

In a similar manner as for electrons, the identification and reconstruction efficiencies of muons are calibrated to account for any residual differences between MC simulated samples and the recorded data. The uncertainties associated with the calibration of muons are propagated through the analyses.

## 4.4 Jets

Color-charged particles such as quarks and gluons cannot be observed freely due to the confinement phenomenon of the strong interaction (Section 1.4). Instead, when a quark or a gluon is produced in a collision, they undergo the so called *showering* and *hadronization* processes. During the showering process, the quarks and antiquarks may branch into  $qg$  and  $\bar{q}g$  pairs, while the gluons may branch into  $q\bar{q}$  or  $gg$  pairs. This branching repeats until the particles reach a scale of  $\sim 1$  GeV. It is around this energy when the hadronization process starts and colored partons combine to form color-neutral bound-states called hadrons. When the energy of the outgoing original parton is high enough, these hadrons form a collimated



stream of particles known as a *jet*. The particles that form this stream are stable or nearly stable, so they are able to reach and interact with the different detector systems of the ATLAS experiment. The tracks of charged hadrons are registered in the tracking system, while their energy is measured in the calorimeters.

The kinematic properties of the original outgoing parton can be derived by clustering the final-state particles measured in the detector into a jet using jet reconstruction algorithms. However, these algorithms can be applied to clusters formed from different kinds of objects, such as partons, truth level particles, topo clusters in the calorimeter, or other objects constructed by combining the information from the tracker and the calorimeter, among other possibilities. The main algorithm used to define and reconstruct jets in ATLAS is the sequential recombination anti- $k_t$  algorithm [135]. The algorithm starts by defining the distance between two objects,  $d_{ij}$ , and the distance between an object and the beam,  $d_{iB}$ , as:

$$d_{ij} = \min\left(\frac{1}{p_{Ti}^2}, \frac{1}{p_{Tj}^2}\right) \frac{\Delta R_{ij}^2}{R^2} \quad (4.1a)$$

$$d_{iB} = \frac{1}{p_{Ti}^2}, \quad (4.1b)$$

where  $i, j$  are the index of two objects,  $p_T$  is the transverse momentum of the  $i^{th}$  object,  $\Delta R_{ij}$  is the angular distance between two objects (Section 3.2.1), and  $R$  is the radius parameter which determines the approximate final size of the jet. Depending on the radius parameter  $R$ , jets can be classified in small- $R$  jets ( $R = 0.4$ ), and large- $R$  jets ( $R = 1.0$ ).

Then, the anti- $k_t$  algorithm proceeds as follows:

1. Search the smallest of the  $d_{ij}$  and  $d_{iB}$  distances for all possible  $i, j$ .
2. (a) If the minimum is a  $d_{ij}$  distance, the  $i$  and  $j$  objects are recombined into a new one following the recombination scheme.
- (b) If the minimum is  $d_{iB}$  distance, then the  $i^{th}$  object is a jet and it is removed from the list of objects to recombine.
3. Repeat until no objects remain in the list.

As it can be inferred from Equations 4.1, the anti- $k_t$  algorithm is dominated by the high  $p_T$  objects. This means that the algorithm prefers to cluster hard objects first, resulting in an area that fluctuates slightly. Thanks to this *soft-adaptable boundary*, the algorithm is safe from infrared and collinear singularities<sup>3</sup>. The anti- $k_t$  algorithm is implemented in ATLAS using the **FastJet** program [136]. In Figure 4.4, a schematic representation of the jet production, detection, and subsequent reconstruction using the anti- $k_t$  algorithm is shown.

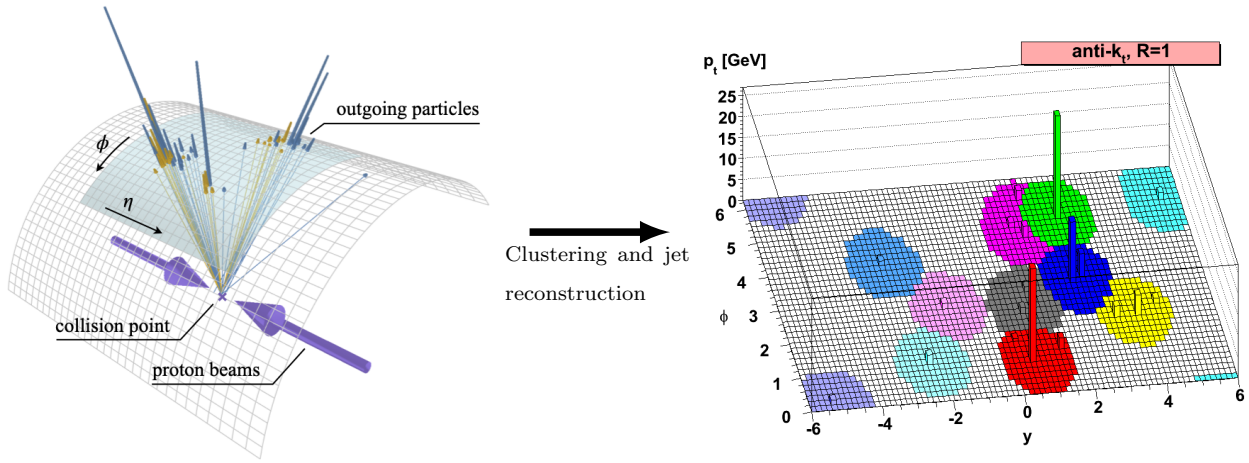


Figure 4.4: Schematic representation of the jet production, detection, and subsequent reconstruction using the anti- $k_t$  algorithm. Left: Illustration of a  $pp$  collision producing two collimated streams of outgoing particles that can be identified as jets. The energy deposition of these particles in the  $\phi - \eta$  plane is also represented [137]. Right: Example of the clustering of the anti- $k_t$  jet reconstruction algorithm in the  $\phi - y$  plane [135]. The two figures do not represent the same event.

In the standard ATLAS Run 2 implementation, the anti- $k_t$  algorithm relies exclusively on the calorimeter topo clusters to reconstruct the jet, overlooking the information provided by the ID about the tracks of charged particles within it. Recently, a new jet definition has been introduced in ATLAS, the so-called *electromagnetic particle flow jets* (EMPflow) [138]. In this new jet definition, the contribution of charged hadrons to the topo clusters is replaced by the more precise ID measurements of their associated track momentum. The introduction of this algorithm improves the resolution in the measured jet momentum, reduces its uncertainties, and leads to a more stable pile-up contribution.

To reduce the contamination from in-time pile-up interactions, the jet-vertex-

<sup>3</sup>Insensitive to soft and collinear gluon emissions, and collinear gluon splitting

tagger (JVT) [139] algorithm is used. The JVT is a likelihood-based algorithm that uses the information of the tracks matched to each jet to create a two-dimensional discriminant that distinguishes between jets originated from the hard scattering, from those originated from pile-up interactions.

At last, the identification efficiency, the reconstruction efficiency, and the jet energy are calibrated to account for residual differences between the MC simulation and the data response. The uncertainties associated with the calibration of jets are propagated through the analyses. A detailed description of the calibration sequence of large- $R$  jets in ATLAS is given in Section 4.8.

## 4.5 Identification of $b$ -jets

The identification of jets originating from the hadronization of  $b$  quarks ( $b$ -jets) is crucial in the reconstruction of events containing top quarks, since this particle decays almost exclusively into a  $W$  boson and a  $b$  quark ( $t \rightarrow Wb$ ). The jets originating from  $b$  quarks contain at least a  $B$ -hadron. Due to their relatively long lifetime of  $\sim 1.5$  ps, high- $p_T$   $B$ -hadrons can travel up to a few centimeters before decaying. This results in a typical decay topology with at least one secondary vertex displayed from the primary vertex of the hard-scattering, as illustrated in Figure 4.5. Using the particularities of their topology,  $b$ -tagging algorithms have been developed to discriminate between  $b$ -jets,  $c$ -jets<sup>4</sup>, and light jets<sup>5</sup>.

For `EMPflow` small- $R$  jets, a deep-learning flavor tagger neuronal network called DL1r [141] is used to perform the  $b$ -tagging. The DL1r  $b$ -tagging is based on the distinctive features of  $b$ -hadrons in terms of the impact parameters of tracks and the displaced vertices reconstructed in the inner detector. The inputs of the DL1r network also include discriminating variables constructed by a recurrent neuronal network (RNNIP) [142]. The tracking information needed for the tagging algorithm is provided by the ATLAS tracking system, which covers the  $|\eta| < 2.5$  range, hence only events within this range can be identified as  $b$ -jets.

The output of the DL1r neural network provides three variables with high discriminant power to select  $b$ -jets,  $c$ -jets, and light jets. These individual outputs are combined to build a single discriminant. The working points for this discriminant can be set to four different working points labeled as 60%,

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<sup>4</sup>Jets initiated by a charm quark

<sup>5</sup>Jets initiated by a light quark (up, down, or strange quark) or by gluons

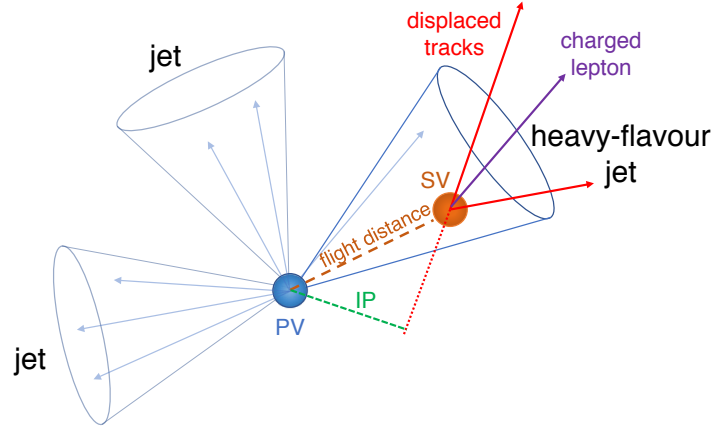


Figure 4.5: Illustration of a collision with a heavy-flavor jet. The heavy-flavor hadrons produced in the primary vertex (PV) decay after propagating for a light distance in the detector, which originates a secondary vertex (SV) and displaced tracks with large values of the impact parameter (IP) [140].

70%, 77%, and 85%. The number on these working points represents the  $b$ -jet efficiency from the most stringent to the most relaxed. The rejection power of  $c$ -jets and light-jets is maximum for the 60% working point. As the jets that pass the conditions of a stringent working point are a subset of the events that pass the conditions of a more relaxed working point, a combination of the four different working points of the DL1r tagger into a single pseudo-continuous variable is also provided. This variable takes an integer value that indicates how many of the fixed working points is the  $b$ -jet candidate able to fulfill. The variable associated with the pseudo-continuous working point is one of the most important inputs provided to the SPA-NET neuronal network of Section 7 to predict the correct jet-to-parton assignment during the event reconstruction.

## 4.6 Missing transverse energy

In collider experiments, the sum of the transverse momenta of all the products of a collision should be effectively zero due to the momentum conservation in the transverse plane to the beam axis. Experimentally, this is computed considering all the detected particles in the detectors. However, the presence of undetected particles such as neutrinos in the SM or other BSM weakly interacting particles, may lead to a momentum imbalance. This imbalance is known as the *missing transverse momentum*,  $E_T^{\text{miss}}$ , and it is calculated from the vector sum of the

$p_T$  of all reconstructed objects (pre-overlap removal, Section 4.7), and with the additional soft terms<sup>6</sup> [143]. The basic set of observables constructed from these quantities are shown in Equation 4.2. They include the previously defined  $E_T^{\text{miss}}$ , its decomposition in the  $x$  and  $y$  axis components,  $E_{x(y)}^{\text{miss}}$ , its angular direction on the transverse plane,  $\phi^{\text{miss}}$ , and the  $W$  boson transverse mass,  $m_T^W$ , used in the case of events which are expected to contain a single leptonically decaying  $W$  boson.

$$E_{x(y)}^{\text{miss}} = - \sum_{i \in \{\text{hard objects}\}} p_{x(y),i} - \sum_{j \in \{\text{soft signals}\}} p_{x(y),j} \quad (4.2a)$$

$$E_T^{\text{miss}} = \sqrt{(E_x^{\text{miss}})^2 + (E_y^{\text{miss}})^2} \quad (4.2b)$$

$$\phi^{\text{miss}} = \tan^{-1}(E_y^{\text{miss}}/E_x^{\text{miss}}) \quad (4.2c)$$

$$m_T^W = \sqrt{2p_T^l E_T^{\text{miss}} (1 - \cos(\phi^l - \phi^{\text{miss}}))} \quad (4.2d)$$

A fake imbalance in the  $E_T^{\text{miss}}$  can arise from the finite resolution of the detectors, badly reconstructed particles, particles outside the detector acceptance, any source of noise, or possible dead regions in the detectors. The uncertainties associated to these effects are evaluated by propagating the uncertainties in each of the reconstructed objects to the  $E_T^{\text{miss}}$ . The uncertainty on the  $p_T$  scale and resolution of the *soft terms* are also evaluated by including the influence of the modeling of the underlying event.

## 4.7 Object overlap removal

The same energy deposits in the detectors can satisfy the selection criteria of different objects at the same time. To solve the ambiguities that can arise

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<sup>6</sup>The soft terms are constructed with all the tracks that are associated with the primary vertex but not associated to any of the reconstructed objects.

from the independent reconstruction of electron, muon, and jet candidates in the detector, the recommended overlap removal procedure of the ATLAS collaboration is applied. Considering all the objects used in the top quark mass measurement of this thesis, the sequential overlap removal algorithm consists of the following steps:

1. Any calorimeter muon found to share a track with an electron is removed.
2. Any electron found to share a track with a muon is removed.
3. Any jet found within a  $\Delta R$  of 0.2 of an electron is removed.
4. Any electron subsequently found within  $\Delta R$  of 0.4 of a jet is removed.
5. Any jet with less than 3 tracks associated to it found within  $\Delta R$  of 0.2 of a muon is removed.
6. Any jet with less than 3 tracks associated to it which has a muon inner-detector track ghost-associated to it, is removed.
7. Any muon subsequently found within  $\Delta R$  of 0.4 of a jet is removed.

## 4.8 Large- $R$ jet definition, calibration, and uncertainties in ATLAS

During the Run 2 of the LHC, it has become relatively frequent to produce signatures of very massive particles such as  $Z$ ,  $W$ , or  $H$  bosons, or top quarks with a high transverse momentum. When one of these massive unstable particles decays hadronically, due to their large transverse momentum, their decay products become collimated (boosted) along the direction of the initial particle. In particular, when a particle of mass  $m$  is produced with a transverse momentum  $p_T$ , then its decay products mostly fall into a cone with an angular size of  $R \approx 2m/p_T$  [144]. This means that, for example, the decay products coming from a hadronically decaying  $W$  boson with  $p_T \gtrsim 200$  GeV or a hadronically decaying top quark with a  $p_T \gtrsim 300$  GeV are expected to be contained in a jet with a radius parameter of  $R \approx 1$ , a large- $R$  jet. An illustration showing the *resolved* and *boosted* regimes in a full hadronic top decay can be found in Figure 4.6, whereas

a recorded ATLAS Run 2 event containing a boosted top quark pair candidate in the  $\mu$ +jets channels can be found in Figure 4.7.

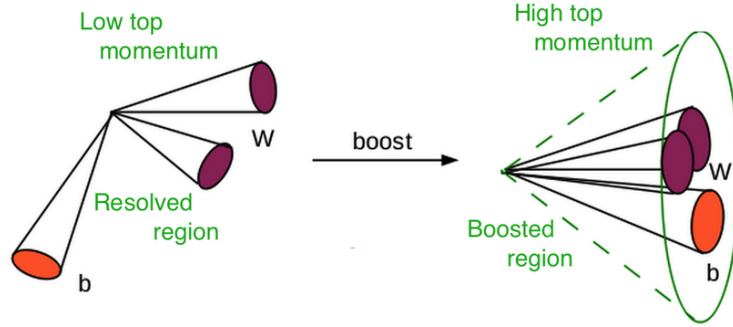


Figure 4.6: Sketch of the resolved and boosted regions (regimes) of the top quark hadronic decay.

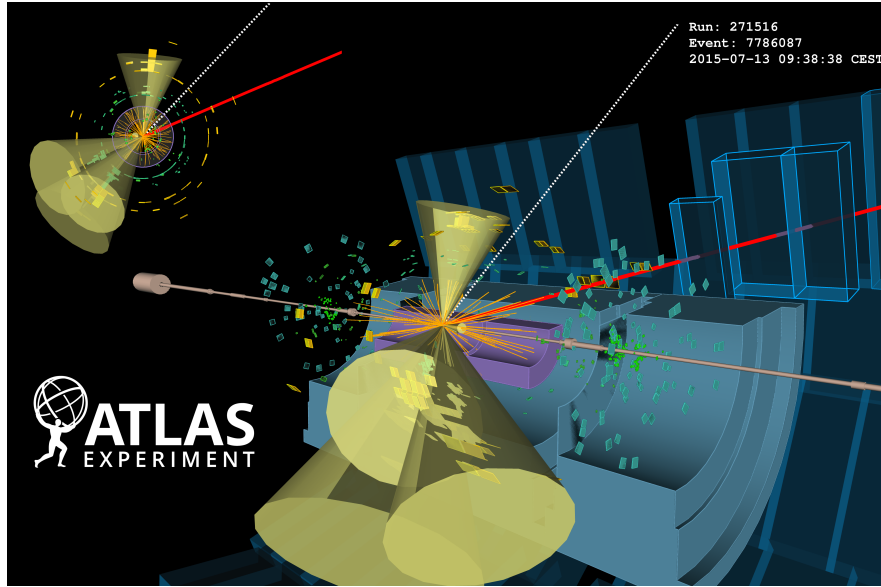


Figure 4.7: Display of a  $t\bar{t}$  event candidate containing a boosted top quark in the  $\mu$ +jets decay channel. The three overlapping small- $R$  jets are identified as coming from a boosted hadronically decaying top quark ( $t \rightarrow Wb$ ,  $W \rightarrow q\bar{q}'$ ). These three small- $R$  jets are reclustered into a single large- $R$  jet, even though it is not explicitly shown [145].

The basic definition of jets in ATLAS can be found in Section 4.4. In the current section, more details about the large- $R$  jets calibration procedure are provided, with a particular focus on the *in-situ* calibration and the implementation of its associated uncertainties into the ATLAS software framework. This section is organized as follows: In Section 4.8.1, the calibration sequence of large- $R$  jets

is described. Section 4.8.2 introduces one of the methods used in the calibration sequence, the forward folding method, then this method is used in Section 4.8.3 to measure the Jet Mass Scale (JMS) and the Jet Mass Resolution (JMR) of large- $R$  jets using the  $Z/W$  mass peak in  $W/Z$ +jets events. At last, in Section 4.8.4, the tool used to implement the JMR uncertainties within the ATLAS software framework is briefly described.

### 4.8.1 Calibration sequence for large- $R$ jets

The sensitivity of many searches and measurements that use large- $R$  jets is highly dependent on the knowledge of the detector responses to the jet transverse momentum,  $p_T$ , and the jet mass,  $m$ . To study and calibrate these responses, the large- $R$  jets in ATLAS follow the stages represented in Figure 4.8.

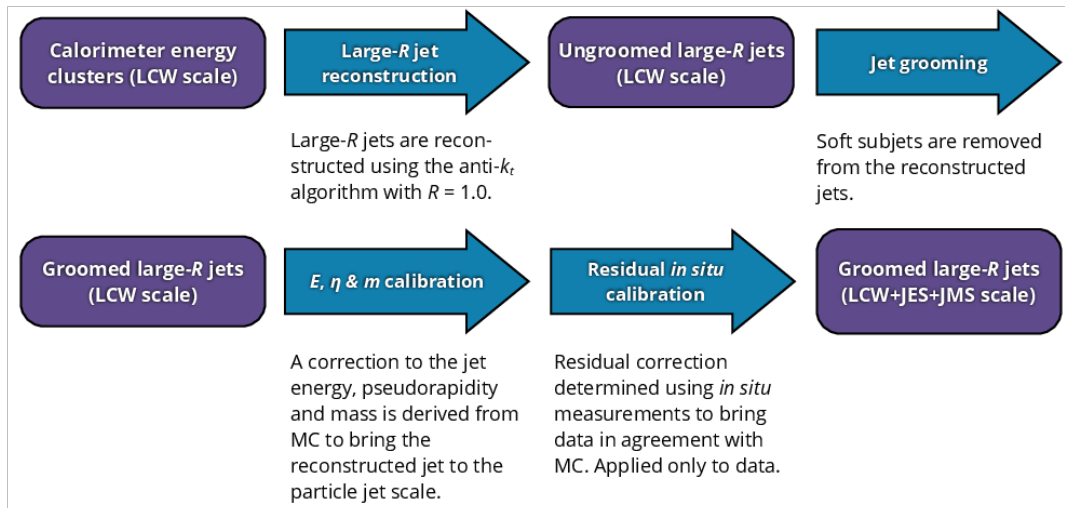


Figure 4.8: Overview of the reconstruction and calibration sequence applied to obtain the standard large- $R$  jet collection used in ATLAS [146].

The reconstruction and calibration procedure of large- $R$  jets starts by reconstructing the jets from the clusters of topologically connected calorimeter cell signals using the anti- $k_t$  algorithm with a radius parameter of  $R = 1.0$ , following the procedure described in Section 4.4.

To reduce the contamination from pile-up interactions, the underlying event, and soft emissions, jets are groomed using the trimming algorithm described in Ref. [147]. This algorithm recombines the constituents of each  $R = 1.0$  jet into sub-jets with  $R = 0.2$ . Then, the constituents of the sub-jets with a



relatively small contribution to the total transverse momentum of the large- $R$  jet,  $p_{\text{T}}^{\text{sub-jet}}/p_{\text{T}}^{\text{jet}} < 0.05$  are removed, and the large- $R$  jet is reconstructed again using only the remaining constituents. The application of jet grooming leads to a significant improvement in the jet energy and mass resolutions.

The groomed large- $R$  jet energy is then calibrated using MC simulated di-jet samples to restore the scale of particle-level jets. The pseudorapidity ( $\eta$ ) of the reconstructed jets is also calibrated to correct a bias between the detector and particle level jets in certain regions of the detector. This calibration is applied as a function of the reconstructed jet energy and pseudorapidity. In this step of the calibration process, the jet mass can be also corrected by combining the jet mass measured in the calorimeters with the mass measurement of the associated charged hadron component of the jet in the Inner Detector. Whether this correction is applied or not gives rise to two different mass definitions, the *calorimeter jet mass*,  $m^{\text{calo}}$ , and the *track-assisted jet mass*,  $m^{\text{TA}}$ :

$$m^{\text{calo}} = \sqrt{\left(\sum_{i \in \text{constituents}} E_i\right)^2 - \left(\sum_{i \in \text{constituents}} \vec{p}_i\right)^2} \quad (4.3)$$

$$m^{\text{TA}} = \frac{p_{\text{T}}^{\text{calo}}}{p_{\text{T}}^{\text{tracks}}} \times m^{\text{tracks}}. \quad (4.4)$$

At last, a residual *in-situ* calibration is applied only to data using data-driven methods to check and correct the residual mismodeling of the simulated detector response and resolution to the jet  $p_{\text{T}}$  and  $m$ . The four quantities that are calibrated at this stage are the Jet Energy Scale and Resolution (JES and JER), and the Jet Mass Scale and Resolution (JMS and JMR). The JES and JER parametrize the  $p_{\text{T}}$  response, whereas the JMS and JMR parametrize the mass response. They are defined as:

$$\text{JES} = \frac{\langle p_{\text{T}}^{\text{data}} \rangle}{p_{\text{T}}^{\text{MC}}} \quad \text{JER} = \frac{\sigma(p_{\text{T}}^{\text{data}})}{\sigma(p_{\text{T}}^{\text{MC}})} \quad (4.5)$$

$$\text{JMS} = \frac{\langle m^{\text{data}} \rangle}{m^{\text{MC}}} \quad \text{JMR} = \frac{\sigma(m^{\text{data}})}{\sigma(m^{\text{MC}})} \quad (4.6)$$

where,  $\langle x \rangle$  and  $\sigma(x)$  represent the mean value and resolution of the variable  $x$ . The calibration of these quantities is determined in two sequential steps: First, the JES and JER are determined using event topologies where the jet being calibrated recoils against a reference object or system with a well-known momentum scale [146]. By applying the conservation of  $p_T$  in the system, the jet energy scale and resolution can be corrected using the  $p_T$  measurement of the reference object in the event. In Figure 4.9, the three topologies used for the JES/JER calibration of large- $R$  jets are schematically represented. In these topologies, the reference object can be a photon or a leptonically decaying  $Z$  boson, for which the  $p_T$  is measured precisely, a system of calibrated small- $R$  jets, or a pre-calibrated large- $R$  jet located in the central region of the detector, which can be used to calibrate large- $R$  jets in the forward region of the detector.

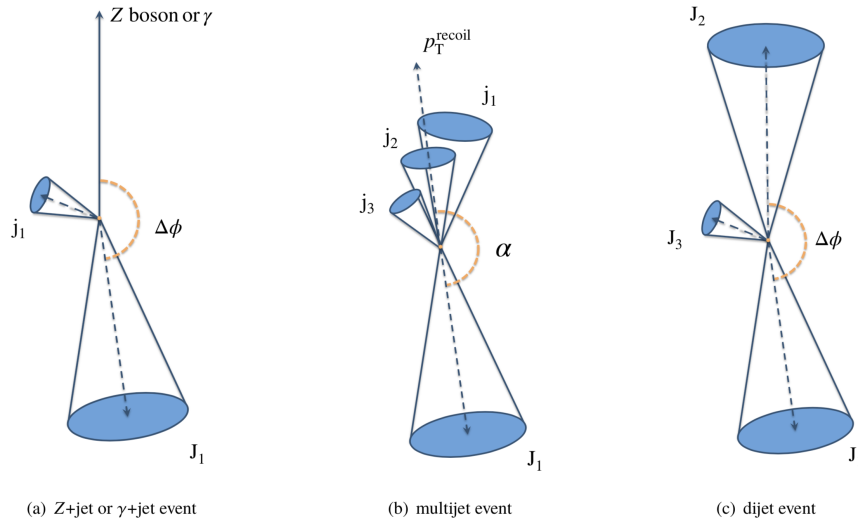


Figure 4.9: Schematic representation of the event topologies used to constrain the JES and JER. (a)  $Z/\gamma$ +jet event, used for the direct balance method. (b) Multijet event with several small- $R$  jets recoiling against a large- $R$  jet. (c) A dijet event, used for the  $\eta$  intercalibration. Figure taken from Ref. [146].

The second step consists of the calibration of the JMS and JMR, which is determined using the  $R_{trk}$  method and forward folding method.

In the  $R_{trk}$  method, the JES (JMS) is determined from the double ratio of track to calorimeter  $p_T$  ( $m$ ) between data and the MC simulation (Equation 4.7). If the simulation describes the detector response properly, the ratio of the double ratios should be one. Any deviation from unity indicates imperfections in the modeling of the detector response and can be used to calibrate it. This method is used to calibrate large- $R$  jets in the  $p_T$  range between 150 to 3000 GeV in the

$|\eta| < 1.2$  range but it can only cover low jet masses.

$$R_{trk} = \frac{\left(\frac{p_T^{\text{calo}}}{p_T^{\text{track}}}\right)^{\text{data}}}{\left(\frac{p_T^{\text{calo}}}{p_T^{\text{track}}}\right)^{\text{MC}}} \qquad R_{trk} = \frac{\left(\frac{m^{\text{calo}}}{m^{\text{track}}}\right)^{\text{data}}}{\left(\frac{m^{\text{calo}}}{m^{\text{track}}}\right)^{\text{MC}}} \quad (4.7)$$

In the forward folding method, the JMS and the JMR are obtained by fitting the mass peak of boosted hadronically decaying resonances. The method was applied for the first time in  $t\bar{t}$  events to fit the large- $R$  jet mass peak of boosted  $W$  boson and top quark candidates. The position and shape of these peaks are related to the relative JMS and JMR between the data and the simulation. An example of these peaked distributions for the calorimeter jet mass is shown in Figure 4.10. Section 4.8.2 contains a detailed description of the forward folding method. The most recent analysis of the in-situ calibration using forward folding is found in Ref. [148]. In this article, the JMS/JMR measurements obtained using  $t\bar{t}$  events are complemented, for the first time, with measurements using  $W/Z$ +jets events. A detailed description of the procedure followed to obtain the *in-situ* JMS/JMR measurements in  $W/Z$ +jets events can be found in Section 4.8.3.

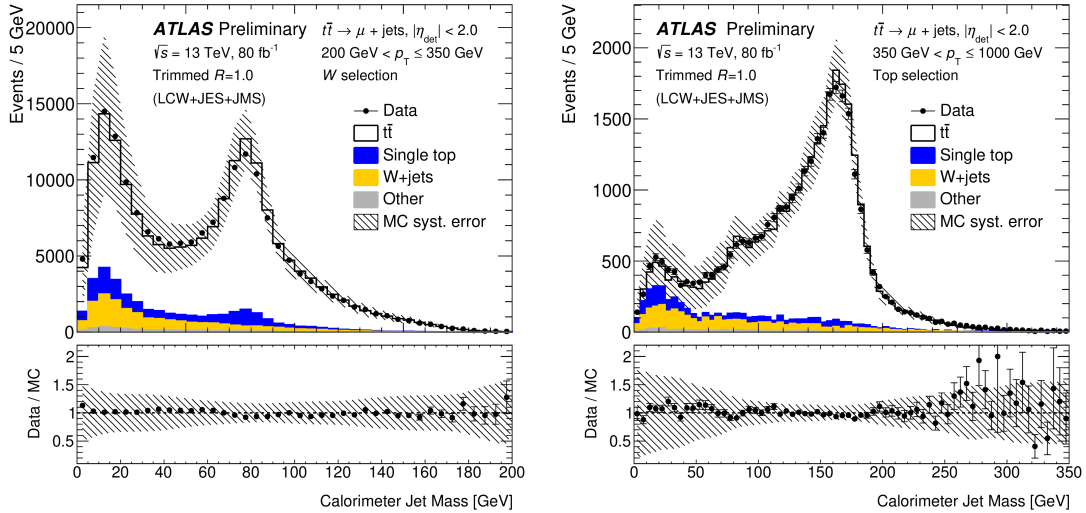


Figure 4.10: Calorimeter jet mass distributions for trimmed large- $R$  jets used for extracting the jet mass scale and resolution using the forward folding method in [148]. The left plot includes the jets that pass the  $W$  selection and on the right the jets that pass the top quark selection in  $t\bar{t}$  events.

### 4.8.2 The forward folding method

The forward folding (FF) method is a technique able to model the response of the detector without assuming a specific shape. This characteristic makes the method perfect to model complex, non-gaussian, and analytically difficult to model transformations such as the detector response to the jet mass. To do so, instead of assuming a specific analytical form, the forward folding method takes the response from the MC simulation. Then, the method takes the particle-level distribution and provides a detector-level distribution where the jet mass response has been modified. Comparing the different modified detector-level distributions with the data enables the determination of the jet mass scale and resolution. At a practical level, the particle level jet mass (truth) is folded, event-by-event, to construct the forward folded mass distribution ( $m_{\text{fold}}$ ) according to the following equation:

$$m_{\text{fold}} = s m_{\text{det}} + (m_{\text{det}} - \langle m_{\text{det}} | m_{\text{truth}} \rangle)(r - s), \quad (4.8)$$

where  $m_{\text{det}}$  is the jet mass for a particular large- $R$  jet in an event,  $m_{\text{truth}}$  is its associated mass at particle level,  $\langle m_{\text{det}} | m_{\text{truth}} \rangle$  is the average detector response derived from simulations,  $s$  is the relative jet mass scale, and  $r$  is the relative jet mass resolution. For values of  $0 \leq (r, s) \leq \infty$ , the jet mass scale and resolution of the  $m_{\text{fold}}$  distribution is, respectively,  $s$  and  $r$  times the scale and resolution of the original simulated detector level jet mass,  $m_{\text{det}}$ . In particular, for  $s = r = 1$  the nominal jet mass response is unaltered, for  $s = 0$  and  $r = 1$  the folded distribution coincides with the truth level one, and for  $r < 1$  resolution of the folded distribution is smaller than the nominal one at detector level.

The alternative detector level distributions obtained by the forward folding procedure of Equation 4.8 are compared to data to find the modified jet mass response that best describes the data. To do so, the  $s$  and  $r$  parameters are determined using the following two-dimensional  $\chi^2$  fit:

$$(r, s) = \arg \min_{(r', s')} \sum_{i=1}^{n_{\text{bins}}} \left( \frac{h_i^{\text{sim}}(r', s') - h_i^{\text{data}}}{\sigma_i} \right)^2, \quad (4.9)$$

where  $h_i^{\text{sim}}$  and  $h_i^{\text{data}}$  represent the content of the  $i^{\text{th}}$  bin of the  $m_{\text{fold}}$  histogram and the  $m_{\text{data}}$  histogram, respectively. Each histogram has a total of  $n_{\text{bins}}$  and the uncertainty  $\sigma_i$  only includes the data and MC statistical error associated with the  $i^{\text{th}}$  bin.

The  $s$  and  $r$  parameters in the fit are then identified as the relative  $\text{JMS} = \text{JMS}^{\text{data}}/\text{JMS}^{\text{MC}}$  and  $\text{JMR} = \text{JMR}^{\text{data}}/\text{JMR}^{\text{MC}}$  values, respectively.

The forward-folding method is only used to estimate the jet energy and mass response of the detector but, in principle, it can be applied to study the detector response of any observable for which particle and detector level information are available. This can be done by replacing the  $m$  in Equations 4.8 and 4.9 by the desired variable that wants to be studied.

### 4.8.3 Measurement of the JMS and JMR for large- $R$ jets using the $Z/W$ mass peak

The measurements of the JMS and JMR using forward folding in  $t\bar{t}$  events lack statistics for  $W$  bosons with  $p_{\text{T}} > 700$  GeV. To complement that analysis, the JMS and JMR are extracted for the first time using the forward folding method in  $W/Z$ +jets event topologies. The main advantage of this topology is that it can be used to study vector bosons produced in a higher  $p_{\text{T}}$  regime than in the  $t\bar{t}$  topology, which increases the transverse momentum coverage of the JMS and JMR measurements. The analysis presented in this section, including the custom boosted  $W/Z$  tagger described in Appendix A, was performed by the author of this thesis during his qualification as an author of the ATLAS collaboration.

To obtain a sample enriched with boosted  $W/Z$ +jets events, the events considered in this analysis are required to fulfill basic selection criteria that consists of having at least two large- $R$  jets with  $p_{\text{T}} > 200$  GeV, a leading large- $R$  jet with  $p_{\text{T}} > 500$  GeV, and all large- $R$  jets are required to be found in the central region of the detector,  $|\eta| < 2$ . This basic selection criteria leads to a distribution that contains  $W/Z$ +jets events but is dominated by multijet background events. To enhance the ratio of the  $W/Z$ +jets signal over the multijet background, a custom  $W/Z$ -jet tagger has been developed using two jet substructure variables which were found to have a good sensitivity in tagging  $W/Z$  jets [149]. These variables are  $D_2$  and the number of tracks associated with the jet,  $N_{\text{trk}}$ . A description of these variables and the optimization studies performed to construct

the custom  $W/Z$  jet tagger are presented in Appendix A. For an event to be considered in the analysis, it has to fulfill the basic selection criteria and the leading  $p_T$  jet has to be tagged as a  $W/Z$ -jet, whereas the subleading jet has to fail the tagger algorithm.

The data samples used in this analysis correspond to the data-taking periods of 2015, 2016, and 2017 for a total integrated luminosity of  $80 \text{ fb}^{-1}$ . The shape and relative contribution of the  $W/Z$ +jets signal and the backgrounds have been estimated using MC simulations. The signal samples have been generated using SHERPA 2.2.1, whereas the multijet background has been estimated using PYTHIA 8.186. Since the forward folding method is only affected by the shape of the distribution and not the global normalization, the total number of events in the simulations is normalized to the total number of events in data after the selection is applied. The analysis is performed for two of the large- $R$  jet mass definitions described in Section 4.8.1, the calorimeter mass,  $m^{\text{calo}}$ , and the track assisted mass,  $m^{\text{TA}}$ . Figure 4.11 shows the resulting jet mass distributions after the basic event selection and the tagging requirements have been applied.

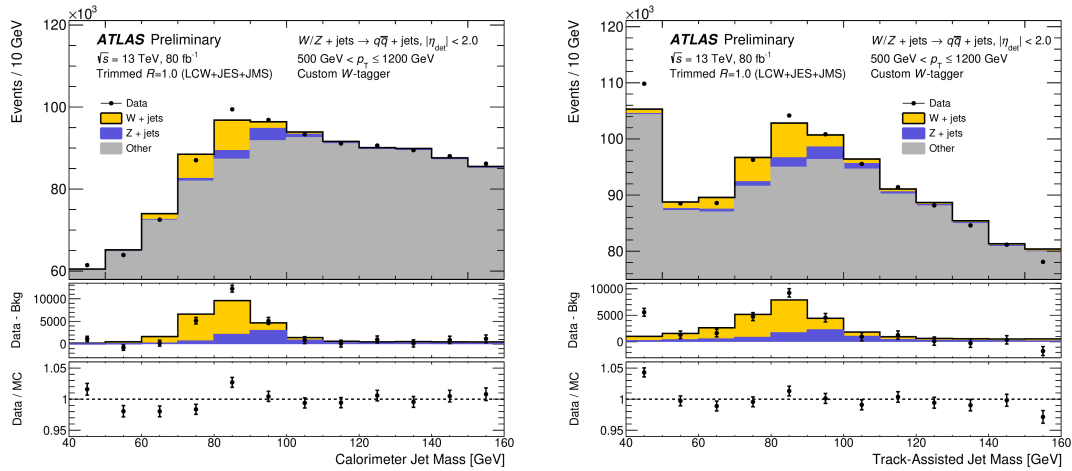


Figure 4.11: Left: calorimeter jet mass distribution for trimmed jets passing the  $W/Z$ +jets selection. Right: the same distribution constructed using track-assisted jets. The *other* category includes all background processes, which are dominated by the multijet production.

Before the forward folding method is applied to extract the data-to-MC relative jet mass scale and resolution, the  $m^{\text{calo}}$  and  $m^{\text{TA}}$  distributions are further divided into four distinct  $p_T$  intervals corresponding to  $[500, 600]$ ,  $[600, 750]$ ,  $[750, 900]$ , and  $[900, 1200]$  GeV. The full signal+background MC predictions are normalized to data independently for each  $p_T$  interval, but the normalization coefficients

vary less than 5% between intervals. Then, the two-dimensional fit described in Section 4.8.2 is performed in the mass region around the  $W/Z$  mass peak, between 50 and 120 GeV. The JMS and JMR measurements resulting from these fits, together with the JMS/JMR measurements performed in  $t\bar{t}$  events, are summarized in Figure 4.12 and 4.13.

A detailed description of the uncertainties associated with the measurements in  $W/Z$ +jets topologies is given in Appendix B. The measurements performed using  $W/Z$ +jets events are found to be compatible with the ones performed with top jets  $t\bar{t}$  events within the uncertainties. This compatibility suggests that the difference between the jet mass scale and response between data and MC is independent of the event topology from which it is extracted. The new JMS/JMR measurements extend the previous  $p_T$  coverage of the measurements up to 1.2 TeV. All the measurements are found to be compatible with one and approximately constant across the  $p_T$  range, which indicates that the JES/JER *in-situ* calibration is sufficient to correct for the JMS/JMR differences between data and simulation. For this reason, no nominal jet mass scale and resolution calibration are applied for the large- $R$  jets in ATLAS. Nevertheless, the uncertainties associated with these quantities are implemented in the ATLAS software framework to be propagated to all the analyses that use large- $R$  jets across the collaboration. In Section 4.8.4, the tool that is used for the implementation of the JMR uncertainties within ATLAS is briefly described.

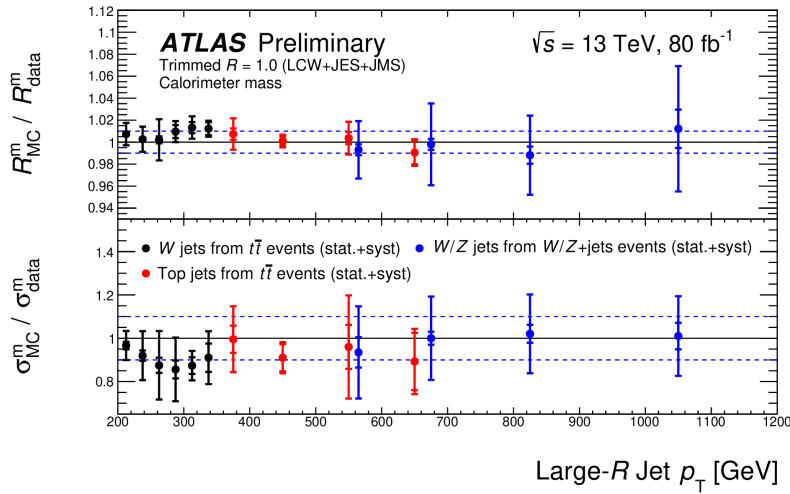


Figure 4.12: The relative jet mass scale and resolution of large- $R$  jets as a function of the jet  $p_T$  for calorimeter mass jets.

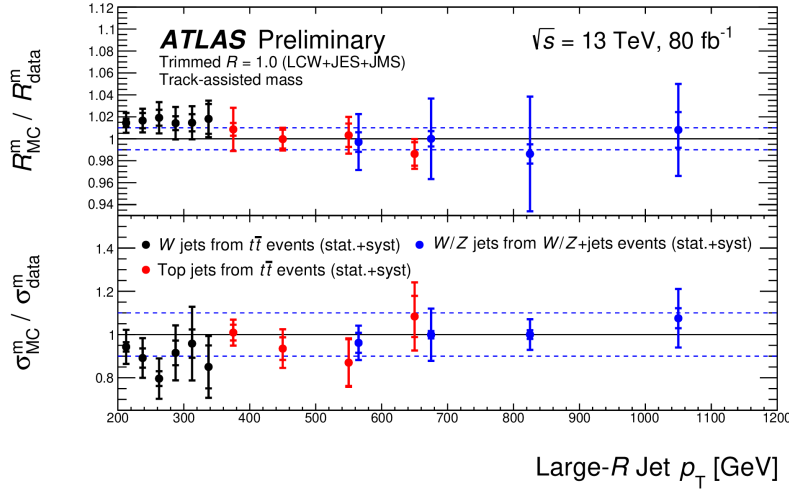


Figure 4.13: The relative jet mass scale and resolution of large- $R$  jets as a function of the jet  $p_T$  for track-assisted mass jets.

#### 4.8.4 Implementation of the large- $R$ jets JMR uncertainties in the ATLAS software framework

The jet mass resolution for large- $R$  jets and their associated uncertainties are derived using the forward folding technique in  $t\bar{t}$  and  $W/Z$ +jets event topologies. In order to apply the derived recommendations across the collaboration, the information extracted from these measurements has to be integrated into the Athena ATLAS software framework. To do so, a tool called the *Forward Folding Jet Smearing Tool* (FFJetSmearingTool) [150] has been developed and integrated into the ATLAS framework. The FFJetSmearingTool was developed by the author of this thesis while qualifying as an author of the ATLAS collaboration, and he continued to maintain and update the tool throughout the entire duration of the thesis.

The FFJetSmearingTool is a C++/ROOT [151] compatible class used to access the current estimate of the uncertainties on the *in-situ* Jet Mass Scale (JMS) and Jet Mass Resolution (JMR) for Run 2 data. However, currently the tool is used to propagate the JMR uncertainties only. The JMS uncertainties are also implemented in the tool, but as of April 2023, the recommended approach is to use the standard gaussian smearing instead of forward folding.

The uncertainties provided via the tool include a large number of terms originated directly from the *in-situ* JMR measurements, and additional



uncertainties addressing differences in the modeling of different jet topologies (QCD vs.  $W/Z/H$ /top jets). These uncertainties are organized in the  $p_T$  vs.  $m$  two dimensional plane, however, as the forward folding measurements do not cover the full phase space, a flat 20% is used in the regions where no measurements are available. A comparison of the JMR uncertainties used in the tool for two different jet mass windows are shown in Figure 4.14. For now, they do not include the measurements in  $W/Z$ +jets topologies.

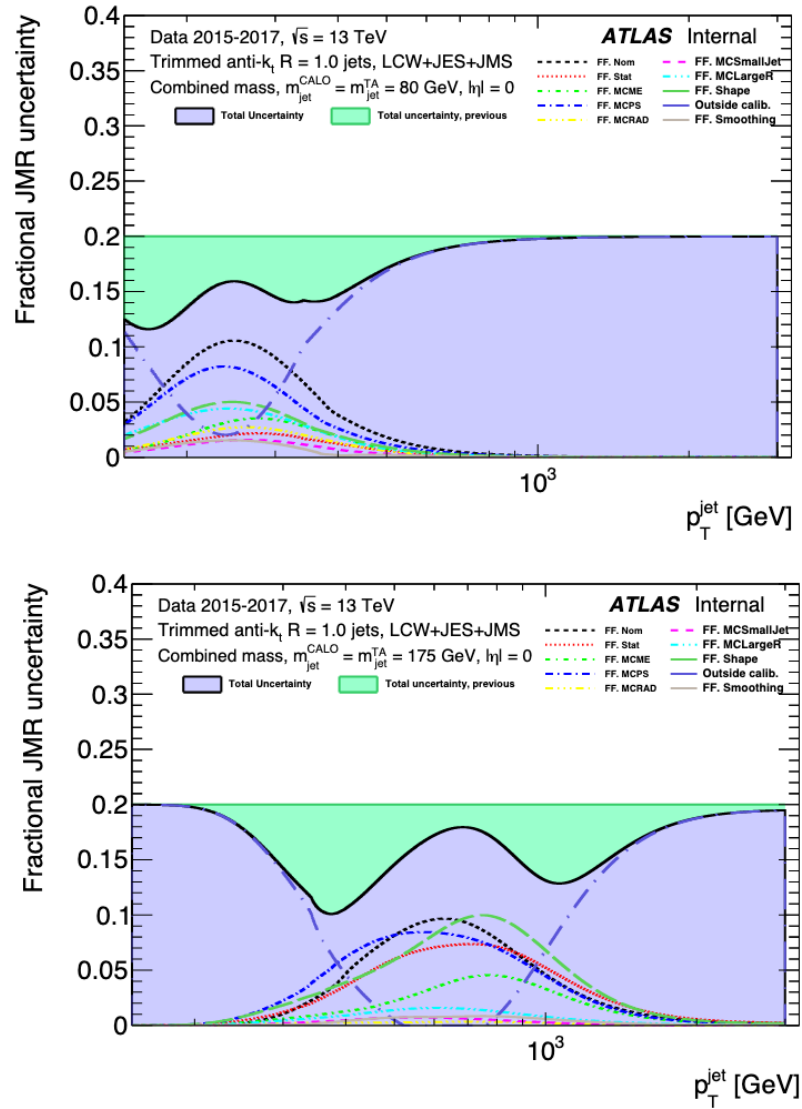


Figure 4.14: The JMR uncertainties implemented in the FFJetSmearingTool compared with the previous recommendation of applying a 20% uncertainty across all  $p_T$  and jet masses values. The recommendations are shown for the two mass values: top:  $m_{\text{jet}}^{\text{Comb}} = 80$  GeV, bottom:  $m_{\text{jet}}^{\text{Comb}} = 175$  GeV

To propagate the *in-situ* JMS and JMR uncertainties across the analyses, the

`FFJetSmearingTool` uses the same technique employed to derive them in the first place, the forward folding method (Section 4.8.2).

Using this method, the tool is able to model properly the non-gaussian response of the detector to the jet mass. Moreover, FF provides a methodology to *un-smear* the original distributions by setting  $r < 1$  in Equation 4.8, something that is not possible to achieve with the previously used *gaussian smearing*.

# Chapter 5

## Top quark mass measurement in semileptonic $t\bar{t}$ +jet events: Analysis overview

This chapter provides a brief overview of the strategy followed to perform the main analysis of this thesis: the top quark pole mass measurement using semileptonically decaying  $t\bar{t}$ +jet events with the full Run 2  $pp$  collision dataset at 13 TeV. This chapter serves as an index, organizing all the information provided in Chapters 6 to 9, thereby facilitating the retrieval of relevant information and highlighting the significance of each chapter within the overall analysis.

The observable used to perform the top quark pole mass measurement presented in this thesis is the  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$ , defined as:

$$\mathcal{R}(m_t^{\text{pole}}, \rho_s) = \frac{1}{\sigma_{t\bar{t}+\text{jet}}} \frac{d\sigma_{t\bar{t}+\text{jet}}}{d\rho_s}(m_t^{\text{pole}}, \rho_s), \quad \rho_s = \frac{2m_0}{\sqrt{s_{t\bar{t}+\text{jet}}}} \quad (5.1)$$

The motivation behind the definition of this observable is discussed in detail in Section 2.3.3, which also contains an overview of the previous measurements that have used this observable.

$\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  is defined in  $t\bar{t}$ +jet topologies, and for this thesis, events at detector level compatible with originating from a semileptonically decaying  $t\bar{t}$ +jet system are selected. The final state products expected from this kind of process are represented by the following diagram:

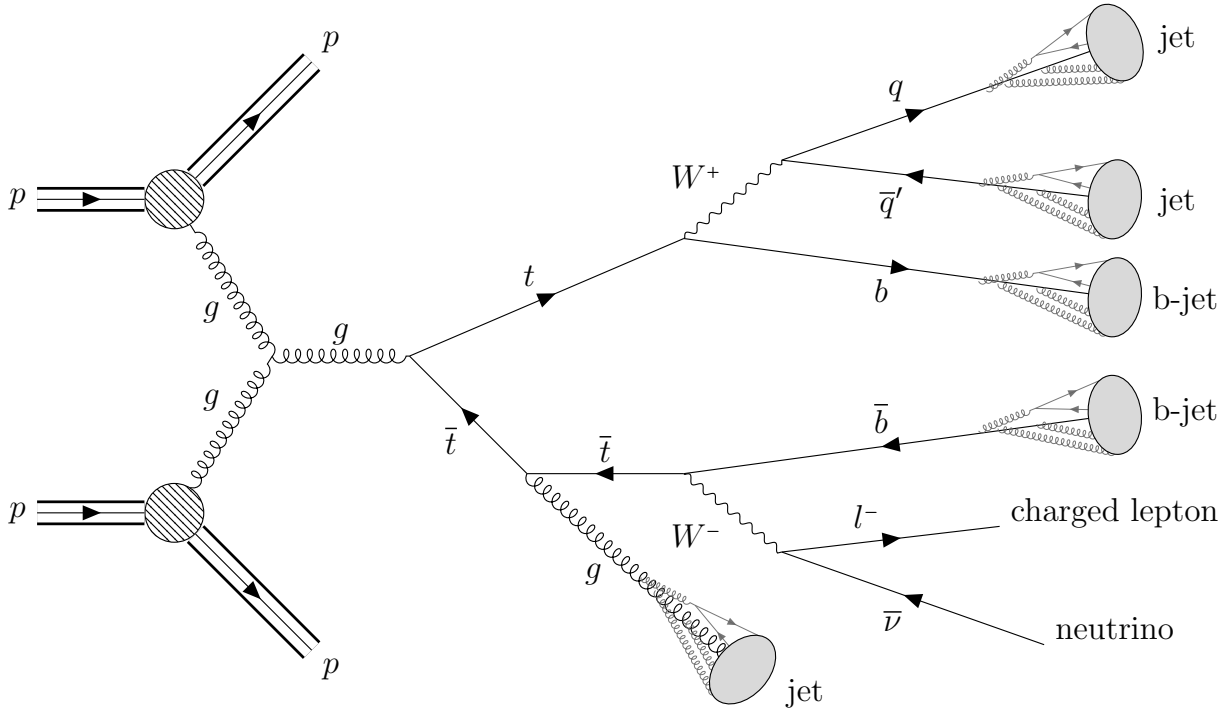


Figure 5.1: Diagram representing the final state products resulting from the semileptonic decay of a top quark pair produced in association with an additional jet in a  $pp$  collision.

In the detector, the experimental signature expected from the final state objects in Figure 5.1 consists of one electron or muon, at least five jets from which two originate from the hadronization of a  $b$  quark, and a significant amount of missing transverse energy to indicate the presence of a neutrino escaping detection.

In Chapter 6, the characteristics of the  $pp$  collisions dataset used in this analysis are described, together with all the simulated samples that are needed to model the various SM contributions that can produce the same experimental signature as the final state objects shown in Figure 5.1. These contributions can originate from various event topologies such as  $t\bar{t}$ , singletop,  $W$ +jets,  $Z$ +jets, diboson, or  $t\bar{t}X$  processes. Events containing fake leptons are also considered in this analysis. Chapter 6 also describes the various alternative simulated samples used in the analysis to estimate the modeling systematic uncertainties affecting the measurement.

In Chapter 7, the event selection and reconstruction of the  $t\bar{t}$  +jet system is described. This process is performed in three distinct steps:

- First, the events from the data and simulated samples that exhibit an

experimental signature compatible with originating from a semileptonically decaying  $t\bar{t}$  +jet event are selected. Additionally, events with exactly four jets, which are only compatible with originating from a  $t\bar{t}$  event topology, are also selected. These events are used to establish a set of control regions where the  $M_{lb}$  observable, described in Section 2.3.1, is reconstructed.

- Secondly, using the events selected in the previous step, a Machine Learning (ML) model implemented in SPA-NET is trained to address the jet-to-parton assignment problem and reconstruct the kinematics of the  $t\bar{t}$  and  $t\bar{t}$  +jet systems.
- At last, an additional set of requirements based on a series of discriminants generated by the ML model are applied to enhance the fraction of correctly matched events, further refining the accuracy of the jet-to-parton assignment.

Chapter 8 provides a description of the procedure used to correct the  $t\bar{t}$  +jet differential cross section with respect to  $\rho_s$  from detector to parton level. This correction is implemented using the Profile Likelihood Unfolding (PLU) technique, a technique which allows for the calculation of this correction while, at the same time, considering the effects of all statistical and systematic uncertainties affecting the analysis in a well-defined statistical framework. Additionally, a series of control regions where the  $M_{lb}$  observable is reconstructed are introduced into the fit in order to perform a simultaneous measurement of  $m_t^{\text{MC}}$  and the parton level differential cross section. This simultaneous measurement effectively mitigates any potential bias that may arise from the assumption of the top quark MC mass in the simulation, ensuring an unbiased determination of the final measured value of the top quark pole mass. Furthermore, the statistical model also incorporates a reparametrization of the unfolded parton level  $\rho_s$  distribution, which enables the extraction of the normalized  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  distribution at parton level directly from the likelihood fit.

Finally, Chapter 9 describes the  $\chi^2$  fit used to extract the top quark pole mass value from the corrected  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  data distribution. This fit is carried out by comparing the unfolded distribution with  $t\bar{t}$  +jet@NLO Fixed Order theory predictions. The chapter also contains the estimation of the uncertainties associated with the theory calculations: the Parton Density Function (PDF) uncertainty, the strong coupling constant ( $\alpha_s$ ) uncertainty, and the

renormalization and factorization scale uncertainties ( $\mu_R$  &  $\mu_F$ , respectively). The final measured value of  $m_t^{\text{pole}}$  and its total uncertainty is reported for various PDF sets.

The author of this thesis, under the guidance of his supervisors and other members of the ATLAS IFIC group, has performed most of the steps involved in the measurement of the top quark pole mass described in this chapter. This includes the derivation of the ntuples used in the analysis from the general ATLAS data and simulated samples; the optimization of the event selection and reconstruction methods, including the construction of the ML model within the SPA-NET framework, its training, and validation; the implementation of the PLU statistical model within the TRExFitter framework, the model employed to correct the data  $\rho_s$  distribution from detector to parton level while simultaneously measuring  $m_t^{\text{MC}}$ ; and the  $\chi^2$  fit used to extract  $m_t^{\text{pole}}$  from the unfolded  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  distribution, including the estimation of the various theory uncertainties. The generation of the  $t\bar{t}$  +jet fixed-order theory predictions, which were essential for this analysis, was carried out by Esteban Fullana and Andrej Saibel.

# Chapter 6

## Data and simulated samples

The measurement of the top quark pole mass described in this thesis is performed using the  $pp$  collisions data at 13 TeV recorded by the ATLAS detector during the Run 2 of the LHC (Chapter 3). To extract interpretable information from the experimentally observed data, it is necessary to compare this data with theory predictions derived from various physics models. These predictions are typically computed using Monte Carlo (MC) event generators, which simulate the different physics processes that are expected to contribute to the experimental data on an event-per-event basis.

The generation of the simulated events begins with the calculation of the Matrix Element (ME) associated with each physics process, which allows for the determination of the kinematics of the parton level particles within the event at a fixed order in perturbation theory. Subsequently, perturbative effects like parton shower cascades and non-perturbative effects such as the hadronization of colored charged particles are simulated. This is followed by the modeling of the response of the ATLAS detector through the simulation of the interactions between the final-state particles and the detector components. Both data and simulated events are then processed using the internal ATLAS software known as ATHENA [152], which performs the object identification and calibration, following the procedures described in Chapter 4.

The sections in this chapter are organized as follows: In Section 6.1, a brief description of the recorded data used for this analysis is given. Section 6.2 provides a comprehensive description of the programs and configurations used to generate the simulated samples for each physics process considered in the

analysis. This includes the description of the baseline samples, commonly referred to as *nominal samples*, as well as the alternative samples used to estimate the systematic modeling uncertainties. At last, Section 6.3 describes the data-driven procedure followed to estimate the fake and non-prompt leptons background.

## 6.1 Data samples

The data used for this analysis was collected from the proton-proton ( $pp$ ) collisions delivered by the LHC during the full Run 2 at a center-of-mass energy of  $\sqrt{s} = 13$  TeV and with a bunch spacing of 25 ns in the laboratory frame. The full Run 2 data-taking period corresponds to the data taken during the years 2015, 2016, 2017, and 2018, which adds up to a total integrated luminosity of  $140.1 \text{ fb}^{-1}$ , with an uncertainty of 0.83 % [121].

## 6.2 Simulated samples

The samples used to model the signal and background processes are simulated using MC event generators, with the exception of the fake and non-prompt lepton background, which is derived using a data-driven method (Section 6.3). These samples are used to assess the data/prediction agreement, evaluate the signal and background efficiencies and uncertainties, and to correct the data from detector to parton level.

The MC simulated samples are split into three production campaigns, depending on the pile-up conditions that they represent. The mc16a campaign corresponds to the pile-up conditions of the LHC during the data taking in 2015 and 2016 (weighted by their integrated luminosity), while the mc16d and mc16e campaigns correspond to the pile-up conditions of 2017 and 2018, respectively. The pile-up in the LHC run is implemented in the simulations by overlaying a number of collisions of simulated soft and hard scatter events (*minimum bias* events) on top of the processed event, in the proper ratios [153]. The number of overlaid pile-up events follows the average number of interactions distributions given in Figure 3.7 of Section 3.2.6. To properly simulate both in-time and out-of-time pile-up, the pile-up events are implemented with precise timing and bunch spacing.



A summary of the MC programs and settings used to produce all the nominal (baseline) signal and background samples can be found in Table 6.1, while a summary of the alternative samples used for evaluating some of the modeling systematic uncertainties is found in Table 6.2. In the following, a brief description of each of the MC samples used in the analysis is provided.

Table 6.1: Summary of the MC generator programs and settings used to simulate the nominal signal and background processes considered in the analysis. All samples have been produced using the NNPDF3.0NLO PDF set in the Matrix Element calculation.

| Sample              | Generator         | Shower       | Normalisation | Cross section [pb] |
|---------------------|-------------------|--------------|---------------|--------------------|
| $t\bar{t}$          | POWHEG + EVTGEN   | PYTHIA 8.230 | NNLO+NNLL     | 831.76             |
| Single top ( $Wt$ ) | POWHEG + EVTGEN   | PYTHIA 8.230 | (app.)NLO     | 71.7               |
| Single top ( $t$ )  | POWHEG + EVTGEN   | PYTHIA 8.230 | (app.)NLO     | 70.43              |
| Single top ( $s$ )  | POWHEG + EVTGEN   | PYTHIA 8.230 | (app.)NLO     | 3.35               |
| $W$ +jets           | SHERPA 2.2.1      |              | NNLO          | 20080.0            |
| $Z$ +jets           | SHERPA 2.2.1      |              | NNLO          | 2107.0             |
| Diboson             | SHERPA 2.2.2      |              | NLO           | 176.0              |
| $t\bar{t}Z$         | MADGRAPH5_aMC@NLO | PYTHIA 8.210 | NLO           | 0.88               |
| $t\bar{t}W$         | MADGRAPH5_aMC@NLO | PYTHIA 8.210 | NLO           | 0.60               |
| $t\bar{t}H$         | MADGRAPH5_aMC@NLO | PYTHIA 8.230 | NLO           | 0.51               |

Table 6.2: Summary of the alternative  $t\bar{t}$  and single-top MC samples used for the estimation of the modeling systematic uncertainties. The samples are normalized to the nominal cross section of the  $t\bar{t}$  and single-top samples.

| Sample                                   | Generator         | Shower       | Comment                              |
|------------------------------------------|-------------------|--------------|--------------------------------------|
| $t\bar{t}$ FastSim                       | POWHEG + EVTGEN   | PYTHIA 8.230 | ATLFASTII simulation                 |
| $t\bar{t}$ $h_{\text{damp}}$ variation   | POWHEG + EVTGEN   | PYTHIA 8.230 | $h_{\text{damp}} = 3m_t^{\text{MC}}$ |
| $t\bar{t}$ Powheg+Herwig                 | POWHEG + EVTGEN   | HERWIG 7.2.1 | HERWIG PS model                      |
| $t\bar{t}$ $p_T^{\text{hard}}$ variation | POWHEG + EVTGEN   | PYTHIA 8.306 | $p_T^{\text{hard}} = 1$              |
| $t\bar{t}$ Underlying Event A14 tune     | POWHEG + EVTGEN   | PYTHIA 8.230 | A14 eigenvector variations           |
| $t\bar{t}$ Colour Reconnection           | POWHEG + EVTGEN   | PYTHIA 8.230 | CR0, CR1, and CR2 tunes              |
| $t\bar{t}$ Recoil to Top                 | POWHEG + EVTGEN   | PYTHIA 8.245 | Alternative recoil scheme            |
| Single top FastSim                       | POWHEG + EVTGEN   | PYTHIA 8.230 | ATLFASTII simulation                 |
| SingleTop Powheg+Herwig                  | POWHEG + EVTGEN   | HERWIG 7.0.4 | HERWIG PS model                      |
| SingleTop aMC@NLO+Pythia                 | MADGRAPH5_aMC@NLO | PYTHIA 8.230 | aMC@NLO ME                           |

### 6.2.1 Nominal simulated samples

#### $t\bar{t}$ nominal sample

The nominal  $t\bar{t}$  MC sample has been generated using the `hvg` package of `Powheg-Box-v2` [154–157]. In this package, the ME of the heavy quark production is calculated at next-to-leading-order (NLO) precision in quantum chromodynamics (QCD). The parton structure is described using the NNPDF3.0NLO PDF set. This sample is produced assuming a top quark MC mass of  $m_t^{\text{MC}} = 172.5$  GeV. The  $h_{\text{damp}}$  parameter that effectively controls the emission of the first gluon is set to 1.5 times the top quark mass. The sample is normalized to the inclusive production cross section of  $\sigma(t\bar{t}) = 831.76$  pb. This cross section is calculated at next-to-next-to-leading order (NNLO) in QCD including the resummation of next-to-next-to-leading logarithm (NNLL) soft-gluon terms using `TOP++2.0` [60–66].

The ME generator is then interfaced with `PYTHIA 8.230` [158] to simulate the parton shower, fragmentation, hadronisation, and the underlying event. The A14 tune [159], together with the NNPDF2.3LO PDF set, is applied for the `PYTHIA 8` showering. Heavy flavor decays (primarily B and D mesons) are modeled using the `EVTGEN 1.6.0` program [160]. The detector response is simulated using a model of ATLAS built in `GEANT4` [161, 162]. The same model of the ATLAS detector in `GEANT4` is used for the simulation of the detector response in all the nominal signal and background samples.

#### Single-top nominal samples

The nominal sample that describes single-top quark processes is split into three production channels: the  $s$ -channel, the  $t$ -channel, and the  $Wt$ -channel. These three processes are generated using the `POWHEG` generator for the ME calculation [163, 164] and then interfaced with `PYTHIA 8.230` for the simulation of the PS and hadronisation. The configuration of `PYTHIA 8` is the same as in the nominal  $t\bar{t}$  sample. To remove the overlap between  $t\bar{t}$  and single-top in the  $Wt$ -channel, the diagram removal technique [165] is used. The samples are normalized to the approximate NNLO cross section calculated in Ref. [166, 167].

### **$W$ and $Z$ boson production in association with additional jets**

Events with a  $W$  or  $Z$  boson produced in association with additional jets are simulated using SHERPA 2.2.1 [168]. The matrix elements are calculated at NLO for up to two additional partons, and LO for up to four partons using the Comix [169] and OpenLoops [170, 171] libraries. Samples produced with SHERPA include the simulation of the hard scattering, the parton shower, the hadronization, and the heavy flavor decays; hence no external PS generator program is needed. The configuration of SHERPA uses a dedicated tune provided by the authors and the NNPDF3.0NNLO PDF set. The  $W$ +jets and  $Z$ +jets samples are normalized to the cross section predicted at NNLO [172].

### **Diboson**

Several samples are produced to simulate diboson ( $VV$ ) processes such as  $ZZ$ ,  $WW$ , and  $WZ$ . The ME of these processes are produced using SHERPA v2.2.1 and v2.2.2 [168], where the NNPDF3.0NNLO PDF set and a tune provided by the authors is used for the two versions of the generator. The matrix elements are computed at NLO accuracy in QCD for up to one additional parton, and at LO for up to three additional partons. These samples are normalized to the NLO QCD predicted cross sections [173].

### **$t\bar{t}X$ and other rare processes**

Events where a  $t\bar{t}$  pair is produced in association with a  $Z$  or  $W$  boson ( $t\bar{t}V$ ) are produced using MADGRAPH5\_aMC@NLO and then interfaced with PYTHIA 8.210 for the simulation of the parton shower and hadronization. The NNPDF3.0NLO PDF set is used for the calculation of the ME, while the A14 tune and the NNPDF2.3LO PDF set are used for the PS simulation. These events are normalized to the NLO QCD+EW cross section calculation [174].

Events where a  $t\bar{t}$  pair is produced in association with a Higgs boson ( $t\bar{t}H$ ) are generated using POWHEG and then interfaced with PYTHIA 8.230 for the simulation of the parton shower and hadronization. The NNPDF3.0NLO PDF set is used for the calculation of the ME, while the A14 tune and the NNPDF2.3LO PDF set are used for the PS simulation. The parameter associated with the mass of the Higgs boson is set to  $m_H = 125$  GeV, and the events are normalized to the

theoretical predictions in Reference [175].

Other rare processes, such as the production of a  $t\bar{t}$  pair in association with two  $W$  bosons ( $t\bar{t}WW$ ) and the production of three and four top quarks ( $ttt$ ,  $tttt$ ), are also taken into account. These samples are produced using MADGRAPH5\_aMC@NLO with the NNPDF3.0NLO PDF set and then interfaced with PYTHIA 8.186. The A14 tune and the NNPDF2.3LO PDF set are used for the PS simulation, and the samples cross sections are normalized to their corresponding QCD theoretical predictions [176].

## 6.2.2 Alternative simulated samples

### $t\bar{t}$ alternative samples

To estimate the *modeling systematic uncertainties* in the  $t\bar{t}$  sample, the uncertainties associated with the non-perturbative part of the MC generator which can only be described by phenomenological models, a collection of alternative  $t\bar{t}$  MC samples are produced. Table 6.2 contains a summary of the configuration of the nominal sample and all the alternative ones described in this section.

The alternative samples used to evaluate the modeling systematic uncertainties are produced using the fast simulation of the ATLAS detector, ATLFASTII [161], to save computing resources and speed up the simulation process. The main difference between the full simulation of the detector and ATLFASTII is that the latter uses an approximation of the detector geometry, parameterizes the hadronic showers in the electromagnetic and hadronic calorimeters, and simplifies the energy deposition models in each calorimeter layer. A version of the nominal  $t\bar{t}$  sample with the fast simulation of the detector is produced to be compared with the alternative samples.

To assess the uncertainty associated with the choice of the POWHEG  $h_{\text{damp}}$  parameter on the nominal  $t\bar{t}$  sample, an alternative sample with the identical configuration as the nominal sample, but with this parameter varied to three times the top quark mass, is produced.

For evaluating the impact of the Parton Shower and hadronization models, an alternative  $t\bar{t}$  sample that replaces the PYTHIA 8 showering program with HERWIG 7.2.1 [177, 178] is produced. The HERWIG configuration uses the HERWIG 7.2.1 default set of tuned parameters [178, 179] and the MMHT2014LO

PDF set [180].

The impact of the NLO matching uncertainty in the  $t\bar{t}$  sample is assessed following the approach described in Ref. [181]. This evaluation requires the production of an alternative sample where the  $p_T^{\text{hard}}$  parameter in PYTHIA 8 is varied from the nominal value of  $p_T^{\text{hard}} = 0$  to  $p_T^{\text{hard}} = 1$ .

To assess the impact of the underlying event (UE) model in the analysis, the corresponding eigenvector of the nominal A14 tune in PYTHIA 8 is varied up and down by one standard deviation, which result into two alternative samples.

The impact of the Color Reconnection (CR) model in PYTHIA is evaluated by comparing three different samples with varied tunes of the CR model: CR0, CR1, and CR2 [182]. A discussion about the differences between these models is provided during the description of their associated uncertainty in Section 8.2.

The impact of the recoil scheme for the gluon radiation in PYTHIA is evaluated using an alternative sample where the nominal *recoil-to-colored* scheme is varied to the *recoil-to-top* scheme.

At last, to measure  $m_t^{\text{MC}}$  and test the independence of the reconstruction and unfolding procedure with respect to this parameter, a set of samples with varied values of the top quark mass parameter in the nominal MC are produced. These samples include a total of six fast simulated samples with the top quark MC mass set to 169, 171, 172, 172.25, 172.75, 173, and 176 GeV, and two fully simulated samples with  $m_t^{\text{MC}} = 171$  and 174 GeV.

### Single top alternative samples

As in the case of the  $t\bar{t}$  signal, to estimate some of the systematic modeling uncertainties related to the single-top background, a set of alternative samples is used. These alternative samples are produced using the ATLFASSTII fast simulation of the ATLAS detector; hence a version of the nominal single top samples using ATLFASSTII is produced for comparison reasons.

The uncertainty originating from the choice of the scheme used to remove the overlap between the  $t\bar{t}$  and the single top  $Wt$ -channel is evaluated using a sample with an alternative diagram subtraction (DS) scheme [165].

For the impact of the PS and the hadronization model, an alternative sample that uses the nominal ME generator but interfaced with HERWIG 7.1.3 has been

produced. The HERWIG configuration uses the HERWIG 7.1.3 default set of tuned parameters [178, 183] and the MMHT2014LO PDF set [180].

To assess the uncertainty associated with the matching scheme, a sample that simulates the ME using MADGRAPH5\_aMC@NLO and interfaces it with PYTHIA 8.230 is used. The configuration of MADGRAPH is the same as in the corresponding alternative  $t\bar{t}$  sample.

All the single-top samples are normalized to the approximate NNLO cross section calculated in Reference [166, 167].

### 6.3 Fake and non-prompt leptons background

The selection of semileptonically decaying  $t\bar{t}$  or  $t\bar{t}$  +jet events requires the identification of one electron or muon compatible with originating from the hard scattering of the event. However, not all leptons that pass the analysis selection originated from the hard-scattering (i.e., they are not *prompt leptons*). Some of the reconstructed leptons originate from the decay of secondary particles with a relatively long lifetime (*non-prompt leptons*) or are, in reality, non-leptonic objects such as photons or jets that are identified as leptons (*fake leptons*). The misidentification of these objects as *prompt leptons* gives rise to the so called *non-prompt* and *fake leptons* backgrounds. In this analysis, the two backgrounds are estimated together and are referred to as *fake leptons*. For more information about the electron and muon definitions in ATLAS, see Sections 4.2 and 4.3.

The fake lepton background is difficult to simulate because the probability of a non-leptonic object being reconstructed as a lepton is small, but the cross section of multijet processes where they may arise is high. A large number of events would be needed to estimate this background accurately so, instead of using MC simulations, the fake lepton background normalization and kinematics are typically estimated using data-driven techniques.

To estimate the fake lepton background in this analysis, the *Matrix Method* [184, 185] is used. This method relies on the construction of two samples with different selection criteria for the leptons. The first of these samples has the nominal selection criteria used in the analysis, whereas the second sample is enriched in *fake leptons* by using a *looser* quality and isolation working points for the leptons (see Sections 4.2 and 4.3). These samples are referred to in the

following as *tight* and *loose* samples, and the total number of events passing each selection ( $N^{\text{tight}}$  and  $N^{\text{loose}}$ ) can be expressed as:

$$\begin{aligned} N^{\text{tight}} &= N_{\text{real}}^{\text{tight}} + N_{\text{fake}}^{\text{tight}} \\ N^{\text{loose}} &= N_{\text{real}}^{\text{loose}} + N_{\text{fake}}^{\text{loose}}, \end{aligned} \tag{6.1}$$

where  $N_{\text{real}}^{\text{tight(loose)}}$  is the number of *tight (loose)* events which origin is a *prompt lepton*, and  $N_{\text{fake}}^{\text{tight(loose)}}$  is the number of *tight (loose)* events which origin is a *non-prompt lepton* or a *non-leptonic* object. Since the *tight* sample is a subset of the *loose* sample, the real and fake lepton selection efficiencies can be defined as:

$$\begin{aligned} \epsilon_{\text{real}} &= \frac{N_{\text{real}}^{\text{tight}}}{N_{\text{real}}^{\text{loose}}} \\ \epsilon_{\text{fake}} &= \frac{N_{\text{fake}}^{\text{tight}}}{N_{\text{fake}}^{\text{loose}}}. \end{aligned} \tag{6.2}$$

Combining Equations 6.1 and 6.2, the total number of fake events in the *tight* sample can be rewritten as:

$$N_{\text{fake}}^{\text{tight}} = \frac{\epsilon_{\text{fake}}}{\epsilon_{\text{real}} - \epsilon_{\text{fake}}} (\epsilon_{\text{real}} N^{\text{loose}} - N^{\text{tight}}). \tag{6.3}$$

The real and fake lepton selection efficiencies are measured for electrons (muons) in a fake enriched region obtained by requiring exactly one electron (muon), four or more jets, zero *b*-tagged jets, and  $E_{\text{T}}^{\text{miss}} < 20$  GeV and  $m_{\text{T}}^W < 60$  GeV. These efficiencies depend on the kinematics of the lepton and are measured as a function of its  $p_{\text{T}}$  and  $|\eta|$ . To correctly account for this dependence, the fake lepton background is estimated by taking each event of the data sample that satisfies the *loose* selection criteria for leptons and applying a *fake weight* to it. The *fake weight* that corresponds to each event is calculated using a per-event version of Equation 6.3 that can be expressed as:

$$w_i^{\text{fake}} = \begin{cases} \frac{\epsilon_i^{\text{fake}}}{\epsilon_i^{\text{real}} - \epsilon_i^{\text{fake}}} (\epsilon_i^{\text{real}} - 1) , & \text{if lepton } i \text{ is tight} \\ \frac{\epsilon_i^{\text{fake}}}{\epsilon_i^{\text{real}} - \epsilon_i^{\text{fake}}} \epsilon_i^{\text{real}} , & \text{if lepton } i \text{ is loose} \end{cases} \quad (6.4)$$

where the position of the real and fake indices in the efficiencies has been changed to make the equation more legible. An important characteristic of the *fake weight* is that it takes a positive (negative) value for events that pass the *loose* lepton selection criteria but fail (pass) the *tight* lepton selection criteria. This means that the contribution of each individual event to the background estimation can also be positive or negative.



# Chapter 7

## Event selection and reconstruction using SPA-Net

The measurement of the top quark pole mass ( $m_t^{\text{pole}}$ ) using the  $\rho_s$  variable requires a complete reconstruction of the  $t\bar{t}$  +jet system in the detector, whereas the measurement of the top quark MC mass ( $m_t^{\text{MC}}$ ) using the  $M_{lb}$  observable requires only a partial reconstruction of  $t\bar{t}$  system. To select and accurately reconstruct the events with a signature compatible with these topologies, a three-step process is followed. First, the events that contain the objects expected from these event topologies are selected. A set of basic kinematic requirements is imposed on these objects to ensure their accurate reconstruction and calibration, and to mitigate the contamination from several background processes. Secondly, using the events selected in the previous step, the  $t\bar{t}$  and  $t\bar{t}$  +jet systems are reconstructed using an event reconstruction technique based on Symmetry Preserving Attention Neural Networks (SPA-NETs) [186]. Finally, once the objects observed at detector level are assigned to their predicted origins (jet-to-parton assignment), an additional set of requirements is imposed. These requirements are based on a collection of discriminants generated by the SPA-NET machine learning model, and they are used to enhance the fraction of correctly matched events within the sample.

The sections in this chapter are organized as follows: In Section 7.1, the basic data quality requirements, trigger flags, and object definitions used in the analysis are presented. Section 7.2 describes the event preselection, which consists of the first set of requirements imposed to select the events whose experimental signature is compatible with originating from a semileptonically decaying  $t\bar{t}$  or  $t\bar{t}$  +jet event. Section 7.3 introduces the SPA-NET framework and describes its implementation

in the analysis to reconstruct the event kinematic properties. In Section 7.4, the performance of this SPA-NET model is studied in detail, and the final event selection is defined. At last, Section 7.5 contains a summary of the final selection used in the analysis.

## 7.1 Data quality requirements and object definitions.

### 7.1.1 Data quality requirements

To ensure the quality of the recorded data used in the analysis, only data events taken under stable beam conditions and with all the relevant subdetectors fully operational are considered. This requirement means that the events have to be contained in the luminosity blocks specified in the *Good Run Lists* (Section 3.2.8). Events collected during noise bursts of the LAr and Tile calorimeters are also excluded. The presence of a primary vertex is ensured by requiring the presence of at least two tracks with  $p_T > 500$  MeV matched to this vertex. To remove events with fake jets originating from cosmic events, non-collision backgrounds, or fake signals due to detector noise, the jet cleaning and overlap removal techniques described in Section 4.4 and 4.7 are applied. If one of the jets does not fulfill the cleaning criteria, the whole event is removed.

Then, to ensure the presence of at least one electron or muon, the events are required to pass one of the single-electron or single-muon triggers defined on the HLT. These triggers have a  $p_T$  threshold of 24 GeV for electrons and 20 GeV for muons in the data taken during 2015, which is then raised to 26 GeV for both electrons and muons during the subsequent data-taking periods of 2016, 2017, and 2018. This raise in the  $p_T$  threshold is implemented to address the increase in the instantaneous luminosity observed in data taken during the latter years. The same trigger requirements is applied to the simulated events.

Additionally, to enhance the detection efficiency for higher  $p_T$  leptons, events that pass similar single-lepton triggers, but without isolation requirements and with a relaxed quality criteria, are also considered. These triggers encompass a muon trigger with a  $p_T$  threshold of 50 GeV and without isolation requirements, an electron trigger with a  $p_T$  threshold of 60 GeV and without isolation requirements,

and an electron trigger with a  $p_T$  threshold of 120(140) GeV for the year 2015 (2016, 2017, and 2018), again without isolation requirements, and with a relaxed quality criteria in comparison to the other electron triggers.

Finally, any event containing a muon with a large error on the  $q/p$  fraction is removed, as these muons tend to have a significantly worse momentum resolution compare to those that pass this veto.

### 7.1.2 Object selection

In terms of the object definitions of Chapter 4, the specific  $p_T$ , quality, and isolation requirements for electrons, muons, and jets are summarized in Table 7.1 and described in further detail below.

The electron candidates considered in the analysis are required to have  $p_T > 25$  GeV, to be found in the range of  $|\eta| < 2.47$  (excluding  $1.37 < |\eta| < 1.52$ ), to be compatible with originating from the primary vertex of the event,  $d_0/\sigma(d_0) < 5$  and  $|z_0 \sin\theta| < 0.5$  mm, and to fulfill the **TightLH** identification quality and the **PLVTight** isolation requirements. For the data-driven estimation of the fake and non-prompt electron background (Section 6.3), a *looser* criteria for the electron identification quality and isolation is set. These *looser* electrons are required to fulfill the **MediumLH** identification quality, and no isolation requirement is imposed. All the other cuts are kept as in the case of the nominal (*tight*) selection.

The muon candidates considered in the analysis are required to have  $p_T > 25$  GeV, to be found in the range of  $|\eta| < 2.5$ , to be compatible with originating from the primary vertex of the event,  $d_0/\sigma(d_0) < 3$ , and  $|z_0 \sin\theta| < 0.5$  mm, to fulfill the **Medium** track quality requirement, and to pass the **PFlowTight.FixedRad** isolation criteria. For the estimation of the fake and non-prompt muon background, the *looser* muon definition used is the same as the nominal, except that no isolation requirement is imposed.

The jet candidates considered in the analysis are reconstructed using the **EMPflow** jet definition with a radius parameter of  $R = 0.4$  (small- $R$  jets). They are required to have a  $p_T > 25$  GeV, and to be found in the range of  $|\eta| < 2.5$ . To suppress the jets originating from pile-up collisions, the Jet Vertex Tagger (JVT) discriminant (Section 4.5) is required to be bigger than 0.5 for jets with  $p_T < 120$  GeV. For the identification of  $b$ -jets, the DL1r  $b$ -jet tagging algorithm described in Section 4.5 is used.

Table 7.1: Summary of object definition used in this analysis. The object definitions for the fake/non-prompt lepton background estimation are stated where they differ from the nominal definition.

| <b>Reconstructed object</b> |             |
|-----------------------------|-------------|
| Property                    | Requirement |

| <b>Electrons</b>          |                                                                               |
|---------------------------|-------------------------------------------------------------------------------|
| Kinematics                | $p_T > 25 \text{ GeV} \ \& \  \eta  < 2.47$ , (excl. $1.37 <  \eta  < 1.52$ ) |
| Identification (nominal)  | <b>TightLH</b>                                                                |
| Identification (fake el.) | <b>MediumLH</b>                                                               |
| Isolation (nominal)       | <b>PLVTight</b>                                                               |
| Isolation (fake el.)      | <b>None</b>                                                                   |
| Impact parameter          | $ d_0/\sigma(d_0)  < 5$ , $ z_0 \sin \theta  < 0.5 \text{ mm}$                |

| <b>Muons</b>           |                                                                |
|------------------------|----------------------------------------------------------------|
| Kinematics             | $p_T > 25 \text{ GeV} \ \& \  \eta  < 2.5$                     |
| Identification         | <b>Medium</b>                                                  |
| Isolation (nominal)    | <b>PflowTight.FixedRad</b>                                     |
| Isolation (fake muons) | <b>None</b>                                                    |
| Impact parameter       | $ d_0/\sigma(d_0)  < 3$ , $ z_0 \sin \theta  < 0.5 \text{ mm}$ |

| <b>Jets</b>        |                                                             |
|--------------------|-------------------------------------------------------------|
| Algorithm          | anti- $k_t$ ( $R = 0.4$ , <b>EMPFLOW</b> )                  |
| Kinematics         | $p_T > 25 \text{ GeV}$ if $ \eta  < 2.5$                    |
| Pile-up Mitigation | $JVT > 0.5$ for $p_T < 120 \text{ GeV} \ \& \  \eta  < 2.4$ |
| $b$ -tagging       | DL1r (70% efficiency and pseudo-continuous working points)  |

## 7.2 Event preselection

The goal of the preselection is to select the events in the detector with an experimental signature compatible with originating from a semileptonically decaying  $t\bar{t}$  or  $t\bar{t}$  +jet event. To include the  $t\bar{t}$  and  $t\bar{t}$  +jet signatures at the same time and define different analysis regions in terms of the  $b$ -tagged jet multiplicity, an inclusive preselection over the physics objects is used. The event preselection requires the presence of:

- Exactly one electron or muon with  $p_T > 25$  GeV ( $p_T > 27$  GeV) for the 2015 (2016, 2017, 2018) data-taking periods. The presence of a second lepton with  $p_T > 25$  GeV is vetoed.
- A significant amount of missing transverse energy and  $W$  boson transverse mass to indicate the presence of an undetected neutrino originated from the leptonic decay of a  $W$  boson,  $E_T^{\text{miss}} > 30$  GeV and  $m_T^W > 30$  GeV.
- The presence of at least four jets with  $R = 0.4$ , with at least one of them passing the 70% efficiency working point of the DL1r  $b$ -tagger.

The event yields after the preselection are compared to the SM expected contributions in Table 7.2. Additionally, Figures 7.1 to 7.3 show the distribution of several important kinematic variables, which include the inputs of the machine learning model trained to reconstruct the  $t\bar{t}$  and  $t\bar{t}$  +jet systems (Section 7.3). The uncertainty band in Figures 7.1 to 7.3 correspond only to the statistical uncertainty in data and the cross section normalization uncertainties of each SM process. The cross section uncertainties associated with each SM process are 6.1% for  $t\bar{t}$  [187], 5.3% for singletop [187], and a conservative 50% for the  $W$ +jets,  $Z$ +jets, and fake lepton. This is considered a conservative uncertainty since the inclusive  $W/Z$ +jets cross section is measured with a precision higher than 50%, however, for high jet multiplicities is estimated to be higher. Additionally, the contributions of diboson and  $t\bar{t}X$  processes are combined into a single category referred to as *others*, which also has a 50% normalization uncertainty.

A good level of agreement is observed for the Data/Prediction event yields shown in Table 7.2. Overall, the kinematic distributions shown in Figures 7.1 to 7.3 also show a good level of compatibility between data and the prediction. However, some trends are noticeable in the momentum distribution of jets, leptons,

and in the MET. In particular, these distributions are predicted to be harder in the simulation than in the observed data. This is a well-known feature that was observed in previous measurements involving top quark pairs Ref. [188, 189]. This phenomenon is expected due to missing higher order corrections in the  $t\bar{t}$  MC simulation and it is covered by the modeling uncertainties, which are not included in these plots.

In accordance with the analysis strategy outlined in Chapter 5, the events that pass the preselection are used to train a machine learning model designed to reconstruct the  $t\bar{t}$  and  $t\bar{t}$  +jet systems. This model is implemented using the SPA-NET framework, which is introduced in the following section.

Table 7.2: Event yields for the preselected events split into the two lepton flavor orthogonal regions,  $e$ +jets and  $\mu$ +jets.

|                      | Preselection $e$ +jets | Preselection $\mu$ +jets |
|----------------------|------------------------|--------------------------|
| $t\bar{t}$           | 2947425 (84.7%)        | 3036326 (84.8%)          |
| Single Top           | 175610 (5.1%)          | 178783 (5.0%)            |
| $W$ +jets            | 233554 (6.7%)          | 273988 (7.6%)            |
| $Z$ +jets            | 54928 (1.6%)           | 41271 (1.2%)             |
| Diboson+ $t\bar{t}X$ | 22565 (0.6%)           | 23229.9 (0.6%)           |
| Fake leptons         | 45540.2 (1.3%)         | 29079.3 (0.8%)           |
| Total pred.          | 3479622.2              | 3582677.2                |
| Data                 | 3437242                | 3501047                  |
| Data/Prediction      | 0.99                   | 0.98                     |

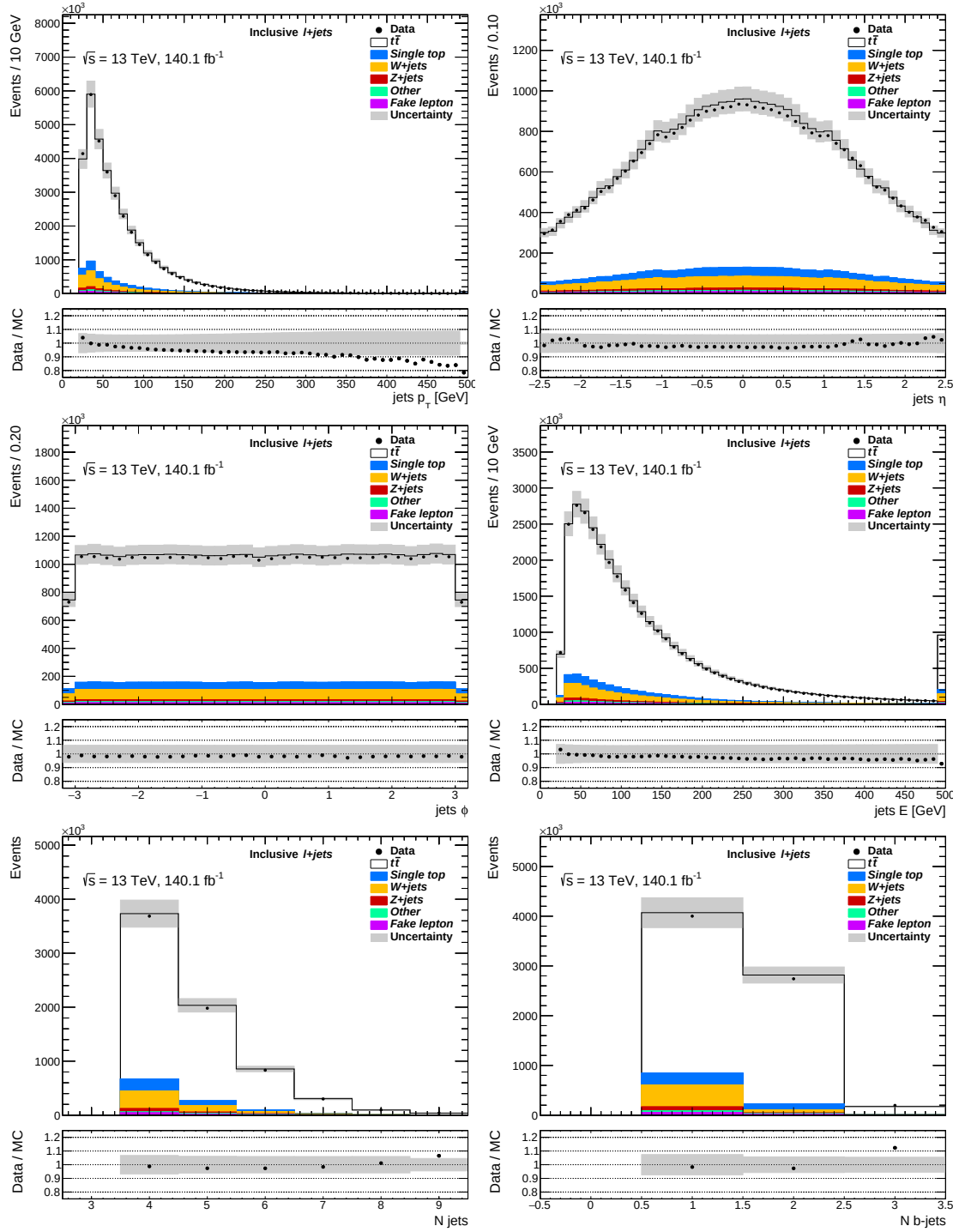


Figure 7.1: Data/prediction comparison for several basic kinematic variables of the inclusive  $l+jets$  preselection. The grey bands show the uncertainty originating from the finite statistics in the MC samples, as well as the normalization uncertainty of each signal/background process. The last bin in each distribution contains the overflow events.

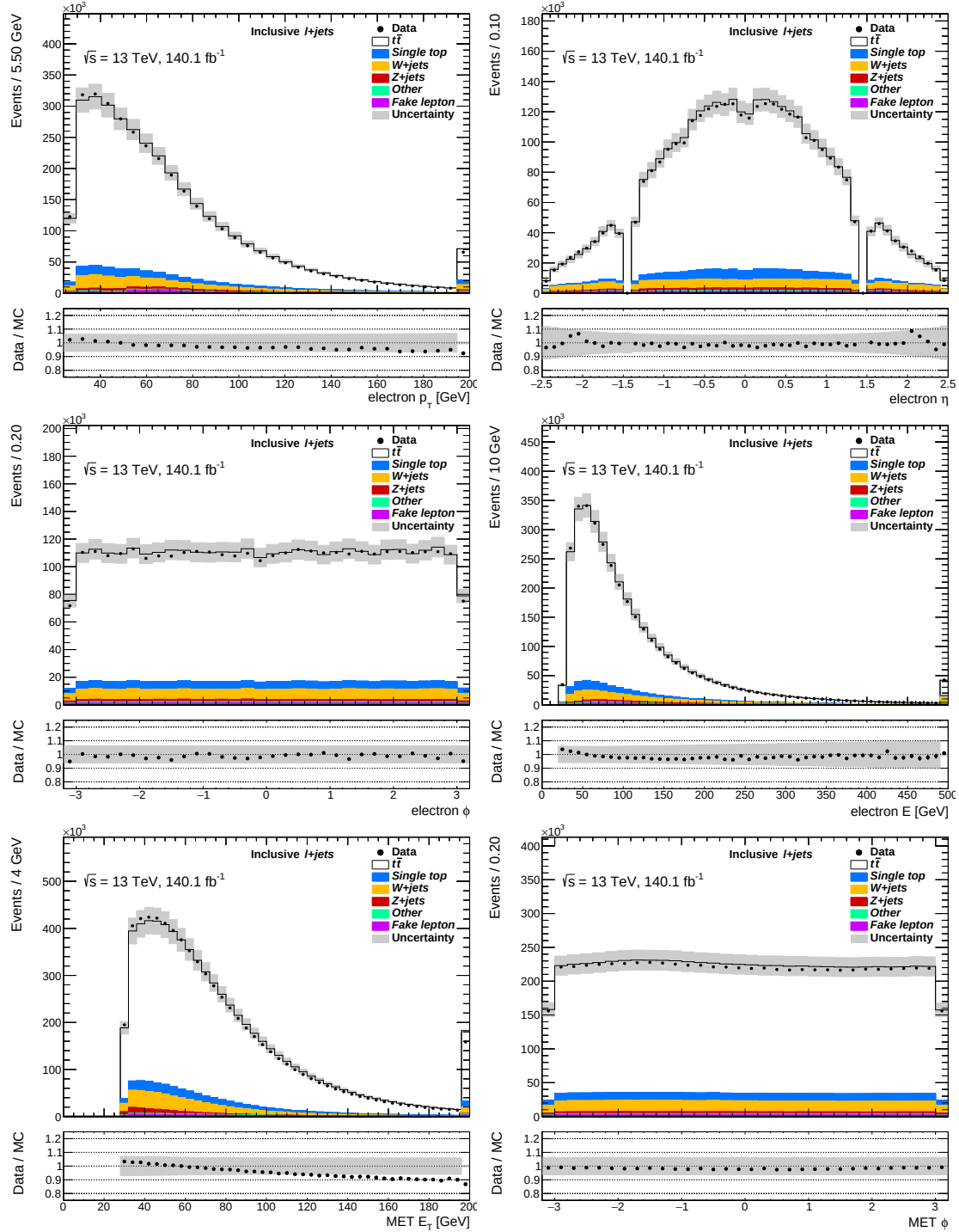


Figure 7.2: Data/prediction comparison for several basic kinematic variables of the inclusive  $l$ +jets preselection. Similar to Figure 7.1.



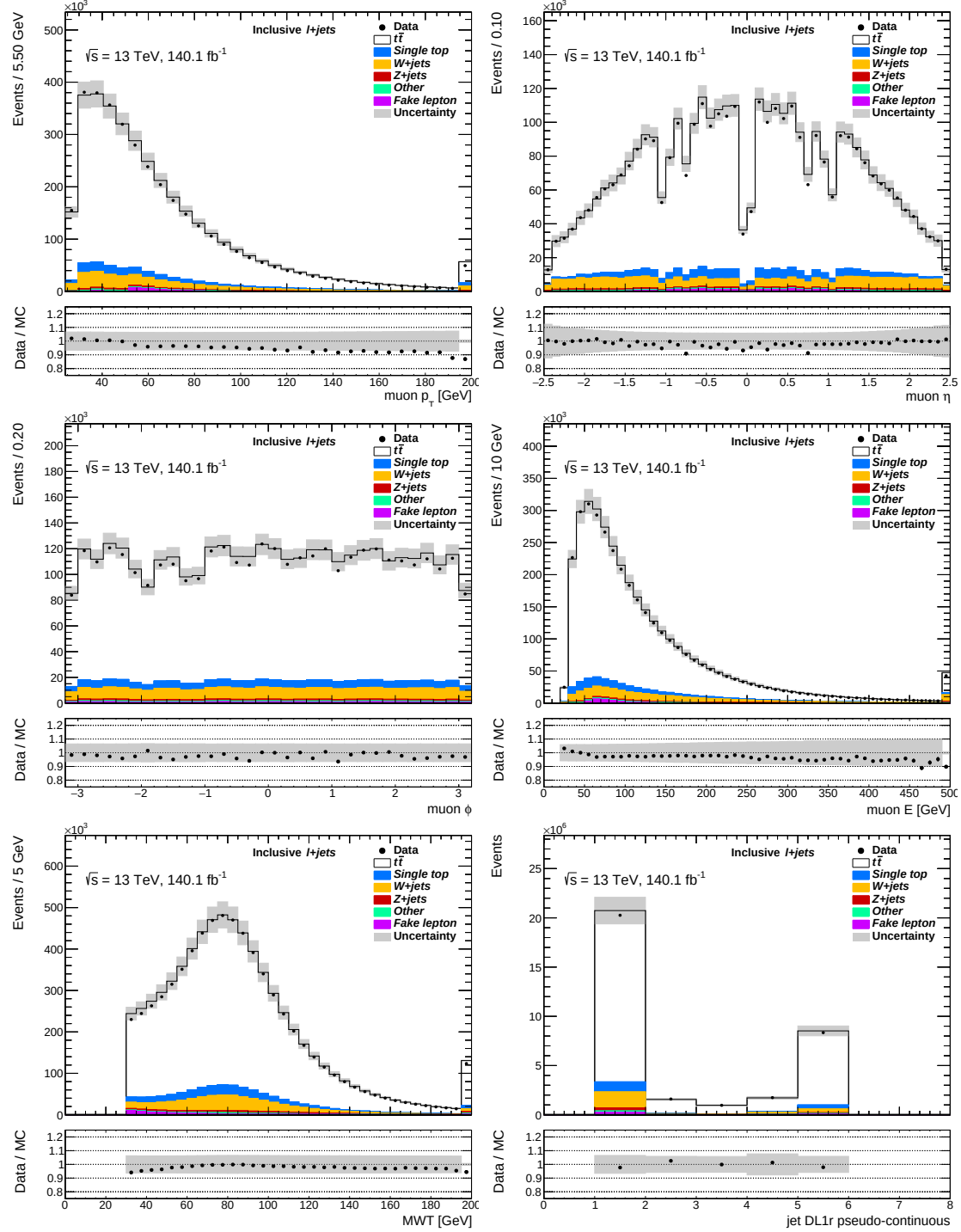


Figure 7.3: Data/prediction comparison for several basic kinematic variables of the inclusive  $l$ +jets preselection. Similar to Figure 7.1.

## 7.3 Reconstruction of the $t\bar{t}$ and $t\bar{t}$ +jet systems using SPA-Net

### 7.3.1 Introduction to SPA-Net

The Symmetry Preserving Attention Networks (SPA-NETs) are a class of neural networks which are constructed with an architecture that reflects the underlying invariances of the problem that is being studied, and trained using generalized attention mechanisms. These kinds of networks were introduced for the first time to solve the jet-parton assignment problem in all-hadronic  $t\bar{t}$  decays [190], but recently have been adapted to be used in any arbitrary event topologies [186]. In the MC studies performed in these references, SPA-NETs outperformed all alternative kinematic-based reconstruction techniques it was compared with when solving the jet-to-parton assignment problem. Another advantage of SPA-NETs with respect to other reconstruction methods such as KLFITTER [191] (Appendix C.2), is that SPA-NETs are trained to identify the decay products of each particle unambiguously without evaluating all the possible permutations, which make them have higher run-time performance for events with large jet multiplicities.

The schematic flowchart of the high-level structure of SPA-NET is shown in Figure 7.4. The network architecture is composed using five distinct elements, each of which is defined as follows:

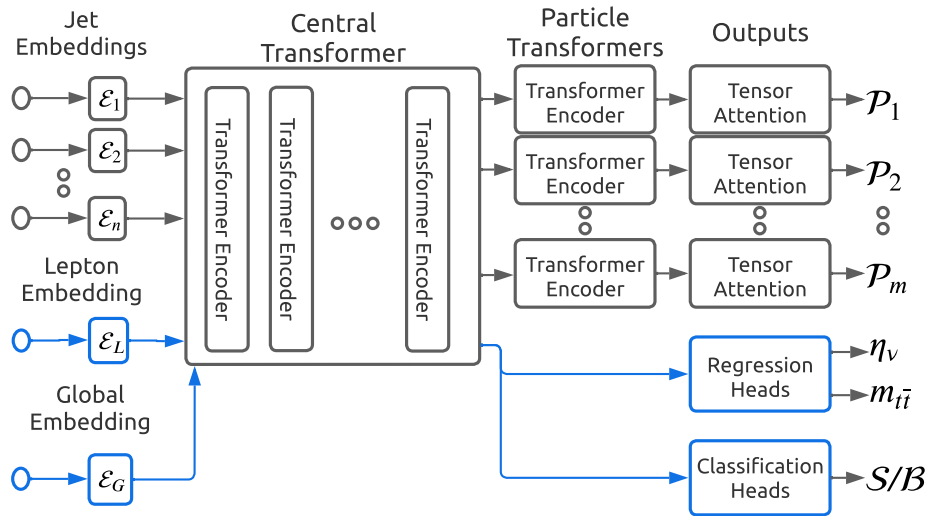


Figure 7.4: Schematic flowchart of the high level structure of SPA-NET [186].

An **embedding** is a machine learning architecture designed to map the input data, represented as a high-dimensional vector, into a low-dimensional latent space that captures the underlying dependencies and relationships between the original elements of the vector of data. In the context of SPA-NET, the jet, lepton, and global embeddings take as inputs the kinematic properties of the corresponding objects ( $p_T$ ,  $\eta$ ,  $\phi$ ,  $E$ , etc) and the flavor information ( $b$ -tag, lepton-tag, etc), and map them into a vector in the latent space which captures all the correlations and interdependencies between the original inputs. Generally speaking, embeddings simplify doing ML on large inputs and improve the efficiency of the models. However, they have the disadvantage that they reduce the interpretability of the models they are part of.

A **transformer encoder** is a ML architecture that uses an attention-based mechanism to map an input sequence into a series of hidden representations, which are then fed to a decoder or to other ML models. The attention mechanism gives the encoder access to all the sequences of elements at each time step, but at the same time, it allows it to selectively place more importance on the parts that are more important for the different positions of the output sequence. This property increases the efficiency of the model when learning the correlations and dependencies between the input and output. A brief description of the architecture of the transformers can be found in Appendix D.1. In the context of SPA-NET, the central stack of transformer encoders learns from the embeddings generated from the different detector level objects and combines their information to create a vector in the hidden representation that contains the information about the dependencies between the different input objects.

A **tensor attention** is a supervised ML architecture used to perform the jet-to-parton assignment via an attention mechanism. The invariances of the physics problem can be introduced by using *symmetric attention tensors* for each group of indistinguishable target particles<sup>1</sup>. For the training of this model, the outputs of the tensor attention of each particle are merged to produce a *combined symmetric loss function*, which also respects the invariances of the system. In the context of SPA-NET, for each parton level particle, there is a tensor attention preceded by an additional transformer encoder. The output of the tensor attention associated with each parton level particle has two outputs:

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<sup>1</sup>An example of two indistinguishable target particles is the two light quarks originating from the hadronic decay of a  $W$  boson (neglecting charge/mass effects).

- A vector containing a discriminant which evaluates the probabilities that each possible permutation of the detector level objects corresponds to the correct assignment with the target parton level particle.
- A discriminant that evaluates the probability that the decay product of the target parton level particle is present among the detector level objects.

The outputs of these two discriminants are known as the *assignment probability* and the *detection probability*, respectively. The permutation with the highest value of the assignment probability variable is chosen as the correct permutation. Both the assignment and the detection probabilities are expressed in arbitrary units (i.e., they are not constrained to the range between 0 and 1).

A **regression head** is a supervised ML architecture designed to predict the value of an output, which is typically a real number. The training of this model is performed through the minimization of the distance between the target value and the predicted value in each training step by means of a loss function. In the context of SPA-NET, regression heads are used to predict the value of one or more of the features of the input event, such as the neutrino  $\eta$  or the invariant mass of the  $t\bar{t}$  system at parton level ( $m_{t\bar{t}}$ ).

A **classification head** is a supervised ML architecture designed to identify the category that an input belongs to, which is typically represented with a discrete value such as an integer. As in the case of the regression heads, the training is also done using a loss function. In the context of SPA-NET, classification heads are used to classify the input data into signal or one of the background categories.

### 7.3.2 Implementation of SPA-Net in $t\bar{t}$ +jet event topologies and the $M_{lb}$ observable

#### Input variables

As introduced in the analysis strategy described in Section 5, the aim of the SPA-NET implementation in the analysis is not only the selection of the correct jet-to-parton matching, but also the regression of the neutrino  $\eta$  and  $p_T$ .

To predict the correct jet-to-parton association, SPA-NET needs to have access to the most relevant information about the objects being matched. This allows the model to learn the patterns, correlations, and dependencies between these objects

and the parton level particles they originate from. Moreover, the properties of the lepton are also related to the properties of the  $b$ -jet associated with the same top decay, so its addition improves the performance of the network. Furthermore, the missing transverse energy information of the event is also considered, primarily for the regression of the neutrino  $p_T$  and  $\eta$ , but also to increase the accuracy of the jet-to-parton association. The specific inputs provided to the SPA-NET model are summarized in Table 7.3 and further described here below.

Table 7.3: List of the input objects and variables considered in the SPA-NET model. This table also includes the configuration of the normalization layer for each variable and a comment motivating the choice of the various inputs.

| Object  | Input variable             | Normalization | Comments                                                                                                                                     |
|---------|----------------------------|---------------|----------------------------------------------------------------------------------------------------------------------------------------------|
| Jets    | $p_T$                      | Log. norm.    | Kinematic properties and flavor information of the jets for jet-to-parton assignment                                                         |
|         | $\eta$                     | norm.         |                                                                                                                                              |
|         | $\sin(\phi)$               | norm.         |                                                                                                                                              |
|         | $\cos(\phi)$               | norm.         |                                                                                                                                              |
|         | $E$                        | Log. norm.    |                                                                                                                                              |
|         | pseudo-cont. $b$ -tag      | None          |                                                                                                                                              |
| Leptons | $p_T$                      | Log. norm.    | Kinematic properties and flavor information of the lepton to help with the jet-to-parton assignment and neutrino $p_T$ and $\eta$ regression |
|         | $\eta$                     | norm.         |                                                                                                                                              |
|         | $\sin(\phi)$               | norm.         |                                                                                                                                              |
|         | $\cos(\phi)$               | norm.         |                                                                                                                                              |
|         | $E$                        | Log. norm.    |                                                                                                                                              |
|         | $e$ -tag                   | None          |                                                                                                                                              |
| Global  | $\mu$ -tag                 | None          | Global information of the event for neutrino $p_T$ and $\eta$ regression                                                                     |
|         | $p_T^{\text{miss}}$        | Log. norm.    |                                                                                                                                              |
|         | $\sin(\phi^{\text{miss}})$ | norm.         |                                                                                                                                              |
|         | $\cos(\phi^{\text{miss}})$ | norm.         |                                                                                                                                              |

The information that characterizes the kinematic properties of an object is its associated four-vector; hence this information is provided to SPA-NET by introducing as inputs the  $p_T$ ,  $\eta$ ,  $\sin(\phi)$ ,  $\cos(\phi)$ , and energy ( $E$ ) of the lepton and each of the jets in the event. The  $\phi$  component of the four-vector is transformed into  $\sin(\phi)$  and  $\cos(\phi)$  to deal with the instabilities that arise when working with periodic variables (circular variables), the so-called *circularity problem*<sup>2</sup>.

<sup>2</sup>For example, the  $1^\circ$  and  $359^\circ$  angles on a circle are numerically distant, but they are actually spatially close. This happens because the circle has a breakpoint at  $0^\circ$ , which creates a discontinuity in the numerical values without affecting their spatial proximity.

Moreover, to increase the efficiency in the jet-to-parton matching for  $b$ -jets, the jet  $b$ -tagging information is provided to SPA-NET by including as input the pseudo-continuous DL1r  $b$ -tagger described in Section 4.5. An  $e$ -tag and a  $\mu$ -tag flag are also provided as inputs of SPA-NET to allow it to learn the kinematic and response differences between the two lepton flavors. The possibility of adding other jet variables, such as a quark/gluon-tagger based on the number of tracks inside a jet, was studied but finally rejected because it was only valid for small- $R$  jets with  $p_T > 50$  GeV and  $|\eta| < 2.1$ , which does not cover the full phase space used in this analysis.

At last, the general information associated with the missing transverse energy is provided to SPA-NET by including as inputs  $p_T^{\text{miss}}$ ,  $\sin(\phi^{\text{miss}})$ , and  $\cos(\phi^{\text{miss}})$ , where  $\phi^{\text{miss}}$  is divided into two functions as in the case of the kinematic  $\phi$  of the jets and the lepton.

The different features used as inputs of the ML model are expressed within numerical ranges that may be several orders of magnitude apart<sup>3</sup>. These big numerical differences between the input values usually affect the relevance that the ML model assigns to each feature, reducing, overall, the learning rate and stability of the model. A common technique employed to address this issue consists of normalizing the inputs to a similar numerical range during the *pre-processing step*. In the case of SPA-NET, the pre-processing step is introduced into the network by adding a normalization layer at the start of the model, which normalizes the desired features based on the range in the training dataset statistics. Additionally, the normalization layer can also apply a logarithmic transformation to the input values to reduce the variance of the feature before normalization.

## Output variables

The output variables provided by the SPA-NET implemented in this analysis consist of the outputs generated by each of the final elements of the network. These include the tensor attention associated with the hadronically decaying top quark ( $t^{\text{had}}$ ), the leptonically decaying top quark ( $t^{\text{lep}}$ ), and the extrajet at parton level. Additionally, there are two regression heads dedicated to the regression of the neutrino  $p_T$  and  $\eta$ .

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<sup>3</sup>The input associated with an object's  $p_T$  is expressed in MeV, and its typical value is  $\sim 10^6$  MeV, whereas the  $\sin(\phi)$  input is constrained in the  $-1 < \sin(\phi) < 1$  range.

For each tensor attention, the predicted jet-to-parton assignment and its probability, and the detection probability are provided, while the output of the neutrino  $\eta$  and  $p_T$  regression heads are the predicted values for these magnitudes. A summary of the outputs provided by the SPA-NET implemented in this analysis is found in Table 7.4.

Table 7.4: List of the output categories and variables provided by the SPA-NET model. The assignment probability variables are vectors with multiple entries. The probabilities are expressed in an arbitrary interval (not between 0 and 1).

| Category         | Output variable                                                                             | Comments                                                                    |
|------------------|---------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------|
| Assignment prob. | $t^{\text{had}}$ assign. prob.<br>$t^{\text{lep}}$ assign. prob.<br>extra-jet assign. prob. | Predicted jet-to-parton assignment and its probability                      |
| Detection prob.  | $t^{\text{had}}$ det. prob.<br>$t^{\text{lep}}$ det. prob.<br>extra-jet det. prob.          | Probability that all decay products of a parton are found at detector level |
| Regressions      | neutrino $p_T$<br>neutrino $\eta$                                                           | Regressed neutrino $p_T$ & $\eta$                                           |

### Training of SPA-Net model

The samples with which the SPA-NET model is trained correspond to the nominal  $t\bar{t}$  samples produced with POWHEG +PYTHIA 8, where the top quark MC mass parameter set to  $m_t^{\text{MC}} = 172.5$  GeV (Section 6.2). The three samples corresponding to the production campaigns that reproduce the pile-up conditions during the 2015+2016, 2017, and 2018 data-taking periods are used simultaneously during the training to produce a single general model that can be applied to all Run 2 data without distinctions. No significant loss in the network performance is observed with respect to a model specifically trained and tested with the MC samples corresponding to the pile-up conditions of a single year. After the event preselection, a total of  $\sim 58$ M simulated  $t\bar{t}$  events remain, from which around 14.8M, 18.5M, and 24.7M correspond to each of the MC production campaigns, roughly reproducing the relative luminosity of each data-taking period.

To ensure that the training and testing datasets are statistically independent, the 58M preselected events composing the  $t\bar{t}$  sample described above are split into two samples, one containing the events numbered as *even* and another one

containing the events numbered as *odd*. The corresponding SPA-NET models trained using the *even* and *odd* samples are also referred to as *even* and *odd* models, respectively. Additionally, the events in the training dataset are split into 95% for the actual training, and 5% for the validation after each training step.

The events in the dataset can be categorized as complete (*matchable*) events or partial (*unmatchable*) events, depending on whether all the final state products associated with the parton level objects are found within the acceptance of the detector or if one or more of these objects fall outside the acceptance, respectively.

A detector level object is considered matched to a parton level object if it is located within a cone of  $\Delta R = 0.4$ . Specifically, for the jet-to-parton matching in  $t\bar{t}$  +jet events outlined in this note, a sequential approach is employed to prevent potential ambiguity arising from various scenarios, such as multiple parton level objects matched to the same detector level object or vice versa. This sequential procedure iterates over the different detector level jets, attempting to match the  $b$  quark originated from the leptonic decay of the top quark first, followed by the  $b$  quark from the hadronic decay of the top quark, then the up and down-type quarks from the hadronically decaying  $W$  boson (in that order), and finally, the additional parton level jet. The first parton level object in this sequence that fulfills the  $\Delta R$  requirement is assigned to the corresponding detector level jet. Additionally, if multiple detector level objects match the same parton level object, the one with a lower  $\Delta R$  value takes precedence for selection. This comprehensive approach ensures a proper treatment of all possible scenarios, avoiding any potential for ambiguous classifications.

Conventional reconstruction methods based on permutations are typically only applicable to complete events since their scoring functions are unsuitable for partial events. However, as SPA-NET uses a partitioned approach to solve the jet-to-parton assignment problem, where an independent tensor attention is used for each parton level object, the training loss function can be modified to only account for the objects that are actually found at detector level, making it possible to learn from events where the  $t\bar{t}$  +jet system is incomplete. Due to this learning capability, the network designed to reconstruct  $t\bar{t}$  +jet events can also reconstruct the  $t\bar{t}$  system alone in events with exactly four jets, allowing the use of this network to calculate the  $M_{lb}$  observable without requiring a separate network for this task. There is no significant loss in the reconstruction efficiency of the  $M_{lb}$  matching when using the  $t\bar{t}$  +jet trained model, with respect to a model specifically trained



to reconstruct only the  $t\bar{t}$  system. Moreover, incorporating partial events during the training increases the effective size of the training dataset and may decrease the generalization bias, as these events are present in recorded collision data.

The symmetry between the two quarks originating from the hadronically decaying  $W$  boson is introduced into the architecture of the network by using symmetric attention tensors for the tensor attention associated with these two particles.

This implementation of SPA-NET was performed while being in close contact with the authors of the SPA-NET framework, so their recommendations on the choice of the hyper-parameters<sup>4</sup> used during the training of the network were followed (Appendix D.2). These hyper-parameters include a dropout rate of 10% during the training of the network, which means that during each training iteration, a random selection of 10% of the neurons are set to zero (dropped out). This technique effectively trains different networks within the model, forcing the model to learn to rely on alternative neurons and not to become too reliant on any particular set. Overall, this technique helps to mitigate overfitting when considering the complete model, which includes all the neurons.

Each network was trained using a total of 4x GPU Nvidia Tesla Ampere A100 40GB SXM4 running in parallel, which were provided by the ARTEMISA cluster [192]. The training was done with a batch size of 2048 for a total of 200 epochs using the AdamW optimizer [193] with  $L_2$  regularization [194] on all parameter weights. The evolution of the model accuracy when evaluating the network performance after each training step over the validation sample is shown in Figure 7.5.

After 200 epochs<sup>5</sup>, the network's validation accuracy curve has reached its maximum performance and does not show signs of overtraining, as further discussed in Appendix D.3. The maximum in the validation accuracy is found around 0.30, which means that, from the whole  $t\bar{t}$  preselected sample, 30% of the events have all the decay products of the  $t\bar{t} + \text{jet}$  system matched properly. This accuracy is relatively low because it is calculated using all event regions, including those with  $n_{\text{jets}} = 4$ , for which it is impossible to match the semileptonic decaying  $t\bar{t} + \text{jet}$  system properly.

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<sup>4</sup>The hyper-parameters are configurable parameters of the model that control the learning process.

<sup>5</sup>A single iteration through the entire training dataset is known as an epoch.

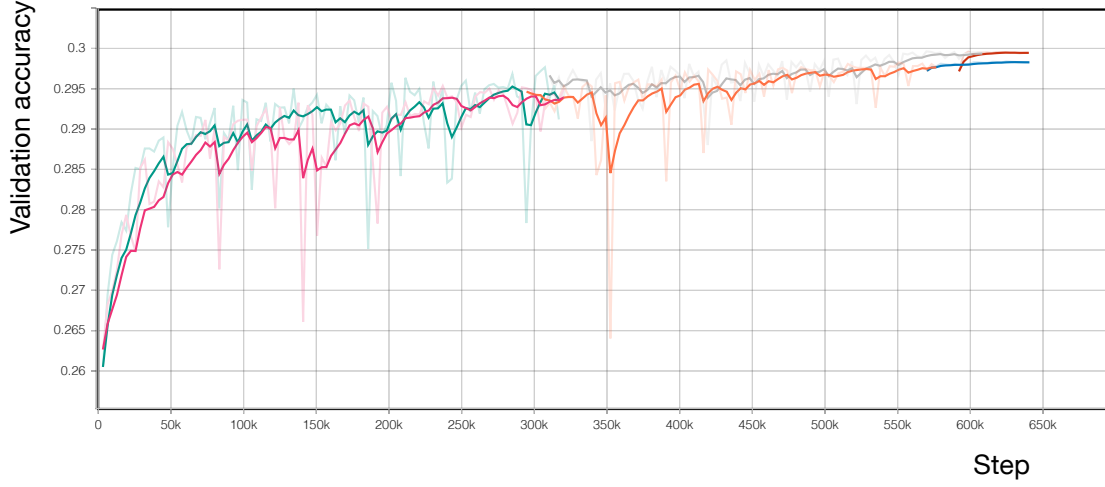


Figure 7.5: Validation accuracy curve for the SPA-NET  $t\bar{t}$  +jet models. The combination of the pink, orange, and blue lines represents the curve for the network trained over *even* events, while the combination of the green, grey, and red lines represents the curve for the network trained over *odd* events. Each curve is formed by three different color lines, which represent the three different training jobs sent to the grid for completing the training.

In Table 7.5, the SPA-NET matching efficiencies for each of the parton level objects is shown for the  $t\bar{t}$  +jet matchable events, the events for which all the decay products of the original particles are found at detector level. The Event Fraction column in this table contains the proportion of matchable events for each jet multiplicity, where the Inclusive  $n_{\text{jets}}$  category comprises all events with  $n_{\text{jets}} \geq 4$ . The overall matching efficiency for *matchable events* is  $\sim 63.8\%$ .

Table 7.5: SPA-NET matching efficiencies for the all the  $t\bar{t}$  +jet *matchable events* that pass the preselection requirements.

| $n_{\text{jets}}$ | Event Fraction | SPA-NET Efficiency |                  |          |       |
|-------------------|----------------|--------------------|------------------|----------|-------|
|                   |                | $t^{\text{had}}$   | $t^{\text{lep}}$ | extrajet | All   |
| $= 5$             | 0.309          | 0.734              | 0.867            | 0.828    | 0.718 |
| $\geq 6$          | 0.469          | 0.639              | 0.836            | 0.773    | 0.558 |
| <b>Inclusive</b>  | 0.184          | 0.686              | 0.851            | 0.800    | 0.638 |

For the construction of the  $M_{lb}$  observable, it is not necessary to properly match all the jets in the event, it is enough only to match correctly the  $b$  quark associated with the leptonically decaying top quark, as this is the only jet used in the calculation of the observable. The matching efficiency of this jet, in the case of only considering events where  $t^{\text{lep}}$  is matchable, is shown in Table 7.6. The Event

Fraction column contains the proportion of events where the  $t^{\text{lep}}$  is matchable for each jet multiplicity category. For the phase space region with  $n_{\text{jets}} = 4$ , the one where the  $M_{lb}$  observable is studied, the matching efficiency is  $\sim 84.2\%$ .

Table 7.6: SPA-NET matching efficiencies for the leptonic decaying top using the events that pass the preselection and for which this particle is *matchable*.

| $n_{\text{jets}}$ | Event Fraction | SPA-NET Efficiency<br>$t^{\text{lep}}$ |
|-------------------|----------------|----------------------------------------|
| $= 4$             | 0.731          | 0.842                                  |
| $= 5$             | 0.788          | 0.835                                  |
| $\geq 6$          | 0.823          | 0.816                                  |
| <b>Inclusive</b>  | 0.766          | 0.834                                  |

The efficiencies presented in Table 7.5 and 7.6 are cross-validated using the SPA-NET models trained with both, *even* and *odd* samples, resulting in differences at the 1/1000 level or below.

## 7.4 Performance of the SPA-Net model and final event selection

The SPA-NET matching efficiencies studied during the training are calculated for specific regions of the phase space, where one or more parton level particles were matchable with their corresponding detector level associated objects. However, these regions cannot be selected in recorded data as the true origin of the detector objects is unknown. In this section, the matching efficiencies and the outputs of the SPA-NET model are studied for the regions that are actually used for the top quark pole mass measurement analysis. The information obtained from these outputs is used to apply a final event selection designed to enhance the fraction of correctly matched events.

### Categorization of the events into multiple event regions

At the preselection stage, all the events with a signature compatible with originating from a semileptonic decaying  $t\bar{t}$  or  $t\bar{t} + \text{jet}$  event are selected and used for the training of the SPA-NET model. Nevertheless, for the maximum likelihood fit described in Chapter 8, the events are divided into multiple orthogonal

categories (regions) to increase the sensitivity of the analysis to the top quark pole mass and the top quark MC mass. This division is carried out based on the jet multiplicity and the  $b$ -tagged jet multiplicity. A summary of all the regions considered in the analysis and the observable constructed in each one of them is given in Table 7.7. A description of the motivation behind each division is given here below:

Table 7.7: Summary of the various orthogonal regions used in the analysis together with their lepton flavor, jet and  $b$ -tagged jet multiplicities, the variable used in the measurement, and its motivation.

| Region      | leptons              | $n_{\text{jets}}$ | $n_{b\text{-tagged}}$ | Variable | Motivation                  |
|-------------|----------------------|-------------------|-----------------------|----------|-----------------------------|
| SRIjets5j2b | $e^\pm$ or $\mu^\pm$ | $\geq 5$          | 2                     | $\rho_s$ | Unfold to parton level      |
| SRIjets5j1b | $e^\pm$ or $\mu^\pm$ | $\geq 5$          | 1                     | $\rho_s$ | Unfold to parton level      |
| CRIjets4j2b | $e^\pm$ or $\mu^\pm$ | 4                 | 2                     | $M_{lb}$ | Sensitive $m_t^{\text{MC}}$ |
| CRIjets4j1b | $e^\pm$ or $\mu^\pm$ | 4                 | 1                     | $M_{lb}$ | Sensitive $m_t^{\text{MC}}$ |

- According to the jet multiplicity, the sample is split into events with exactly four jets,  $n_{\text{jets}} = 4$ , and events with five or more jets,  $n_{\text{jets}} \geq 5$ . This split is based on whether or not the experimental signal is compatible with originating from a  $t\bar{t}$  +jet system. For the regions where the  $t\bar{t}$  +jet system can be reconstructed, the distribution of the  $\rho_s$  variable is calculated and used for the fit. For the regions where only the  $t\bar{t}$  system can be reconstructed, the  $M_{lb}$  variable is calculated and added to the fit to increase the sensitivity to the top quark MC mass (Section 2.3.1).
- According to the  $b$ -tagged jet multiplicity, the events are further divided into two categories, one containing the events with  $n_{b\text{-jets}} = 1$  and another one containing the events with  $n_{b\text{-jets}} = 2$ . Events with  $n_{b\text{-jets}} \geq 3$  are removed from the analysis as they are affected by significantly higher  $b$ -tagging uncertainties. The background contamination is expected to be lower in the category with exactly two  $b$ -tagged jets than in the category with exactly one  $b$ -tagged jet. Therefore, dividing the events into these categories increases the sensitivity of the analysis while keeping a significant portion of the signal events.

The performance of the network is studied separately for each region in the analysis since signal and control regions study different variables, and two and

one  $b$ -tagged regions have different contamination of *unmatchable* and *incorrectly matched* events. Nevertheless, this section only contains plots constructed in the SRljets5j2b signal region and the CRLjets4j2b control region in order to make the section more readable. A collection of supplementary performance plots for these and the other regions is provided in Appendix D.5.

### Reconstruction of the neutrino four-vector using SPA-Net

One of the main goals of implementing the SPA-NET model in the analysis is to reconstruct the non-detected neutrino associated with the semileptonic  $t\bar{t}$  decay. To perform this reconstruction, the neutrino  $p_T$  and  $\eta$  regressed using the ML model are combined with the measured  $\phi^{\text{miss}}$  to construct the neutrino four-vector, under the assumption that the mass of the neutrinos is negligible. In Figure 7.6, the performance of the SPA-NET neutrino reconstruction is compared with the neutrino reconstructed using an alternative algorithm based on the  $W$  mass constraint, as described in Appendix C.1.

The neutrino  $p_T$  reconstructed from the  $W$  mass constraint algorithm exhibits a systematic overestimation across the entire phase space. Moreover, since this algorithm sets the neutrino  $p_T$  to be equal to  $E_T^{\text{miss}}$ , it is unable to properly reconstruct neutrinos with a  $p_T$  smaller than the preselection requirement imposed on this variable, leading to a region of the phase space without any entry. The neutrino  $p_T$  regressed using the SPA-NET model does not have that limitation and shows a much better overall performance across the full phase space.

The neutrino  $\eta$  reconstructed from the  $W$  mass constraint algorithm exhibits a concentration of unphysical solutions that accumulate at  $\eta = 0$ . This feature is also avoided in the case of the SPA-NET model, which does not present that mathematical limitation.

The comparison between data and the SM prediction for the components of the neutrino four vector reconstructed using SPA-NET model and  $\phi^{\text{miss}}$  is shown in Figure 7.7. Overall, good level of agreement is observed for all the kinematic variables. However, as with kinematic distributions in Figures 7.1 to 7.3, the neutrino  $p_T$  and energy is predicted to be harder in the simulation than in the observed data. Nonetheless, this discrepancy is covered by the modeling systematic uncertainties.

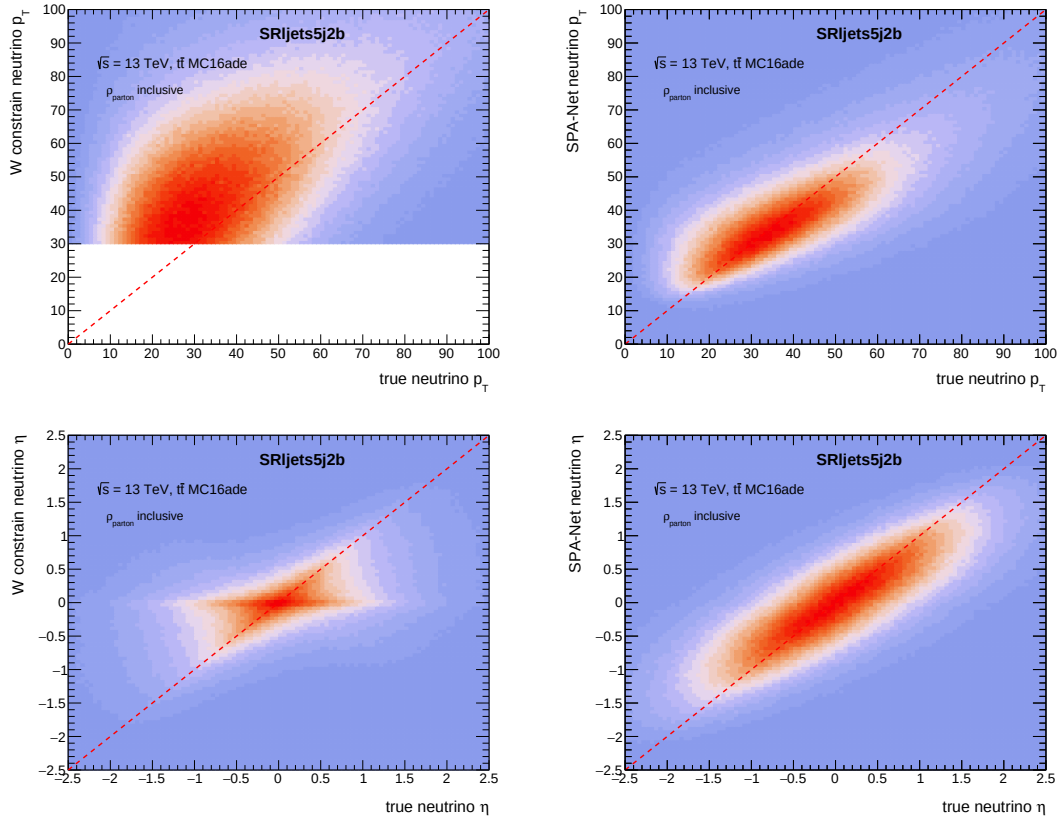


Figure 7.6: Neutrino  $p_T$  and  $\eta$  reconstructed using the  $W$  mass constraint (left) and the regression outputs of the SPA-NET model (right). The two reconstruction methods are applied over the signal region SRIjets5j2b. The white band in the neutrino  $p_T$  predicted by the  $W$  mass constraint is due to the  $E_T^{\text{miss}} > 30$  GeV requirement in the event preselection.

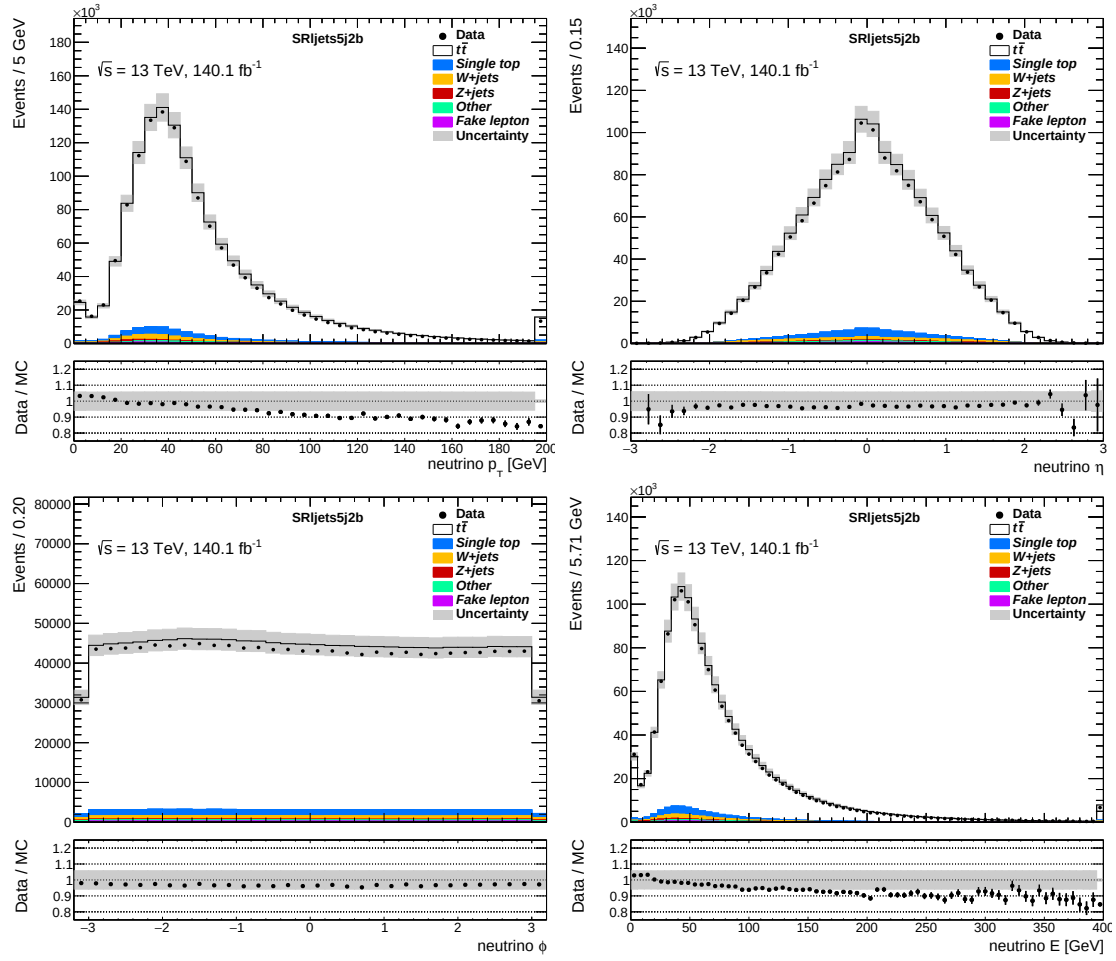


Figure 7.7: Data/prediction comparison for the four vector components of the neutrino reconstructed using the SPA-NET regression outputs and  $\phi^{\text{miss}}$ .

### SPA-Net performance in $t\bar{t}$ +jet event topologies and $\rho_s$ reconstruction

To evaluate the performance of the SPA-NET reconstruction in a specific signal region of the analysis and compare it with the alternative reconstruction methods presented in Appendix C, five different metrics are evaluated:

- The percentage of *correctly matched* events.
- The percentage of *incorrectly matched* events.
- The percentage of *unmatchable* events.
- The fraction of remaining events after the cuts introduced by the algorithm.
- The resolution in the reconstructed  $\rho_s$  variable.

These metrics are also used to optimize the performance of the various reconstruction algorithms tested for the reconstruction of the  $t\bar{t}$  +jet system.

In the case of SPA-NET, the optimization of the reconstruction is done by analyzing the discriminant power of the *assignment probabilities* and *detection probabilities* outputs. This discriminant power is assessed by representing the distribution of the *correctly matched*, *incorrectly matched*, and *unmatchable* events for each parton level particle, as illustrated in Figure 7.8. The level of agreement between data and the SM prediction for these SPA-NET outputs is shown in Figure 7.9. A noticeable slope can be observed for high values of the detection probability variables. However, these slopes are covered when accounting for all the systematic uncertainties in the analysis. The good level of agreement indicates that these variables are well modeled in the simulations. Therefore, cuts can be applied to them to enhance the fraction of correctly matched events.

As expected, the distributions shown in Figure 7.8 demonstrate that the *detection probability* variables exhibit a significant discrimination power between *matchable* and *unmatchable* events for each of the parton level particles. Similarly, the *assignment probability* variables exhibit a significant discriminant power between *correctly matched* and *incorrectly matched* events. Consequently, a cut-and-select approach based on these variables lead to an improvement in the fraction of correctly matched events within the samples.

In the case of the signal regions, the variable studied is  $\rho_s$ , which is proportional to the inverse of the invariant mass of the  $t\bar{t}$  +jet system (as defined in



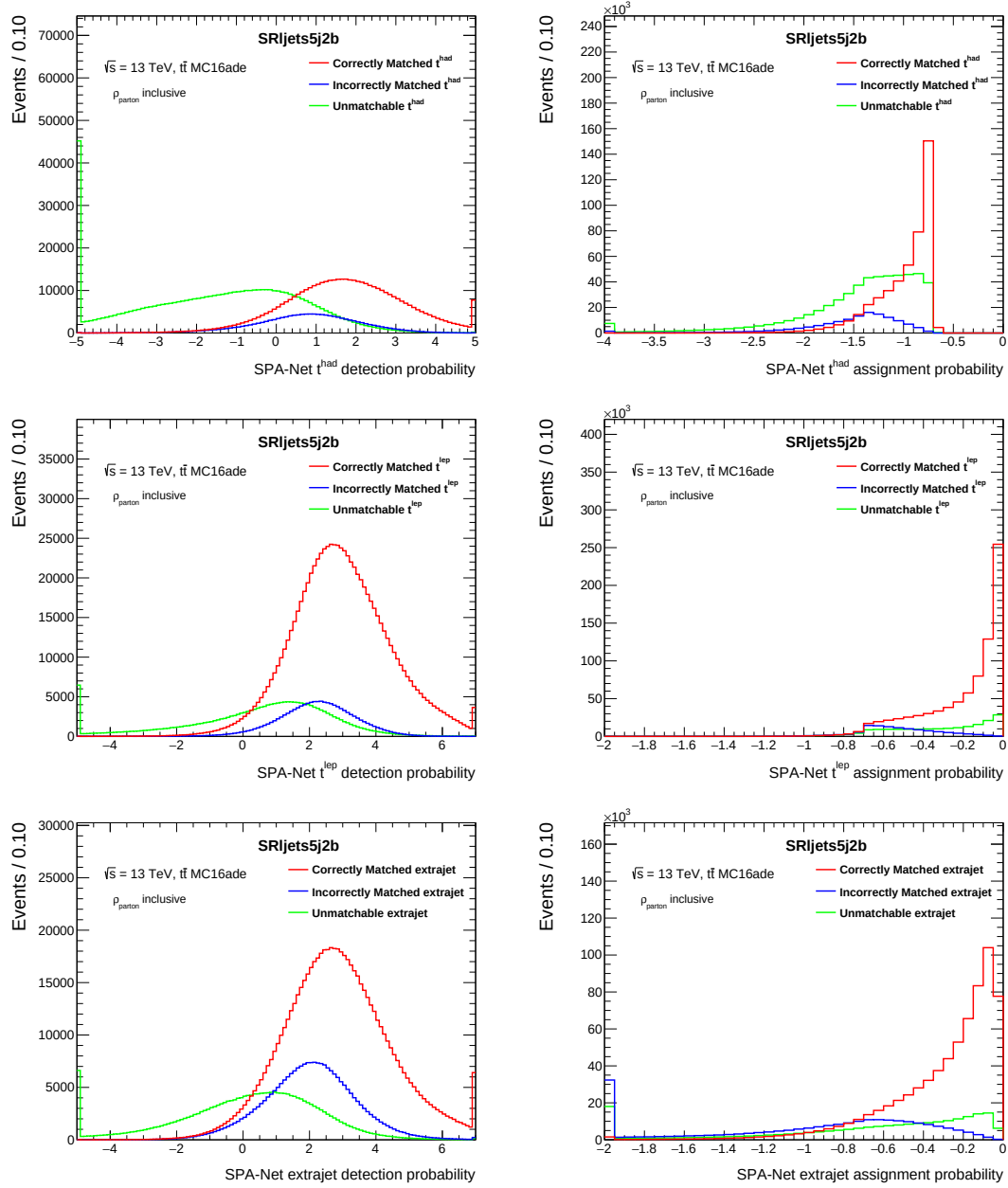


Figure 7.8: SPA-NET predicted detection probability and assignment probability for the hadronically decaying top quark ( $t^{\text{had}}$ ), the leptonically decaying top quark ( $t^{\text{lep}}$ ), and the extrajet. These predictions are performed for the SRljets5j2b signal region.

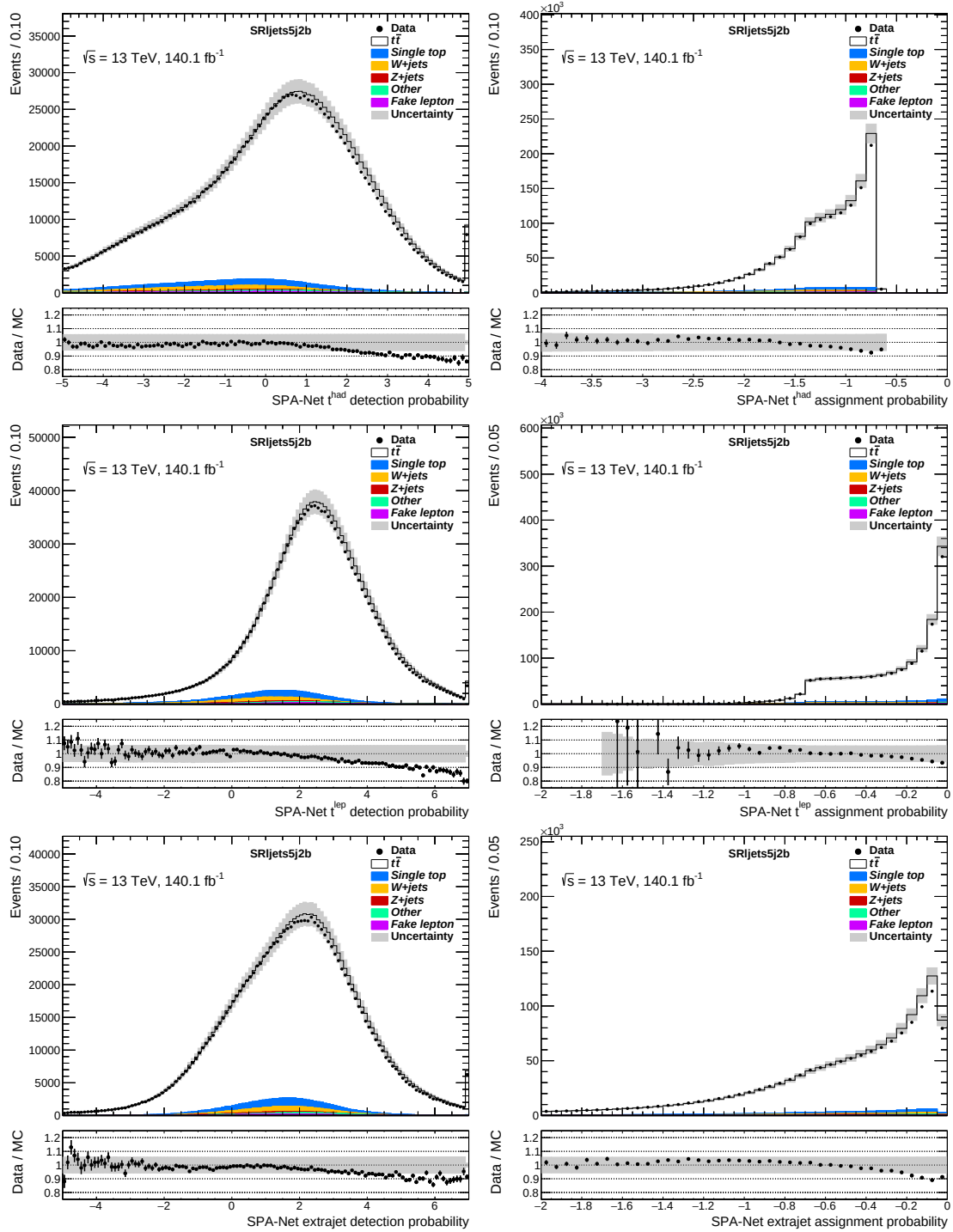


Figure 7.9: Data/prediction comparison for the detector and assignment probabilities of SPA-NET for each parton level particle in the SRljets5j2b signal region.

Equation 2.15). Since  $\sqrt{s_{t\bar{t}+\text{jet}}}$  is unaffected by the permutation of the object assignments within the system, improving the resolution in the reconstruction of  $\rho_s$  relies primarily on the rejection of *unmatchable* events, rather than *incorrectly matched* events. Therefore, only cuts in the *detection probability* variables are imposed to improve the  $\rho_s$  reconstruction while preserving as much statistics as possible. In particular, the final event selection requires the following cuts in all signal regions:

- $t^{\text{had}}$  detection probability  $> 0.5$
- $t^{\text{lep}}$  detection probability  $> 0.5$
- $\text{extrajet}$  detection probability  $> -1$

The requirements imposed in the final event selection have been optimized to improve the resolution of the reconstructed  $\rho_s$  variable, enhance the fraction of correctly matched events, and ensure a similar performance across all signal regions while avoiding any significant bias and preserving a significant portion of the statistics.

Additionally, the four-momenta of the jets identified as originating from the decay of the  $W$  boson are corrected by a factor  $\alpha = \frac{M_W^{PDG}}{M_W^{\text{SPA-NET}}}$ , with  $M_W^{PDG} = 80.4$  [4]. This correction ensures that the mass of the hadronic  $W$  boson candidate corresponds to the one value reported in the PDG, thereby improving the reconstruction of the kinematic properties of the  $t\bar{t} + \text{jet}$  system. The control plots for the  $\alpha$  distribution, as well as for other reconstructed variables after applying the final event selection, are provided in Appendix E.

At last, the event is accepted if the jet labeled as *extrajet* satisfies:

- $p_T^{\text{extrajet}} > 30 \text{ GeV}$
- $|\eta^{\text{extrajet}}| < 2.5$

In Figure 7.10, the resolution in  $\rho_s$  obtained using the SPA-NET reconstruction with the final event selection is compared to the reconstruction algorithm used in the 8 TeV analysis (Appendix C.1) and with the optimized version of KLFITTER (Appendix C.2). Further studies evaluating the performance of the various reconstruction algorithms are available in Appendices D.4 and D.5. SPA-NET

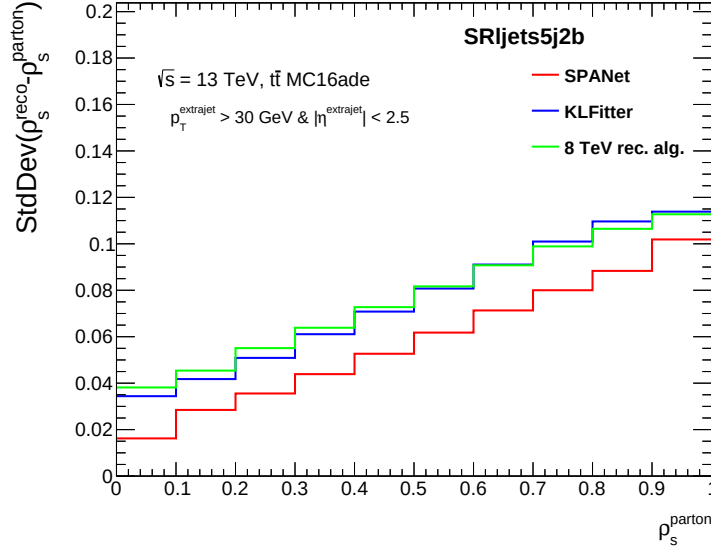


Figure 7.10: Resolution of  $\rho_s$  as a function of its value at parton level for various  $t\bar{t}$  +jet system reconstruction algorithms.

is the reconstruction method that leads to a better resolution in  $\rho_s$  for all the bins in the distribution.

The resulting  $\rho_s$  distribution at detector level after applying the final event selection over the events reconstructed using the SPA-NET model is shown in Figure 7.11. A good level of agreement between data and the SM is observed prediction. Furthermore, since the topologies that originate the background processes lack the presence of one or more of the parton level objects in the  $t\bar{t}$  +jet system, the introduction of the  $t^{\text{had}}$ ,  $t^{\text{lep}}$ , and the extrajet *detection probability* requirements, has the secondary effect of reducing the background contributions. This effect is notable when comparing the reconstructed distribution before and after the final event selection (Appendix D.5).

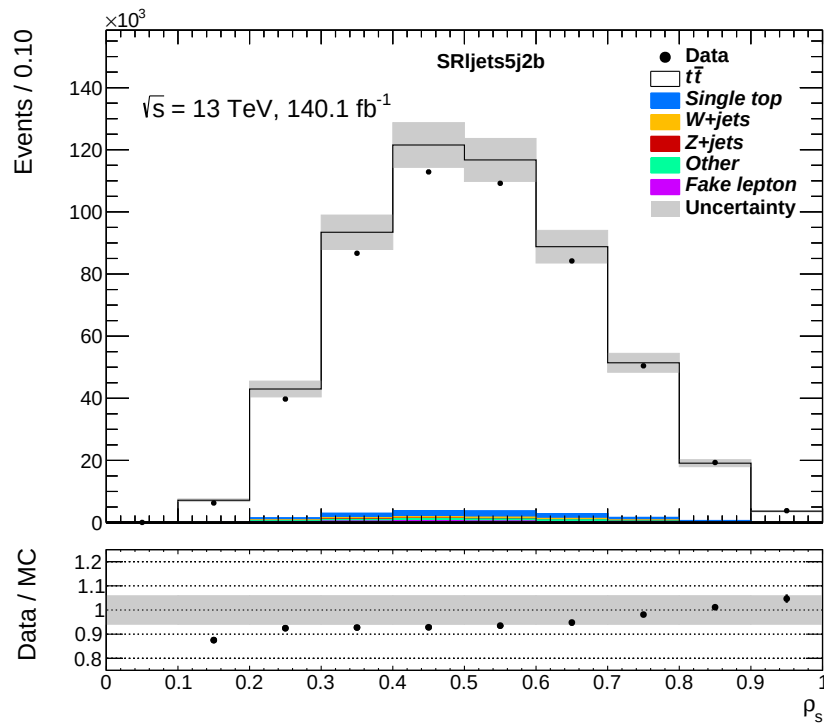


Figure 7.11: Data/prediction comparison for the  $\rho_s$  observable in the  $t\bar{t}$  +jet system using the SPA-NET reconstruction after the final selection cuts on the *detection probabilities* of each parton level particle are imposed.

### SPA-Net performance in $t\bar{t}$ event topologies and $M_{lb}$ reconstruction

In the case of the control regions defined in Table 7.7, the variable of interest is  $M_{lb}$ , so only the SPA-NET output variables related to the reconstruction of this variable are considered. The optimization of the reconstruction of this variable is done by analyzing the discriminant power of the *assignment probability* and *detection probability* for the leptonically decaying top quark. Their separation power is assessed by representing the distribution of the *correctly matched*, *incorrectly matched*, and *unmatchable* events for the leptonically decaying top quark, as illustrated in Figure 7.12. The level of agreement between data and the SM prediction for these SPA-NET outputs is shown in Figure 7.13. A good level of agreement is observed, which means that these variables are well modeled in the simulations, thus cuts can be applied to them to enhance the fraction of correctly matched events.

As in the case of the  $\rho_s$  observable, the  $t^{\text{lep}}$  *detection probability* has a significant discriminant power between *matchable* and *unmatchable* events, while the  $t^{\text{lep}}$  *assignment probability* has a significant discriminant power between *correctly matched* and *incorrectly matched* events.

The  $M_{lb}$  observable is constructed using the lepton and the  $b$ -jet associated with the leptonically decaying top quark. For this reason, this variable is highly affected by the *background* originated from *unmatchable* events, where the  $b$ -jet associated with the leptonically decaying top is outside the acceptance of the detector, as well as the *incorrectly matched* events, where the  $b$ -jet originated from the leptonically top decay is not correctly assigned. Therefore, in contrast to the cuts applied in the signal regions, both a cut in the  $t^{\text{lep}}$  *detection probability* and the  $t^{\text{lep}}$  *assignment probability* are imposed. In particular, the final event selection requires the following cuts in all control regions:

- $t^{\text{lep}}$  detection probability  $> 0.5$
- $t^{\text{lep}}$  assignment probability  $> -0.5$

Additionally, the final event selection only includes events in the interval  $20\text{GeV} < M_{lb} < 160\text{GeV}$ . This choice of fit range mirrors the one used in Ref [195], and it is designed to optimize the precision in the measurement of  $m_t^{\text{MC}}$ . This selection was applied to remove the events with exceptionally high or low values of  $M_{lb}$ , as these tend to introduce a higher uncertainty due to the JES and JER

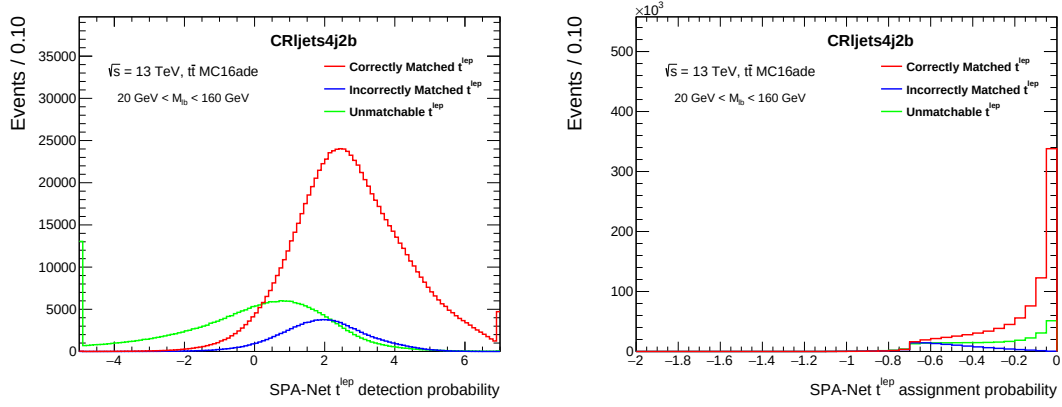


Figure 7.12: SPA-NET predicted detection probability and assignment probability for the leptonically decaying top quark ( $t^{\text{lep}}$ ). These predictions are performed for the CRljets4j2b control region.

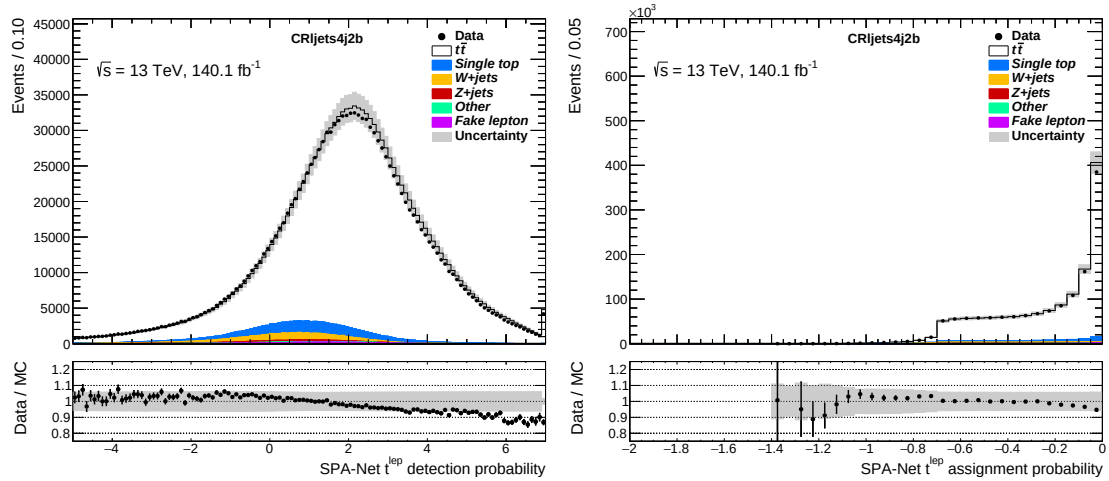


Figure 7.13: Data/prediction agreement for the detector and assignment probabilities of SPA-NET for the leptonically decaying top quark at parton level.

components. Nevertheless, in the present analysis, this particular choice of the fitting range has a minimal impact.

The resulting  $M_{lb}$  distribution at detector level after applying the final event selection over the events reconstructed using the SPA-NET model is shown in Figure 7.14. Similar to the signal regions, a noticeable slope can be observed for high values of the detection probability variable, which is also covered when accounting for all the systematic uncertainties in the analysis.

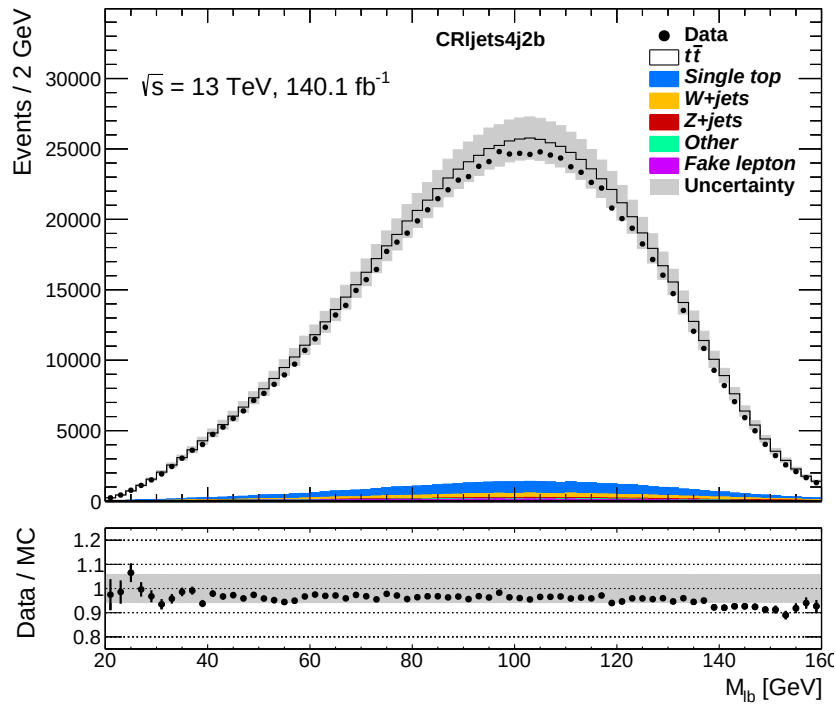


Figure 7.14: Data/prediction agreement for the  $M_{lb}$  observable in the  $t\bar{t}$  system using the SPA-NET reconstruction after the final selection cuts on the *detection* and *assignment* probabilities of the leptonically decaying top are imposed.



## 7.5 Summary of the event selection used in the analysis

To sum up, all the events considered in the analysis have to, first, fulfil the event preselection described in Section 7.2 and summarized in Table 7.8. Then, the  $t\bar{t}$  and  $t\bar{t}$  +jet systems are reconstructed using the SPA-NET ML model described in Section 7.3. The resulting events from the reconstruction are divided into two control and two signal regions according to their jet and  $b$ -jet multiplicity. At last, the final event selection requirements described in Section 7.4 are imposed to obtain the final samples used in the analysis. A summary of the final event selection is shown in Table 7.9

Table 7.8: Summary of the event preselection applied to identify events with a signal compatible with originating from semileptonically decaying  $t\bar{t}$  or  $t\bar{t}$  +jet events.

| Event Preselection        |                                      |                                     |                                   |
|---------------------------|--------------------------------------|-------------------------------------|-----------------------------------|
| Leptons                   | $N_l (l = e^\pm/\mu^\pm) = 1$        | $p_T^l > 25 \text{ GeV}$            | (2015)                            |
|                           |                                      | $p_T^l > 27 \text{ GeV}$            | (2016, 2017, 2018)                |
| Jets                      | $N_{\text{jet}} \geq 4$              | $p_T^{\text{jet}} > 25 \text{ GeV}$ |                                   |
|                           | $N_{b\text{-jet}} \geq 1$            |                                     | (70% eff. WP DL1r $b$ -tagger)    |
| Missing Transverse Energy | $E_T^{\text{miss}} > 30 \text{ GeV}$ | $m_T^W > 30 \text{ GeV}$            | (Same for $e$ and $\mu$ channels) |

Table 7.9: Summary of the Final Event Selection. This selection is applied to the events that pass the Event Preselection. It is designed to increase the resolution in the reconstruction of the  $\rho_s$  variable in the Signal Regions and of the  $M_{lb}$  variable in the Control Regions.

| Final Event Selection |                                                                           |                                         |
|-----------------------|---------------------------------------------------------------------------|-----------------------------------------|
| Signal Regions        | $N_{\text{jet}} \geq 5$                                                   | $t^{\text{had}}$ detec. prob. $> 0.5$   |
|                       | $N_{b\text{-jet}} = 1, 2$                                                 | $t^{\text{lep}}$ detec. prob. $> 0.5$   |
|                       | $p_T^{\text{extrajet}} > 30 \text{ GeV}$ $ \eta^{\text{extrajet}}  < 2.5$ | extrajet detec. prob. $> -1$            |
| Control Regions       | $N_{\text{jet}} = 4$                                                      | $t^{\text{lep}}$ detec. prob. $> 0.5$   |
|                       | $N_{b\text{-jet}} = 1, 2$                                                 | $t^{\text{lep}}$ assign. prob. $> -0.5$ |
|                       | $20 \text{ GeV} < M_{lb} < 160 \text{ GeV}$                               |                                         |



## Chapter 8

# Extraction of the top quark MC mass and the $t\bar{t}$ +jet differential cross section at parton level

This chapter describes the procedure followed to obtain the  $t\bar{t}$  +jet differential cross section as a function of the  $\rho_s$  observable at parton level, while simultaneously determining the top quark mass parameter in the simulation ( $m_t^{\text{MC}}$ ). The measured  $t\bar{t}$  +jet differential cross section is then used in Chapter 9 to extract the top quark mass parameter of the SM Lagrangian in the on-shell renormalization scheme (the top quark pole mass,  $m_t^{\text{pole}}$ ). This chapter is structured as follows: In Section 8.1, an introduction to the binned profile maximum likelihood fitting techniques is outlined. These are the tools used to construct the statistical model employed in this analysis. Section 8.2 provides insight into the origin and treatment of all the relevant sources of uncertainties affecting this fit. The detailed description of the specific statistical model employed in this analysis is given in Section 8.3. Lastly, in Section 8.4, the fit is validated on a detailed Asimov dataset based on the ATLAS MC simulations. At the time of writing this thesis, the analysis on the recorded Run 2 ATLAS dataset remains blinded.

## 8.1 Introduction to the profile maximum likelihood techniques

### Construction of the statistical model in a simplified scenario

The methodology used for performing a profile maximum likelihood fit is introduced in this section by presenting a schematic description of the process followed to construct the statistical model associated with a simplified scenario. In this simplified scenario, a single channel is considered<sup>1</sup>, with only contributions from one signal and one background process, and without considering any systematic uncertainties that could modify the expected number of signal or background events (denoted by  $S$  and  $B$ , respectively).

Within this scenario, a single *parameter of interest* (POI) is introduced into the model, the signal strength ( $\mu$ ) parameter. This continuous parameter is introduced such that  $\mu = 0$  corresponds to the background-only hypothesis, while  $\mu = 1$  corresponds to the signal+background hypothesis.

The probability to observe  $n$  events in data when a total of  $\mu S + B$  are expected from the prediction is described by the following equation [196]:

$$\mathcal{P}(\{x_1 \dots x_n\} | \mu) = \text{Poisson}(n | \mu S + B) \left[ \prod_{e=1}^n \frac{\mu S f_S(x_e) + B f_B(x_e)}{\mu S + B} \right] \quad (8.1)$$

where  $x$  is the discriminatory variable used to perform the measurement, and  $f_S(x)$  and  $f_B(x)$  are the probability density functions for signal and background events, respectively. The value of this discriminant variable for event  $e$  takes the value  $x_e$ , hence the full dataset is denoted as  $\{x_1 \dots x_n\}$ .

When the dataset is fixed,  $\mathcal{P}(\{x_1 \dots x_n\} | \mu)$  only depends on  $\mu$  and is referred to as the *likelihood function*,  $L(\mu)$ . The *extended maximum likelihood fit* formula can be obtained from Equation 8.1 simply by taking the negative logarithm of the likelihood and introducing the definition of the Poisson distribution,  $\text{Poisson}(n | \nu) = \nu^n e^{-\nu} / n!$ . This formula can be expressed as:

---

<sup>1</sup>A *channel* is a region of the data defined by a particular event selection.

$$\begin{aligned}
-\ln L(\mu) &= -n \ln(\mu S + B) + (\mu S + B) + \ln n! - \sum_{e=1}^n \ln \left[ \frac{\mu S f_S(x_e) + B f_B(x_e)}{\mu S + B} \right] \\
&= (\mu S + B) + \ln n! - \sum_{e=1}^n \ln [\mu S f_S(x_e) + B f_B(x_e)]
\end{aligned} \tag{8.2}$$

The  $f_S(x_e)$  and  $f_B(x_e)$  pdfs are estimated from MC simulations by constructing a binned distribution with respect the discriminatory variable ( $x$ ). For any given event  $e$  in which  $x_e$  falls within the bin  $b$  of the distribution, the values of these pdfs can be expressed as:

$$f_S(x_e) = \frac{\nu_b^{\text{sig}}}{S \Delta_b} \quad \text{and} \quad f_B(x_e) = \frac{\nu_b^{\text{bkg}}}{B \Delta_b}, \tag{8.3}$$

where  $\Delta_b$  represents the bin width,  $\nu_b^{\text{sig}}$  ( $\nu_b^{\text{bkg}}$ ) represents the expected number of signal (background) events in the bin, and  $S$  ( $B$ ) denotes the total number of signal (background) events. Since the pdfs are normalized to unity, the total number of signal and background events can be expressed as  $S = \sum_b \nu_b^{\text{sig}}$  and  $B = \sum_b \nu_b^{\text{bkg}}$ , respectively.

Combining Equation 8.1 and 8.3, the probability model can be written as a combination of Poisson distributions for each bin in the histograms:

$$\begin{aligned}
\mathcal{P}(n|\mu) &= \text{Poisson}(n|\mu S + B) \left[ \prod_{b \in \text{bins}} \frac{\mu \nu_b^{\text{sig}} + \nu_b^{\text{bkg}}}{\mu S + B} \right] \\
&= \mathcal{N}_{\text{comb}} \prod_{b \in \text{bins}} \text{Poisson}(n_b | \mu \nu_b^{\text{sig}} + \nu_b^{\text{bkg}}),
\end{aligned} \tag{8.4}$$

where the measured number of events in each bin of the data histogram is denoted by  $n_b$ , and  $\mathcal{N}_{\text{comb}}$  is a constant factor that is dropped when the  $\mathcal{P}\{n|\mu\}$  is interpreted as the likelihood distribution.

## Implementation of systematic uncertainties

The statistical model presented above offers a method to estimate the value of the parameter of interest ( $\mu$ ) via the minimization of the corresponding negative log-

likelihood function. However, the value extracted from the fit does not account for systematic uncertainties. To incorporate the impact of these uncertainties, a set of additional parameters can be introduced into the statistical framework to model their effects. These parameters are usually referred to as *nuisance parameters* (NPs).

The impact of each systematic uncertainty is captured by producing a varied distribution of the observable, which can be compared to the nominal distribution. The difference between these two distributions is parametrized by a single NP whose uncertainty has been previously determined through dedicated auxiliary measurements. To incorporate the prior knowledge provided by the auxiliary measurements, a penalty term is added into the likelihood for each NP. The resulting extended likelihood function with the NPs is expressed as follows:

$$L(\mu)(n|\mu, \vec{\theta}) = \prod_{b \in \text{bins}} \text{Poisson}(n_b|\nu_b(\mu, \vec{\theta})) \times \prod_{j \in \text{syst} + \gamma} \pi_j(\theta_j), \quad (8.5)$$

where  $\theta_j$  represents each of the  $j$  NPs associated with each uncertainty,  $\pi_j(\theta_j)$  denotes the penalty term associated with the prior knowledge for each NP, and  $\nu_b(\mu, \vec{\theta})$  represents the total expected number of events in bin  $b$ , which depends on both the parameter of interest and the nuisance parameters.

In Equation 8.5, the  $\theta_j$  NPs include those associated with each systematic uncertainty, as well as the  $\gamma$  NPs ( $j \in \text{syst} + \gamma$ ). The  $\gamma$  NPs model the total MC statistical uncertainty in each bin, and they are fully decorrelated among different bins.

For every NP, two alternative distributions of the discriminatory variable are provided for each channel. These distributions are constructed using MC samples generated with  $\pm 1\sigma$  variations of the systematic uncertainty associated with the NP. The uncertainties provided by the auxiliary measurements are assumed to follow a Gaussian distribution, hence the penalty terms assigned to them are Gaussian priors,  $\pi_j(\theta_j) = G(\theta_j)$ . The width of the Gaussian priors is set to match the value of the  $\pm 1\sigma$  variations of the associated uncertainty. Additionally, to simplify the interpretation of the NP value, this value is commonly scaled to the width of the uncertainty, making the  $\theta_j = \pm 1$  values correspond to the  $\pm 1\sigma$  variations of the uncertainty, as depicted in Figure 8.1.

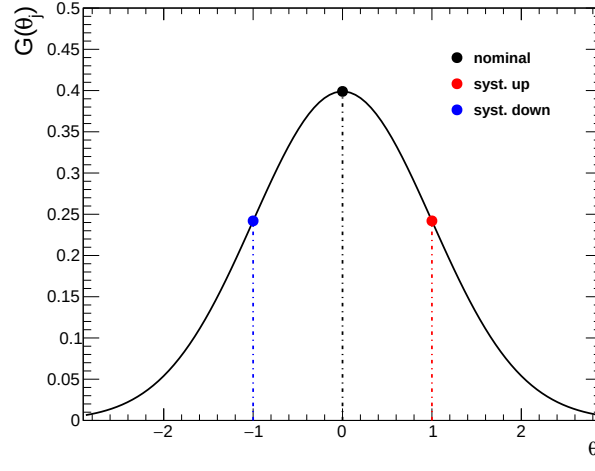


Figure 8.1: Gaussian penalty term associated with each of the  $\theta_j$  NPs that model the effects of each of the  $j$  systematic uncertainties in the statistical model.

The upper plot depicted in Figure 8.2 provides an illustrative example of the impact of a systematic up/down variation on the expected number of events in various bins of a distribution. The effect of this systematic uncertainty can be parametrized in terms of its associated  $\theta_j$  NP by a technique known as *template morphing*, the process used to interpolate the systematic variations to create a continuous parametrization of their effect. The lower plot depicted in Figure 8.2 shows the parametrization of the content of the first bin in terms of the associated  $\theta_j$  continuous NP using a linear interpolation.

However, the effect of each systematic uncertainty is typically decomposed into a pure normalization and a pure shape effect, represented by the  $\eta(\theta)$  and  $\sigma_b(\theta)$  functions, respectively. The shape effect is parametrized using a linear interpolation, as shown in Equation 8.6, while the normalization effect is parametrized using an exponential interpolation, as depicted in Equation 8.7.

$$\sigma_b(\theta) = \sigma_b^0 + I_{\text{lin},b}, \quad \text{where} \quad I_{\text{lin},b}(\theta, I_b^0, I_b^+, I_b^-) = \begin{cases} \theta(I_b^+ - I_b^0) & \theta \geq 0 \\ \theta(I_b^0 - I_b^-) & \theta < 0 \end{cases} \quad (8.6)$$

$$\eta(\theta) = I_{\text{exp}}, \quad \text{where} \quad I_{\text{exp}}(\theta, I^0, I^+, I^-) = \begin{cases} (I^+/I^0)^\theta & \theta \geq 0 \\ (I^-/I^0)^{-\theta} & \theta < 0 \end{cases} \quad (8.7)$$

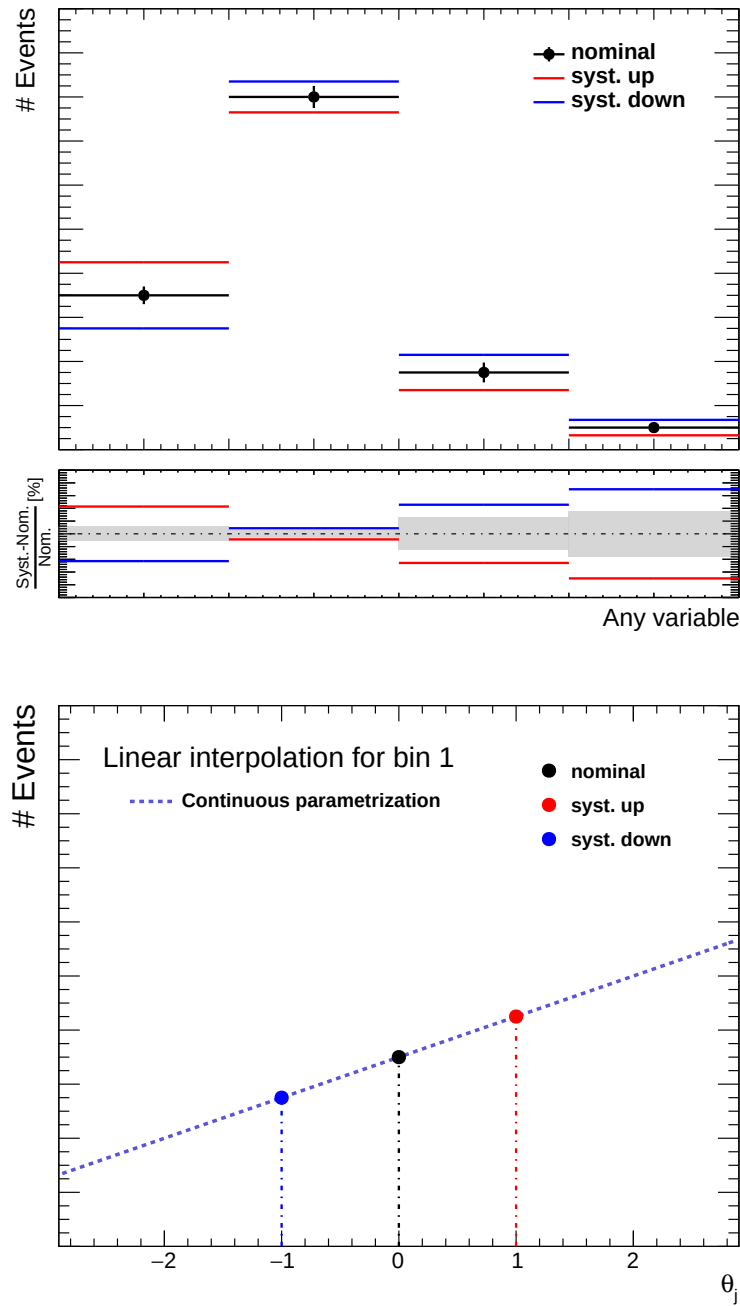


Figure 8.2: Top: Schematic example of the effect of a systematic uncertainty on a distribution. The red/blue lines depict the up/down effect of the systematic variation, while the black line represents the nominal distribution along with its uncertainty. Bottom: Linear interpolation of the systematic uncertainty effect on the first bin of the distribution. The linear interpolation enables the creation of a continuous parametrization of the systematic uncertainty effect as a function of its associated  $\theta_j$  NP.



The  $I^0$  and  $I^\pm$  parameters in these equations represent the expected event yield for the nominal prediction and the systematic up/down variations associated with the  $\theta$  NP, while  $\sigma_b^0$  represents the shape component of the nominal sample.

The choice to use an exponential interpolation for the parametrization of the normalization effect, rather than a linear interpolation, is driven by the necessity to prevent negative contributions to the normalization, which is crucial to preserve the physical interpretability of the effect.

### Minimization of $-\ln L$

The goal of the profile likelihood technique is to determine the most probable values of the POIs in the statistical model, along with their associated uncertainties and correlations. The most probable values of these POIs correspond to the values that minimize the negative logarithm of the likelihood,  $-\ln L$ .

In **HistFactory** [196], the framework used to implement the profile maximum likelihood statistical model used in this analysis, the minimization of the  $-\ln L$  is performed using the MIGRAD minimization technique in the MINUIT program [197], which is an implementation of the *Davidon–Fletcher–Powell* algorithm [198–200]. The outcomes of the MIGRAD minimization procedure are the best-fit values for the POI, the post-fit values for the NPs, and the correlation between all these parameters. The uncertainties and correlations between the POIs extracted from the fit are combined to form the covariance matrix ( $V$ ). The elements of this matrix are defined as  $V_{ij} = \rho_{ij}\sigma_i\sigma_j$ , where  $\sigma_i$  represents the uncertainty associated with each of the  $i$  POIs, and  $\rho_{ij}$  denotes the correlation between two POIs.

The uncertainties from the minimization procedure are derived from the quadratic function used by the MIGRAD technique, which results in symmetric uncertainties. However, for a more accurate estimation of the uncertainties, after finding the global minimum using MIGRAD, the MINOS technique [197] can be applied. Unlike MIGRAD, the MINOS technique does not assume a quadratic dependence of  $-\ln L$  around the minimum, resulting in non-symmetric uncertainties on both the POIs and NPs.

## 8.2 Uncertainties in the profile likelihood fit

The uncertainties affecting the correction of the  $\rho_s$  distribution from detector to parton level can be classified, according to their origin, into two groups: statistical and systematic uncertainties.

### 8.2.1 Statistical uncertainties

#### Data statistical uncertainty

The number of events measured in each bin of the histograms studied in this analysis can be treated as independent counting experiments, and therefore, they are described by a Poisson distribution. When the number of events is significantly large, the Poisson distribution can be approximated to a Gaussian distribution, and the uncertainty in the number of events can be approximated as  $\sqrt{N_{events}}$ .

In the case of the statistical model used in this analysis, which is based on the profile likelihood technique described in Section 8.1, the statistical uncertainty associated with data is described in a natural way due to the use of Poisson distributions in the construction of the likelihood in Equation 8.5.

#### MC statistical uncertainties

The MC statistical uncertainties, the uncertainties that arise from the finite statistical power of the MC samples used to describe the signal and background processes, are accounted for by adding an additional NP for each bin in the distributions considered in the analysis. These NPs are called *gammas* ( $\gamma$ ), and they combine the MC statistical uncertainties for all the signal and background processes. The effect of the MC statistical uncertainty in the content of each bin follows a Poisson distribution. Therefore, the associated penalty term is also described by a Poisson distribution.

### 8.2.2 Systematic uncertainties

The systematic uncertainties in the measurement of the top quark MC mass and the unfolded  $\rho_s$  distribution in this analysis can be classified into two categories:

experimental and modeling systematic uncertainties.

The experimental systematic uncertainties propagate the uncertainty of the calibration of the final-state objects used in the analysis to the measurements. A description of the process followed in ATLAS to reconstruct these objects is provided in Chapter 4. These objects include jets, leptons, and the missing transverse energy. Additionally, other effects such as the uncertainty in the total recorded integrated luminosity and the shape of the pile-up distribution in the collision data, are also considered.

The modeling systematic uncertainties arise from the assumptions made in the MC simulations used to predict the distributions expected in data. This category includes the uncertainties related to the normalization of the background processes due to the uncertainty in their associated cross sections, as well as the uncertainties associated with the parton shower and hadronization models, the PDF eigenvectors, variations on the initial and final state radiations, among others.

Each systematic variation studied in this analysis results in a varied detector level distribution for each of the physics processes they affect. Typically, these systematic variations consist of an up and a down variation, where the corresponding systematic is varied  $\pm 1\sigma$  around its nominal value. The systematic uncertainties for which an up and a down variation are available can be directly incorporated into the likelihood function. However, some modeling systematic uncertainties arise from the comparison between the nominal model and an alternative one, resulting in a single variation. For these single-sided variations, the difference between the varied and the reference sample is used as the up variation, and then this variation is symmetrized with respect to the nominal distribution to create the *down* variation.

For the experimental systematic uncertainties, both the normalization and shape components of the uncertainty are considered. However, for modeling uncertainties, the normalization component (Equation 8.6) is dropped and only the shape effect of the systematic is considered. This is done to prevent over-constraints in the associated NP due to the normalization component that would result in an underestimation of the shape effect of the systematic. It is important to note that dropping the normalization component does not result in an underestimation of the uncertainties, as the parameters of interest associated with the signal normalization are allowed to vary freely.

### 8.2.2.1 Experimental systematic uncertainties

#### Luminosity uncertainty

The luminosity calibration relies on multiple redundant luminosity detectors and algorithms with complementary capabilities and different systematic uncertainties. The total integrated luminosity recorded by the ATLAS experiment for the  $pp$  collisions during the full Run 2 is  $140.1 \text{ fb}^{-1}$ , with an uncertainty of 0.83% [121]. All processes for which their normalization factor is estimated from MC simulations are scaled by the measured integrated luminosity to obtain the total expected number of events. The uncertainty in the luminosity measurement is propagated as an up-and-down variation in the total number of expected events for each MC sample.

#### Pile-up reweighting uncertainty

To incorporate the effects of the additional  $pp$  collisions (pile-up) in the simulated samples, a set of minimum-bias events is superimposed onto the hard scattering events. Typically, these MC samples are produced before or during a specific data-taking period, so only the best guess of the data pile-up conditions can be put in the MC. To account for the difference in the pile-up distributions between data and MC simulations, a scale factor is applied to reweight the simulated events. The uncertainty in this factor arises from the uncertainty in the pile-up profile measured in data [122].

#### Lepton reconstruction, identification, isolation and trigger

For charged leptons, the reconstruction, identification, and trigger performances differ between data and the MC simulations. To correct these discrepancies, several scale factors are applied to the simulated events. These scale factors are estimated by means of a tag-and-probe method using events with  $Z$  and  $W$  bosons, as well as  $J/\psi$  hadrons [134, 201]. The uncertainty of the measured scale factors, which includes contributions from statistics, modeling, and systematics, is incorporated into the analysis by varying these factors in the simulation by  $\pm 1\sigma$ .

In the case of muons, the reconstruction scale factors were found to be consistent across different isolation criteria, hence no additional systematic

uncertainty was needed. However, an additional scale factor associated with the track-to-vertex-association (TTVA) efficiency is added for muons.

### Lepton momentum scale and resolution

The detector response for the lepton scale and resolution may differ between the simulated MC events and the recorded data. To correct these potential discrepancies, the MC samples are compared with the reconstructed data distributions of the  $Z \rightarrow l^+l^-$  and  $J/\psi \rightarrow l^+l^-$  mass peaks using methodologies similar to those described in Ref. [134, 202]. In the case of electrons,  $E/p$  studies based on  $W \rightarrow e\nu$  events are also used for this calibration. These studies identified small discrepancies between data and MC, leading to the introduction of correction factors for the electron and muon energy scale and resolution, together with their associated uncertainties. Moreover, an additional energy correction is applied to the electron energy scale in data to account for the *sagitta bias*, a bias in the momentum measurement of the ID caused by the misalignment of this ATLAS sub-detector due to time-dependent movements of the system [203].

### Jet vertex tagger efficiency uncertainty

The jet-vertex tagger (JVT) is a 2-dimensional likelihood constructed from tracking and vertexing information which is designed to distinguish between jets originating from the hard-scattering and jets originating from pile-up [139]. However, it has been observed that the efficiency of jets passing the JVT selection differs between the simulated events and the recorded data. To address this, a scale factor is applied to the simulated events to correct for this discrepancy. This scale factor is derived from  $Z \rightarrow \mu^+\mu^- + \text{jets}$  events and is reported with a single uncertainty that combines several effects. These effects include a 20% uncertainty in the residual contamination from pile-up jets after the pile-up suppression (estimated by using a control region), a systematic uncertainty assessed by comparing different MC generators for the  $Z + \text{jets}$  events, and the statistical uncertainty associated with the derivation of the scale factor.

## Jet energy scale

The jet energy scale (JES) calibration consists of multiple consecutive steps based on test-beam data, LHC collision data, and simulations [204]. The calibration of the JES starts with an area-based subtraction of the per-event pile-up contribution to the  $p_T$  of each jet. A residual subtraction based on the number of primary vertices ( $N_{PV}$ ) and  $\mu$  is also applied. Then, events with a vector boson ( $Z/\gamma$ ) and additional jets are used to calibrate the JES for jets in the central regions of the detector. To calibrate forward jets, dijet events with one forward and one central jet as reference are used. High- $p_T$  jets are calibrated using multi-jet events with one energetic jet and multiple low-energy jets as recoil. The outcomes of these measurements are then combined and decorrelated into a set of 26 eigenvectors that depend on the jet  $p_T$  and  $\eta$ .

Furthermore, eight additional JES NPs are added to account for the uncertainty on the flavour composition of the jets in the event, and the uncertainty on the detector response to different jet flavors. At last, an additional NP is added to account for the modeling of the *punch – through* events, events where a jet constituent passes the whole calorimeters without leaving all the energy in them.

## Jet energy resolution

The jet energy resolution (JER) is determined using both data and simulated events. In data, the JER is measured by comparing the distribution of the transverse momentum balance in events with a jet and a reference object, such as a photon or a leptonically decaying  $Z$  boson ( $Z \rightarrow l^+l^-$ ), between data and in the MC simulations [204]. In MC, the JER is determined using the particle and the truth information stored in simulated dijet events. This determination involves matching the reconstructed jets to their associated particle level jets to then calculate the difference of their jet energy distributions and fill it into histograms. The histograms are then fitted with a Gaussian function, and the width of the Gaussian distribution ( $\sigma$ ) is identified as the JER in the simulation. The JER in simulated events is smeared to match the JER measured in the data, with the smearing factor depending on the jet  $p_T$  and  $\eta$ . The uncertainties originated from JER determination are propagated through the analysis by scaling the MC smearing factors to the simulated jets. After combining and decorrelating the JER uncertainties, a total of 13 NPs are used.

### Flavour tagging

The efficiency of the DL1r  $b$ -tagging algorithm (Section 4.5), as well as the mistagging efficiencies associated with  $c$ - and light- jets, need to be calibrated in order to align the performance in the MC simulations with that in data. To achieve this, flavor-dependent corrective scale factors are derived from data and then applied to the simulations. For  $b$ -tagged jets, the correction factors and their uncertainties are estimated using dileptonic  $t\bar{t}$  events [141, 205], while for  $c$ -jets, they are derived from jets originated from  $W$  boson hadronic decays in  $t\bar{t}$  events [206]. In the case of light-flavor jets, the correction factors are derived from di-jet and  $Z$ +jets events [207, 208]. The scale factors derived from these methods depend on the jet  $p_T$  and  $\eta$ , and their associated uncertainties are a combination of statistical, experimental, and modeling uncertainties that arise during the calibration procedures. Two additional uncertainties are added to account for the extrapolation of  $b$ -tagging efficiency and the  $c$ -jet mistag rate from the phase space region used to determine the correction factors to regions with higher  $p_T$ . After combining and decorrelating some of the uncertainties, their effect can be modeled by a total of 9 NPs for the  $b$ -tagging efficiencies, 5 NPs for the  $c$ -mistag rate, and 5 NPs for the light-flavor mistag rate.

### $E_T^{\text{miss}}$ scale and resolution

The missing transverse energy ( $E_T^{\text{miss}}$ ) is calculated from the vector sum of the  $p_T$  of all reconstructed objects (hard objects) and the additional soft term, which is reconstructed from all the tracks that are not associated to any of the calibrated objects (see Section 4.6). The uncertainties affecting each reconstructed object are propagated to the calculated value of  $E_T^{\text{miss}}$ , hence their effects are already been taken into account. However, the uncertainties in the soft-track component (soft term) have not been considered so far. The uncertainties associated with this term are derived from the agreement between data and MC of the  $p_T$  balance between the hard and the soft term ( $p_T^{\text{hard}} = -p_T^{\text{soft}}$ ) in events with  $Z \rightarrow \mu^+\mu^-$  [143]. The different uncertainty sources derived from this study are combined into a total of three variations: The first variation accounts for an offset along the  $p_T^{\text{hard}}$  axis, and it includes both an up and down variation. The other two variations consider a smearing in the  $E_T^{\text{miss}}$  resolution, one parallel and the other perpendicular to the  $p_T^{\text{hard}}$  axis. These two resolution variations are one-sided.

Table 8.1: Summary of the experimental systematic uncertainties considered in the analysis, together with a brief description of their origins. This table continues in Table 8.2

| Reconstructed object                                                                    |                                                                                                                                 |
|-----------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------|
| Systematic uncertainty name                                                             | Uncertainty origin                                                                                                              |
| <b>Electrons</b>                                                                        |                                                                                                                                 |
| Electron trigger                                                                        | Trigger efficiency calibration for electrons                                                                                    |
| Electron reco.                                                                          | Reconstruction efficiency calibration for electrons                                                                             |
| Electron ID                                                                             | Identification efficiency calibration for electrons                                                                             |
| Electron isol.                                                                          | Isolation efficiency calibration for electrons                                                                                  |
| Electron energy scale<br>Electron energy scale AF2                                      | Energy scale calibration for electrons                                                                                          |
| Electron energy res.                                                                    | Energy resolution calibration for electrons                                                                                     |
| <b>Muons</b>                                                                            |                                                                                                                                 |
| Muon trigger stat.<br>Muon trigger syst.                                                | Trigger efficiency calibration for muons                                                                                        |
| Muon ID stat.<br>Muon ID syst.                                                          | Identification eff. calibration for muons for muons with $p_T > 15$ GeV                                                         |
| Muon ID stat. low $p_T$<br>Muon ID syst. low $p_T$                                      | Identification eff. calibration for muons for muons with $p_T < 15$ GeV                                                         |
| Muon isol. stat.<br>Muon isol. syst.                                                    | Isolation efficiency calibration for muons                                                                                      |
| Muon TTVA stat.<br>Muon TTVA syst.                                                      | Track to vertex association efficiency calibration for muons                                                                    |
| Muon scale                                                                              | Momentum scale calibration for muons                                                                                            |
| Muon sagitta data stat.<br>Muon sagitta res. bias                                       | Momentum resolution correction due to the <i>sagitta bias</i> for muons. It covers charge-dependent local misalignment effects. |
| Muon CB                                                                                 | Direct variations in the track resolution of Combined muons                                                                     |
| <b>Missing transverse energy</b>                                                        |                                                                                                                                 |
| $E_T^{\text{miss}}$ soft term Scale                                                     | Momentum scale calibration of the soft term in the MET calculation                                                              |
| $E_T^{\text{miss}}$ soft term res. perp.<br>$E_T^{\text{miss}}$ soft term res. parallel | Momentum resolution correction of the soft term in the MET calculation                                                          |
| <b>Pile-up reweighting</b>                                                              |                                                                                                                                 |
| Pile-up                                                                                 | Pile-up reweighting to match data $\mu$ profile                                                                                 |
| <b>Luminosity</b>                                                                       |                                                                                                                                 |
| Luminosity                                                                              | Measurement of the total integrated luminosity (2015-2018) in ATLAS                                                             |



Table 8.2: Summary of the experimental systematic uncertainties considered in the analysis, together with a brief description of their origins. This table is a continuation of Table 8.1.

| <b>Reconstructed object</b>                                                                                                                                                                                                           |                                                                                                                                     |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------|
| Systematic uncertainty name                                                                                                                                                                                                           | Uncertainty origin                                                                                                                  |
| <b>Jets</b>                                                                                                                                                                                                                           |                                                                                                                                     |
| JVT                                                                                                                                                                                                                                   | Jet vertex tagger (JVT) calibration                                                                                                 |
| Jet pile-up $p_T$<br>Jet pile-up $\rho$<br>Jet pile-up offset $\mu$<br>Jet pile-up offset NPV                                                                                                                                         | Area-based subtraction of the per-event pile-up contribution to the jet $p_T$                                                       |
| Jet detector {1-2}<br>Jet mixed {1-3}<br>Jet modelling {1-4}<br>Jet statistical {1-6}                                                                                                                                                 | Calibration of the JES in jets in the central region of the detector                                                                |
| Jet $\eta$ intercalib. modelling<br>Jet $\eta$ intercalib. NC. 2018 data<br>Jet $\eta$ intercalib. NC. highE<br>Jet $\eta$ intercalib. NC. neg $\eta$<br>Jet $\eta$ intercalib. NC. pos $\eta$<br>Jet $\eta$ intercalib. total stat.  | Calibration of the JES in jets in the forward region of the detector                                                                |
| Jet single particle high $p_T$                                                                                                                                                                                                        | Calibration of the JES in high- $p_T$ jets                                                                                          |
| Jet flavor composition prop<br>Jet flavor response prop<br>Jet flavor gen. shower<br>Jet flavor gen. shower HF<br>Jet flavor hadro.<br>Jet flavor gen. shower HF<br>Jet flavor hadro. HF<br>Jet flavor shower<br>Jet flavor shower HF | JES uncertainty associated with the jet flavor composition in the event and the detector response to jets of different flavor       |
| Jet punchthrough MC16                                                                                                                                                                                                                 | Modeling of the punch-through events                                                                                                |
| Jet JER {1-12}<br>Jet JER DataVsMC MC16                                                                                                                                                                                               | Calibration of the JER                                                                                                              |
| <b>Flavour tagging</b>                                                                                                                                                                                                                |                                                                                                                                     |
| b-tag eigenvector B{0-8}                                                                                                                                                                                                              | $b$ -jet tagging efficiency calibration                                                                                             |
| b-tag eigenvector C{0-4}                                                                                                                                                                                                              | $c$ -jet miss-tagging efficiency calibration                                                                                        |
| b-tag eigenvector Light{0-4}                                                                                                                                                                                                          | Light-jet miss-tagging efficiency calibration                                                                                       |
| b-tag extrapolation<br>b-tag extrapolation charm                                                                                                                                                                                      | Extrapolation of the $b$ -jet tagging efficiency calibration and the $c$ -jet mistagging efficiency calibration to high- $p_T$ jets |

### 8.2.2.2 Modeling systematic uncertainties

#### Background normalization

The normalization uncertainties for the various background processes considered in the analysis are assumed to be proportional to the uncertainty in their measured cross section. To simplify the fit complexity, only the main background contributions are considered individually, whereas the less relevant ones are grouped. For the single top samples, a 5.3% uncertainty is considered based on the NNLO cross section uncertainty [187]. The  $W$ +jets and  $Z$ +jets contributions are combined into a single  $V$ +jets sample, and a conservative 50% uncertainty on its normalization is considered. All remaining backgrounds, which include  $t\bar{t}W$ ,  $t\bar{t}Z$ ,  $t\bar{t}H$ , diboson, and other rare  $t\bar{t}X$  process, as well as the fake lepton background, are combined into a single contribution, and a conservative 50% uncertainty on its normalization is considered.

#### Parton shower, hadronization, and fragmentation modeling for $t\bar{t}$

To evaluate the impact of the uncertainty arising from the chosen parton shower, hadronization, and fragmentation models, the nominal  $t\bar{t}$  sample produced with POWHEG and interfaced with PYTHIA 8 for the simulation of the PS is compared with an alternative sample produced with the same POWHEG configuration but interfaced with the HERWIG 7 PS model.

A further description of these samples can be found in Section 6.2. The two parton shower modeling programs choose different approaches in the shower modeling. The difference between the two samples is symmetrized and enters the likelihood fit as a NP with only a shape component (the normalization component is dropped).

#### Initial/final state QCD radiation (ISR/FSR)

To estimate the uncertainty associated with the ISR/FSR modeling, five different contributions are considered independently. These contributions originate from variations in several POWHEG and PYTHIA parameters. In particular, the POWHEG parameters varied are the renormalization scale ( $\mu_R$ ), the factorization scale ( $\mu_F$ ), VAR3C, and  $h_{damp}$ . Conversely, the renormalization scale ( $\mu_R$ ) in

PYTHIA is also varied to estimate the uncertainty in the FSR in the parton shower.

For the evaluation of the  $\mu_R$ ,  $\mu_F$ , and VAR3C variations in POWHEG and the  $\mu_R$  variations in PYTHIA, alternative weights are stored within the nominal POWHEG +PYTHIA 8 sample. The  $\mu_R$  and  $\mu_F$  scales are varied by a factor of 2, up and down, from their nominal values. The VAR3C parameter represents a variation of  $\alpha_S$  coupling in the ISR, and it is varied up and down within its uncertainty. The  $\mu_R$  variation in PYTHIA corresponds to a variation of this parameter in the FSR, and it is varied by a factor 2, up and down, from its nominal value. The differences between each pair of up and down variations enter the statistical model as independent NPs.

The  $h_{damp}$  parameter controls the strength of the first radiative emission in POWHEG. To evaluate the uncertainty associated with this parameter, a dedicated POWHEG +PYTHIA 8 sample with  $h_{damp} = 517.5$  GeV (three times the top quark mass in the generator) is used. The difference between this sample and the nominal one is symmetrized and incorporated into the statistical model as a single NP.

### Parton distribution functions modeling (PDFs)

The PDFs are measured by performing a global fit to short-distance scattering data. Therefore, they have experimental uncertainties which are reflected as variations of the individual eigenvectors of the PDF. The nominal  $t\bar{t}$  sample uses the PDF4LHC15 PDF set [209], which has a total of 30 eigenvectors. The effects of the PDF eigenvectors variations are propagated through the analysis using alternative MC generator weights stored within the nominal POWHEG +PYTHIA 8 sample. The value of the strong coupling constant,  $\alpha_S$ , is also varied within its uncertainty in the PDF set. Each individual PDF variation enters the statistical model as an independent NP, where the difference between each variation and the nominal sample is symmetrized, and only the shape component is considered.

### Matrix Element matching uncertainty for $t\bar{t}$

The  $t\bar{t}$  Matrix Element calculated at NLO in QCD using POWHEG has to be matched to the PYTHIA parton shower using a matching scheme. The parameter that controls the matching scheme in PYTHIA is the  $p_T^{\text{hard}}$  matching parameter. This parameter regulates the hardness criterion that vetoes the emissions of additional radiation on the showering, with the goal to avoid an overlap/hole in

the phase space covered by the POWHEG ME and the PYTHIA PS. To estimate the uncertainty associated with the choice of this matching scheme, the  $p_T^{\text{hard}}$  matching parameter is varied from the nominal value of 0 to 1, as recommended in [210]. The difference between these two predictions is symmetrized and introduced as a NP in the statistical model.

### Top quark $p_T$ NNLO reweighting

The kinematic properties of top quarks in  $t\bar{t}$  NLO+PS event generators are known to be mismodeled due to the impact of missing higher orders in the calculation. In particular, the event yield for top quarks produced with high  $p_T$  is overestimated. This leads to skewed distributions for the kinematic properties of some detector level objects, such as the jet  $p_T$ , lepton  $p_T$ , and  $H_T$ , which are also overestimated in the high energy regime. Moreover, this effect is also known to affect other kinematic variables, such as  $M_{t\bar{t}}$ .

The effect of this mismodeling can be mitigated by reweighting the desired parton level distributions to match the distributions predicted by higher-order calculations. However, applying such reweighting only to certain variables results in a loss of precision in the description of other kinematical variables due to cross-correlations, so it is not typically used. Instead, the comparison between the nominal NLO+PS sample and the reweighted sample is considered as an uncertainty. In the current analysis, the reweighting is applied to the parton level top quark  $p_T$  and  $M_{t\bar{t}}$  differential distributions using an *iterative recursive* algorithm to the NNLO-QCD+NLO-EW Fix Order theory predictions from [211].

### Underlying Event

The Underlying Event (UE) is defined as those aspects of a hadronic interaction that are not coming from the primary hard scattering, but rather to the accompanying interactions of the rest of the proton [212]. It is impossible to separate the UE from the hard scattering process on an event-by-event basis. To evaluate the modeling dependence on the UE, the nominal sample is compared with two samples that use the same algorithms for the ME and PS (POWHEG + PYTHIA 8) as the nominal sample, but where the corresponding A14 tune parameters of PYTHIA are varied within their uncertainties (A14up and A14down).

It is important to mention that including this uncertainty on its own is a very conservative approach and involves partial double-counting. During the evaluation of the parton shower, fragmentation, and hadronization modeling uncertainties, two different PS programs are compared (PYTHIA 8 vs. HERWIG 7). As these two programs use different models and tunes for the UE, the difference between them also includes uncertainties originating from the modeling of the UE.

### **Color Reconnection model (CR)**

During the hadronization process, colorless hadrons are formed from colored quark particles. How the sum over colored particles is handled in the hadronization program can affect how events are reconstructed at particle and detector levels. The color reconnection (CR) and the multiple parton interactions (MPI) are modeled in the PYTHIA 8 event generator. Several of these models have been studied within ATLAS [182]. These tunes are denoted as CR0, CR1 and CR2. The CR0 denotes a tune that uses an MPI based model to calculate the probability for different colored partons to reconnect. The CR1 denotes a tune that uses a QCD-based model. In comparison with CR0, the main difference is that it makes a more complete treatment of the QCD multiplet structure that ends up enhancing the production of baryons. The CR2 denotes a tune that uses a gluon-move model. The main difference with CR0 is that, in this model, only gluons are considered for reconnection. CR0 is very similar to the nominal A14 tune. It is only a retuning of the nominal models to be used for comparisons with CR1 and CR2. To calculate the color reconnection uncertainty, the CR2 and the CR1 samples are compared with the CR0 sample. The largest difference compared to CR0 is taken as the final uncertainty.

### **Recoil to Top**

In the decays of colored resonances, such as  $t \rightarrow Wb$ , the radiation patterns are typically described exclusively in terms of the emissions originating from the decay products. This description means that the radiation patterns from the decaying resonance itself are neglected in the parton shower. However, certain MC generators, such as the interface between POWHEG and PYTHIA, incorporate matrix-element corrections that can correct the first emission to the full result, though they are not generally applied to all emissions.

In the case of PYTHIA 8, after the emission of the first gluon, any additional gluon radiation recoils against the  $b$  quark, which significantly affects the modeling of the parton shower, as it determines how the momentum is redistributed between the  $W$  boson and the  $b$  quark. This recoil scheme is called *recoil-to-colored*. However, an alternative recoil scheme called *recoil-to-top* can be set in PYTHIA. This scheme enables the top quark itself to act as the recoiler for the gluon radiation, resulting in more out-of-cone radiation (wider-angle gluon radiation), with energy depositions that do not get reclustered in the  $b$ -jet. As a consequence, the  $b$  quark fragmentation is modified, generating a harder  $b$ -hadron momenta and modifying the  $b$ -jet shape.

The uncertainty associated with the choice of the gluon recoil scheme is estimated by comparing the nominal sample, which uses the recoil-to-coloured scheme, with an alternative sample which uses the recoil-to-top scheme. This comparison probably overestimates the real effect of this uncertainty, as no dedicated tune exists for the recoil-to-top scheme.

### Single top $tW$ and $t\bar{t}$ overlap modeling

At NLO in QCD, there are overlaps between the  $tW$  production and the  $t\bar{t}$  process. In the nominal single top  $tW$  sample, the diagram removal (DR) technique [164] is used to remove the overlap between the two processes. This is not the only possible technique that exists to remove the interference between the two processes. To estimate the uncertainty arising from the chosen technique to handle the interference, an alternative sample generated using the diagram subtraction (DS) scheme [164] is compared with the nominal sample. In the DR approach, all the NLO diagrams that overlap with the  $t\bar{t}$  contributions are removed from the calculation of the  $tW$  amplitude. This technique accounts for the interference term, but it is not gauge invariant. In the DS scheme, a subtraction term is built into the  $tW$  amplitude to cancel out the  $t\bar{t}$  component close to the top quark resonance while respecting gauge invariance. The symmetrized difference between these two samples is considered as the overlap modeling uncertainty.

### Matrix element matching uncertainty for single top

To estimate the matrix element matching uncertainty for single top processes, alternative samples for the three single top processes are generated using

MADGRAPH5\_aMC@NLO interfaced with PYTHIA 8. The difference between these samples and the nominal single top samples produced with POWHEG and interfaced with PYTHIA 8 is symmetrized and considered as the matrix element matching uncertainty for single top processes.

### **Parton shower, hadronization, and fragmentation modeling for single top**

Similar to the estimation of the matrix element matching uncertainty for  $t\bar{t}$  events, several dedicated MC samples with POWHEG interfaced with HERWIG 7 are generated to simulate the three single top channels. The difference between these samples and the nominal single top samples produced with POWHEG and interfaced with PYTHIA 8 is symmetrized and considered as the PS uncertainty for the single top processes.

### **Initial/final state QCD radiation (ISR/FSR) for single top processes**

Similar to the ISR/FSR for  $t\bar{t}$  events, the ISR/FSR uncertainties for single top processes are estimated considering four different contributions independently. These contributions originate from variations in several POWHEG and PYTHIA parameters. In particular, the POWHEG parameters varied are the renormalization scale ( $\mu_R$ ), the factorization scale ( $\mu_F$ ), and VAR3C. Conversely, the renormalization scale ( $\mu_R$ ) in PYTHIA is also varied to estimate the uncertainty in the FSR in the parton shower.

For the evaluation of the  $\mu_R$ ,  $\mu_F$ , and VAR3C variations in POWHEG and the  $\mu_R$  variations in PYTHIA, alternative weights are stored within the nominal POWHEG + PYTHIA 8 sample. The  $\mu_R$  and  $\mu_F$  scales are varied by a factor of 2, up and down, from their nominal values. The VAR3C parameter represents a variation of  $\alpha_S$  coupling in the ISR, and it is varied up and down within its uncertainty. The  $\mu_R$  variation in PYTHIA corresponds to a variation of this parameter in the FSR, and it is varied by a factor 2, up and down, from its nominal value. The differences between each pair of up and down variations enter the statistical model as independent NPs.

## V+jets scale variations

For the  $V$ +jets processes, the uncertainties associated with the renormalization scale  $\mu_R$  and factorization scale  $\mu_F$  are estimated through an independent up/down variation of these scales by a factor two in SHERPA. The reweighting of the nominal  $W$ +jets and  $Z$ +jets samples is used to obtain the alternative distributions.

Table 8.3: Summary of the modeling systematic uncertainties considered in the analysis, together with a brief description of their origins.

| Reconstructed object                     |                                                                                         |
|------------------------------------------|-----------------------------------------------------------------------------------------|
| Systematic uncertainty name              | Uncertainty origin                                                                      |
| <b>MC background normalization</b>       |                                                                                         |
| Single top cross section                 | Normalization uncertainty of the single top samples, 5.3%                               |
| $V$ +jets cross section                  | Normalization uncertainty of the $V$ +jets sample, 50%                                  |
| Others cross section                     | Normalization of the remaining backgrounds, 50%                                         |
| <b><math>t\bar{t}</math> modeling</b>    |                                                                                         |
| $t\bar{t}$ Parton Shower                 | Parton shower, hadronization, and fragmentation (PYTHIA 8 vs. HERWIG 7.2.1).            |
| $t\bar{t}$ $\mu_R$ scale                 | Initial state QCD radiation. $\mu_R$ variations in POWHEG.                              |
| $t\bar{t}$ $\mu_F$ scale                 | Initial state QCD radiation. $\mu_F$ variations in POWHEG.                              |
| $t\bar{t}$ Var3c                         | Initial state QCD radiation. Var3c variations in PYTHIA.                                |
| $t\bar{t}$ matching: $h_{\text{damp}}$   | Initial state QCD radiation. $h_{\text{damp}} = m_t$ vs. $h_{\text{damp}} = 3m_t$       |
| $t\bar{t}$ FSR                           | Final state QCD radiation. $\alpha_S$ variations in PYTHIA.                             |
| PDF4LHC{01-30}                           | Parton distribution function. PDF4LHC15 variations.                                     |
| $t\bar{t}$ matching: $p_T^{\text{hard}}$ | Matrix Element matching, $p_T^{\text{hard}} = 0$ vs. $p_T^{\text{hard}} = 1$ in PYTHIA. |
| $t\bar{t}$ NNLO reweighting              | Reweighting of $p_T^t$ and $m_{t\bar{t}}$ to NNLO.                                      |
| $t\bar{t}$ Underlying Event              | Underlying event. A14 tune variations of PYTHIA.                                        |
| $t\bar{t}$ Color Reconnection            | Color reconnection model. CR2 vs. CR0                                                   |
| $t\bar{t}$ PS recoil model               | Recoil-to-colour vs. Recoil-to-top in PYTHIA.                                           |
| <b>Single top modeling</b>               |                                                                                         |
| Single top Diagram Sub.                  | Single top $tW$ and $t\bar{t}$ overlap modeling. DR vs. DS                              |
| Single top matching                      | Matrix element matching. POWHEG vs. aMC@NLO                                             |
| Single top Parton Shower                 | Parton shower hadronisation and fragmentation. PYTHIA 8 vs. HERWIG 7.1.3                |
| Single top $\mu_R$ scale                 | Initial state QCD radiation. $\mu_R$ variations in POWHEG.                              |
| Single top $\mu_F$ scale                 | Initial state QCD radiation. $\mu_F$ variations in POWHEG.                              |
| Single top Var3c                         | Initial state QCD radiation. Var3c variations in PYTHIA.                                |
| Single top FSR                           | Final state QCD radiation. $\alpha_S$ variations in PYTHIA                              |
| <b><math>V</math>+jets variations</b>    |                                                                                         |
| $V$ +jets $\mu_R$ scale                  | Initial state QCD radiation. $\mu_R$ variations in SHERPA.                              |
| $V$ +jets $\mu_F$ scale                  | Initial state QCD radiation. $\mu_F$ variations in SHERPA.                              |



### 8.3 Definition of the statistical model

The statistical model used in this analysis to extract the top quark mass parameter in the Monte Carlo ( $m_t^{\text{MC}}$ ) and the normalized  $t\bar{t}$  +jet differential cross section with respect to  $\rho_s$  at parton level is based on the profile likelihood techniques described in Section 8.1. A total of four different binned distributions are used to construct the model, which corresponds to the four orthogonal categories summarized in Table 7.7 after applying the requirements described in the final event selection (Section 7.4). The four regions defined in this analysis are divided into two Signal Regions (SR), where the  $\rho_s$  observable is calculated, and two Control Regions (CR), where the  $M_{lb}$  observable is calculated. As described in Chapter 7, the  $\rho_s$  observable is chosen for its sensitivity to the top quark pole mass, and its associated differential distribution is unfolded to parton level to measure the top quark pole mass. The  $M_{lb}$  variable is chosen because it is sensitive to the top quark mass parameter in the Monte Carlo ( $m_t^{\text{MC}}$ ), allowing for a precise determination of this parameter at detector level.

#### Expected number of events in the signal and control regions

The general structure of the likelihood function implemented in the statistical model used to measure  $m_t^{\text{MC}}$  and the  $t\bar{t}$  +jet differential cross section at parton level is the same as the one defined in Equation 8.5. However, in this case, the expected number of events in the signal and control regions is expressed as:

$$\nu_i^{\text{SR}}(\vec{\mu}_{t\bar{t}+\text{jet}}, m_t^{\text{MC}}, \vec{w}, \vec{\theta}) = \sum_{k=1}^{n_{\text{bin}}^{\rho_s}} S_i^k(\mu_{t\bar{t}+\text{jet}}^k, m_t^{\text{MC}}, \vec{\theta}) + \sum_j B_i^j(w_j, \vec{\theta}), \quad (8.8)$$

$$\nu_i^{\text{CR}}(\mu_{t\bar{t}}^{\text{CR}}, m_t^{\text{MC}}, \vec{w}, \vec{\theta}) = s_i(\mu_{t\bar{t}}^{\text{CR}}, m_t^{\text{MC}}, \vec{\theta}) + \sum_j b_i^j(w_j, \vec{\theta}). \quad (8.9)$$

In Equation 8.8,  $S_i^k$  represents the expected number of signal events in bin  $i$  of a SR that originate from bin  $k$  of the  $\rho_s$  parton level distribution.  $B_i^j$  represents the expected number of background events in the bin  $i$  of a SR from the  $j$  process.  $\mu_{t\bar{t}+\text{jet}}^k$  is the POI normalization factor associated with the bin  $k$  of the  $\rho_s$   $t\bar{t}$  +jet parton level distribution. Finally,  $w_j$  is the background normalization NP associated with process  $j$ , and  $\vec{\theta}$  is the vector of NPs describing all other systematic uncertainties considered in the analysis.

In Equation 8.9,  $s_i$  represents the expected number of signal events in bin  $i$  of a CR that originate from the entire  $t\bar{t}$  process, which contains all  $t\bar{t}$  events produced in association with any number of jets, including zero jets. The normalization factor associated with this process is  $\mu_{t\bar{t}}^{\text{CR}}$ . The 'CR' superscript denotes that this POI is considered decorrelated from the  $\mu_{t\bar{t}+\text{jet}}^k$  POIs. Decorrelating these parameters follows a conservative approach in which the measurement of the cross section in the CRs does not affect the measurement of the normalization factors in the SRs. In this manner, the only common parameters between the signal and control regions are the top quark MC mass parameter,  $m_t^{\text{MC}}$ , and the NPs associated with the experimental systematic uncertainties, while the POIs and the NPs associated with the  $t\bar{t}$  modeling systematic uncertainties are decorrelated between signal and control regions. At last,  $b_i^j$  is the expected number of background events in the CR bin  $i$  from the  $j$  process.

### Direct extraction of $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$ via a redefinition of the POIs

The goal of the measurement of the  $\mu_{t\bar{t}+\text{jet}}^k$  normalization factors is the extraction of the  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  distribution at parton level, which is the normalized version of the distribution constructed from the  $\mu_{t\bar{t}+\text{jet}}^k$  parameters. However, instead of extracting the  $\mu_{t\bar{t}+\text{jet}}^k$  parameters and then normalizing the distribution, an alternative approach is to extract the normalized distribution from the maximum likelihood fit directly. This is accomplished by expressing the  $\mu_{t\bar{t}+\text{jet}}^k$  parameters in terms of the relative normalization factors.

In this alternative approach, a new normalization factor for the total cross section of the combined folded distributions, denoted as  $\mu_{t\bar{t}+\text{jet}}^{\text{tot}}$ , is introduced. Subsequently, the  $\mu_{t\bar{t}+\text{jet}}^k$  normalization factors are replaced by  $\mu_{t\bar{t}+\text{jet}}^k = \mu_{t\bar{t}+\text{jet}}^{\text{rel},k} \cdot \mu_{t\bar{t}+\text{jet}}^{\text{tot}}$ , where  $\mu_{t\bar{t}+\text{jet}}^{\text{rel},k}$  are the relative normalization factors for each parton level bin. Finally, as the  $\mu_{t\bar{t}+\text{jet}}^{\text{rel},k}$  factors are not independent of each other, one of the relative factors is substituted by:

$$\mu_{t\bar{t}+\text{jet}}^{\text{rel},j} = (1 - \sum_{i,i \neq j}^{n_{\text{bin}}} \mu_{t\bar{t}+\text{jet}}^{\text{rel},i} (N_i/N)) / (N_j/N), \quad (8.10)$$

where  $N_i$  is the number of events in each parton level bin, and  $N$  is the total number of events at parton level. In this analysis, the choice is to substitute the

first bin of the distribution ( $j = 1$ ). However, this choice is arbitrary and does not affect the final outcome of the measurement.

### Folding of the parton level $\rho_s$ distribution

The  $S_i^k$  functions in Equation 8.8 describe the relation between the content in each parton level bin and its contribution to the various distributions in the SRs considered in the analysis. Using this relation, the problem of obtaining the parton level distribution associated with a detector level distribution, the unfolding problem, can be transformed into a typical problem of fitting the normalization of multiple distributions, for which the profile likelihood techniques are suitable. This adaptation of the profile likelihood technique for solving the unfolding problem is known as *Profile Likelihood Unfolding* (PLU).

The distributions associated with the  $S_i^k$  functions are computed by *folding* the parton level  $\rho_s$  distribution to detector level. The folding procedure consists of performing a matrix multiplication between the truth level distribution and the *response matrix*, which results in a reco level distribution associated with each truth level bin. The response matrix represents the combination of the selection efficiency, migration matrix, and acceptance following the equation:

$$R_{ij} = f_j^{\text{eff.}} \cdot M_{ij} \cdot 1/f_i^{\text{acc.}} , \quad (8.11)$$

where the indices  $i$  and  $j$  represent each of the truth and reco level bins, respectively. The formal definition of each of these variables is as follows:

- The **efficiency factor**,  $f_j^{\text{eff.}}$ , is defined as the truth level events that fulfill the reco level selection and the truth level selection, divided by all the events that pass the truth level requirements only, bin by bin.
- The **migration matrix**,  $M_{ij}$ , contains the events that fulfill both the truth and reco level requirements. It describes the migration of the events produced in each truth level bin to the different reco level bins. The migration matrix is normalized to the number of entries in each truth level bin, row by row.
- The **acceptance factor**,  $f_i^{\text{acc.}}$ , is defined as the truth level events that fulfill

the reco level selection and the truth level selection, divided by all the events that pass the reco level requirements only, bin by bin.

Based on the definition of the  $f_j^{\text{eff.}}$ ,  $f_i^{\text{acc.}}$ , and  $M_{ij}$ , each factor and matrix element must be  $\leq 1$ .

In the case of the nominal  $t\bar{t}$  POWHEG +PYTHIA 8 sample, the resulting efficiency factor, migration matrix, and acceptance factor for the SRljets5j2b signal region are depicted in Figure 8.3. These quantities have been obtained using the final  $\rho_s$  binning used in the analysis. The corresponding plots for the SRljets5j1b can be found in Appendix F.1.

The resulting folded distributions associated with each bin of the  $\rho_s$  parton level distribution are depicted in Figure 8.4. This figure includes the parton level distribution, with each bin colored in a distinct color, and the resulting folded distributions at detector level. With this approach, the unfolding problem is transformed into a problem of fitting the normalization factor of each of the folded distributions at detector level.

Each of the systematic uncertainties described in Section 8.2.2 have an associated modified response matrix. To evaluate the impact of these uncertainties on the folded  $t\bar{t}$  +jet distributions, the folding procedure is repeated by applying the modified response matrix on the original parton level distribution. This approach ensures that the efficiency, migration, and acceptance effects of the corresponding systematic uncertainty are properly considered, while removing any additional impact from the differences between the various parton level distributions. The theory uncertainties associated with the computation of the parton level distribution itself are evaluated in Section 9.2.

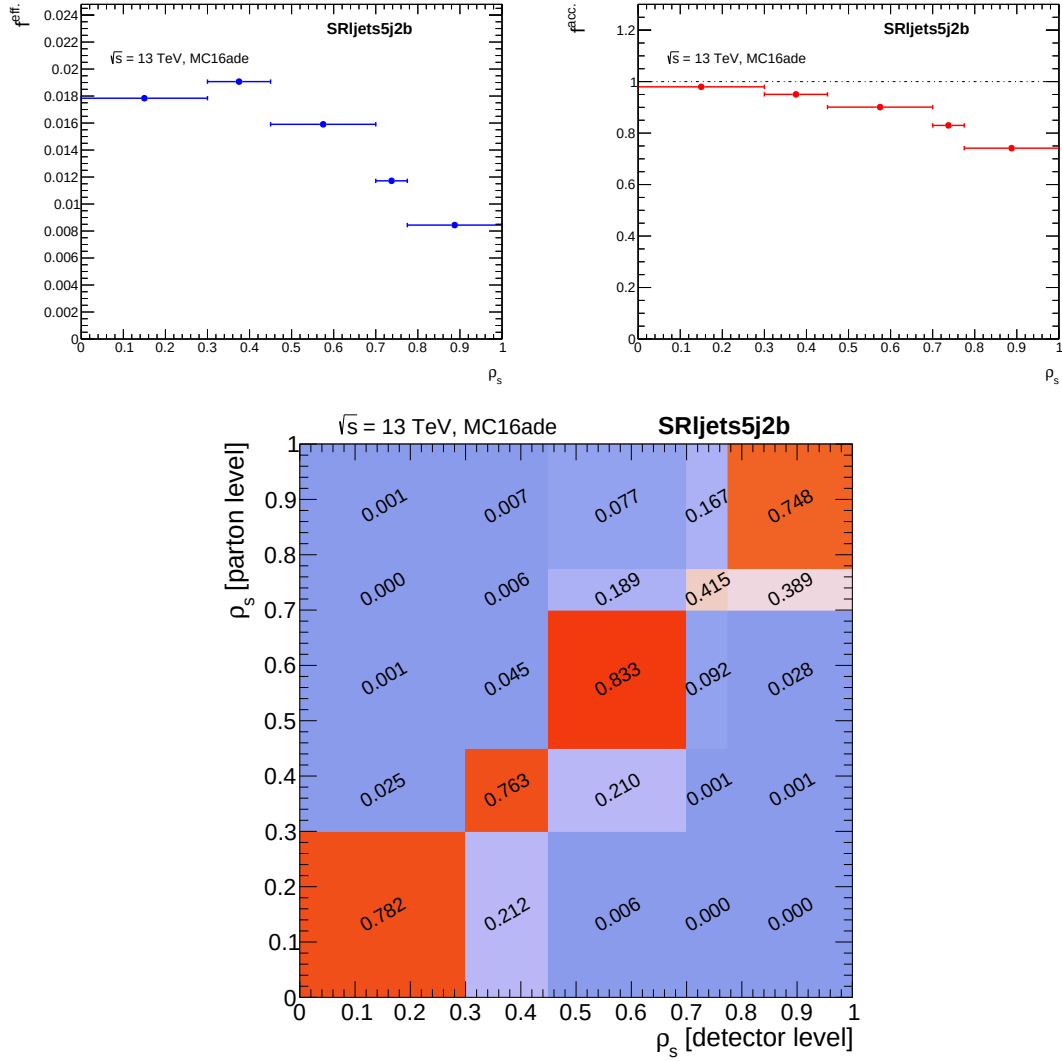


Figure 8.3: Efficiency factor (top-left), acceptance factor (top-right), and migration matrix (bottom) used for the folding of the nominal  $t\bar{t}$  sample from parton to detector level. These factors and migration matrix are shown for the SRIjets5j2b signal region.

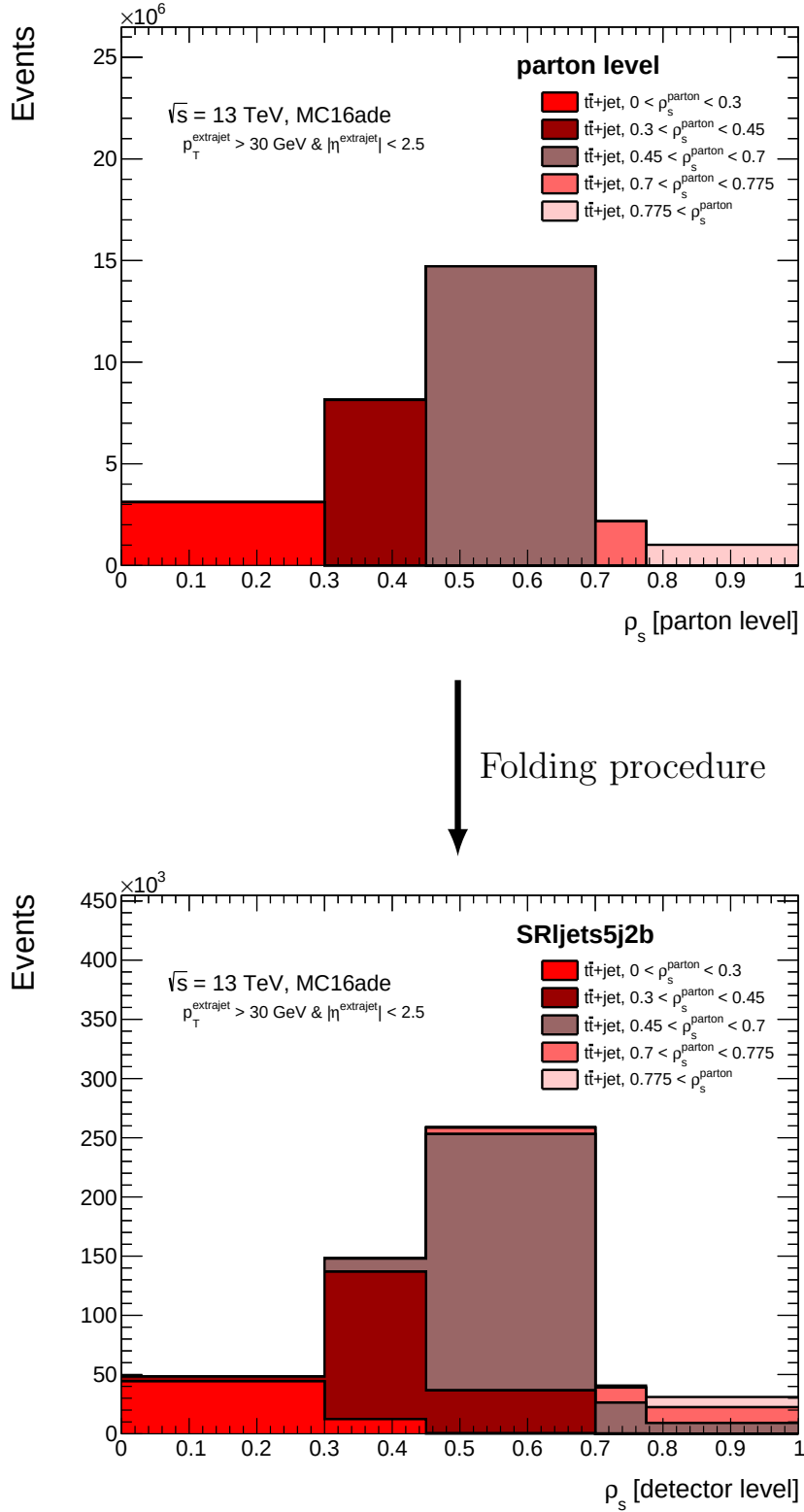


Figure 8.4: Top:  $\rho_s$  parton level distribution for the nominal  $t\bar{t}$  MC sample used in the analysis. Bottom:  $\rho_s$  detector level distribution for the SRIjets5j2b signal region obtained by folding the parton level distribution with the corresponding response matrix. Each bin in the parton level distribution contributes to multiple bins at detector level.

## 8.4 Fit validation and expected precision using the Asimov dataset

### The Asimov dataset

Within the particle physics community, it is a widely adopted practice to assess the fit properties and the expected precision of the measurements before analyzing the recorded data. This evaluation is performed by using what is known as the *Asimov* dataset [98]. The Asimov dataset is constructed by combining all the simulated signal and background contributions considered in the analysis and setting the statistical uncertainty of the resulting distributions in this dataset to  $\sqrt{N_i^{\text{events}}}$  for each bin  $i$ , mimicking the statistical uncertainty of a recorded data sample.

By employing the Asimov dataset as a substitute for the data sample in the fit, the analysis can be optimized while keeping the measurement *blinded* from the recorded data. This practice is a key part of the code of good practices, as it significantly reduces the risk of introducing any bias into the analysis due to the prior expectations of the researchers. Consequently, employing the Asimov dataset until the final result is reported improves the reliability and integrity of the final measurement.

The top quark mass measurement presented in this thesis is currently under approval from the ATLAS collaboration. Therefore, all the results reported in this section and Chapter 9 are based on the Asimov dataset. Once the analysis successfully completes all the necessary review stages, it will be unblinded, and the final results derived from recorded data will be reported.

### Input distributions

As mentioned in Section 8.3, the statistical model constructed for the measurement of the top quark MC mass parameter ( $m_t^{\text{MC}}$ ) and the extraction of the  $t\bar{t}$  +jet differential cross section at parton level utilizes two signal and two control regions. The distributions used in the analysis are shown in Figure 8.5. The  $t\bar{t}$  samples depicted in the SRs are internally subdivided into the different folded samples corresponding to each parton level bin, as shown in Figure 8.4.

In the case of the  $M_{lb}$  variable, the associated distributions are divided into five bins of equal width in the range  $20 \text{ GeV} < M_{lb} < 160 \text{ GeV}$ . This binning has been

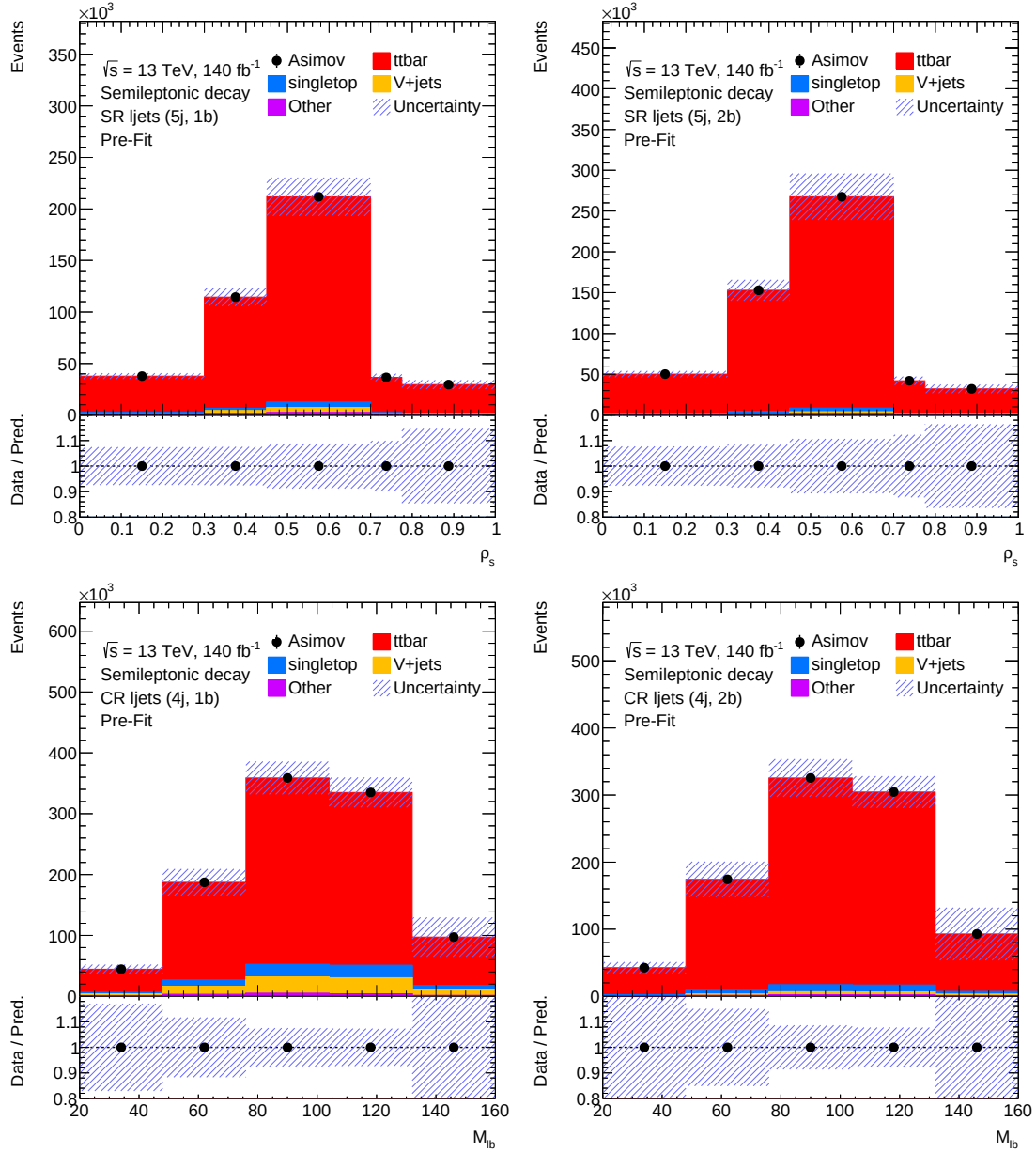


Figure 8.5: Comparison between the Asimov dataset and the pre-fit MC predictions for the two signal regions (top) and the two control regions (bottom) considered in the analysis. The error bands show the total pre-fit uncertainty associated with each bin, which includes all systematic uncertainties.



employed in previous analyses that also use the  $M_{lb}$  observable to constrain the top quark MC mass NP [213]. It provides a good compromise between being narrow enough to capture the observable's sensitivity to  $m_t^{\text{MC}}$ , while being wide enough to minimize migrations effects. Moreover, the binning is chosen to be sparse to avoid over-constraining the NP of the statistical model. The same binning is used for both control regions of the analysis. To mitigate the contribution of top quarks produced in the off-shell region, the underflow and overflow events are excluded from the distributions.

For the  $\rho_s$  variable, the corresponding distributions are binned following the bin edges:  $\rho_s = \{0, 0.3, 0.45, 0.7, 0.775, 1\}$ . This binning has been chosen after studying the resolution of the  $\rho_s$  variable after the final event selection, the diagonality of the migration matrix, and the purity and stability of these bins. The core idea underlying the chosen binning is to isolate two regions of the  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  parton level distribution from the others. First, the region with  $0.45 < \rho_s < 0.7$ , as in this region the  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  distributions for different  $m_t^{\text{pole}}$  intersect, thus its sensitivity to the top quark mass is limited. Secondly, the threshold regions with  $0.775 < \rho_s$ , as it exhibits the highest sensitivity to the top quark mass (Figure 2.16). Additionally, this binning is also chosen to be sparse to avoid over-constraining the NP of the statistical model. Different binning configurations have been tested for the analysis, providing consistent results with respect to the nominal binning selection (Appendix G.4). The same binning is used for both signal regions of the analysis. The overflow events are added to the last bin of the distribution.

#### Fit validation and $m_t^{\text{MC}}$ linearity test: Statistical uncertainty only

In addition to the Asimov dataset constructed using the nominal  $t\bar{t}$  sample, which was produced with the top quark MC mass parameter set at  $m_t^{\text{MC}} = 172.5$  GeV in the simulation, a collection of alternative Asimov samples are also constructed to validate the fit procedure. These alternative Asimov datasets are constructed analogously to the nominal one, with the exception that the nominal  $t\bar{t}$  sample is substituted by one of the alternatives  $t\bar{t}$  samples produced with various values of  $m_t^{\text{MC}}$ , as described in Section 6.2.2.

Subsequently, the maximum likelihood fit to extract  $m_t^{\text{MC}}$  and the parton level differential distribution is performed using the nominal statistical model for each of the Asimov datasets, but only including the statistical uncertainty and the top quark MC mass NP. In this *statistics only* fit, it is expected to observe a

good agreement between the fitted values of  $m_t^{\text{MC}}$  and the input values set in the production of each sample. Furthermore, in Appendix G.2, the parton level  $\mathcal{R}$  distributions obtained after unfolding the various Asimov datasets are used to extract once again the top quark MC mass at parton level. This latter test ensures that the differential distribution is also extracted without any bias.

The values of the top quark MC mass parameter used in the simulation and its corresponding extracted value from the fit are shown in Table 8.4. The agreement with the input values is assessed in the linearity plot of Figure 8.6, where only the  $m_t^{\text{MC}}$  values extracted from the statistics only fit in each Asimov dataset are plotted.

A good level of agreement is observed between the fitted and the input values, with a non-closure of  $|m_t^{\text{MC, fit}} - m_t^{\text{MC, IN}}| < 82$  MeV for all extracted values, including those that do not correspond to the up and down variations of the NP, 171 and 174 GeV, showing that the shape effect of the MC top quark mass in each bin of our distributions is linear.

Table 8.4: Summary of the fitting procedure tests with the statistics only and the full systematic model for the Asimov datasets produced with various values of  $m_t^{\text{MC}}$ . The up/down variations for the  $m_t^{\text{MC}}$  NP are constructed with the samples produced with  $m_t^{\text{MC}} = 171$  GeV and  $m_t^{\text{MC}} = 174$  GeV, respectively. A good agreement between the input and the fitted values is observed.

| Input $m_t^{\text{MC}}$ [GeV] | Detector sim. | Fit setting | $m_t^{\text{MC}}$ NP | Fitted $m_t^{\text{MC}}$ [GeV] |
|-------------------------------|---------------|-------------|----------------------|--------------------------------|
| 169.00                        | ATLFASTII     | Stat.       | $-2.317 \pm 0.024$   | $169.024 \pm 0.036$            |
| 171.00                        | ATLFASTII     | Stat.       | $-1.000 \pm 0.025$   | $171.002 \pm 0.038$            |
| 172.00                        | ATLFASTII     | Stat.       | $-0.341 \pm 0.026$   | $171.989 \pm 0.039$            |
| 172.50                        | ATLFASTII     | Stat.       | $+0.000 \pm 0.027$   | $172.500 \pm 0.041$            |
| 173.00                        | ATLFASTII     | Stat.       | $+0.343 \pm 0.028$   | $173.014 \pm 0.042$            |
| 174.00                        | ATLFASTII     | Stat.       | $+1.000 \pm 0.028$   | $173.999 \pm 0.043$            |
| 176.00                        | ATLFASTII     | Stat.       | $+2.388 \pm 0.030$   | $176.082 \pm 0.045$            |
| 171.00                        | Full sim.     | Stat.       | $-0.999 \pm 0.025$   | $171.002 \pm 0.037$            |
| 174.00                        | Full sim.     | Stat.       | $+0.999 \pm 0.028$   | $173.999 \pm 0.041$            |
| 171.00                        | Full sim.     | Stat.+Syst. | $-1.063 \pm 0.266$   | $170.905 \pm 0.400$            |
| 174.00                        | Full sim.     | Stat.+Syst. | $+1.029 \pm 0.264$   | $174.043 \pm 0.396$            |
| 172.50                        | Full sim.     | Stat.       | $+0.000 \pm 0.026$   | $172.500 \pm 0.039$            |
| 172.50                        | Full sim.     | Stat.+Syst. | $+0.000 \pm 0.276$   | $172.500 \pm 0.414$            |

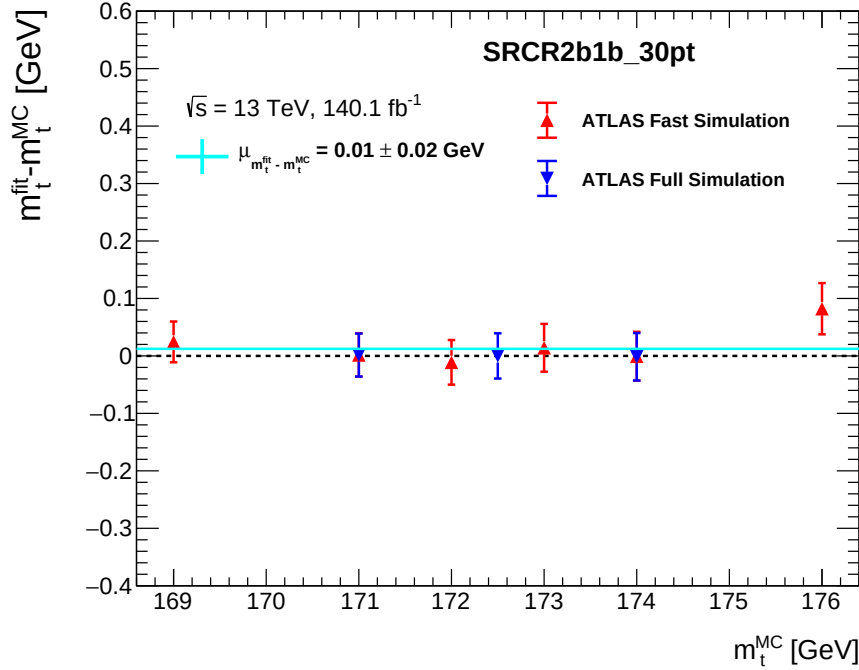


Figure 8.6: Difference between the top quark MC mass extracted from the associated NP of the profile maximum likelihood Stat. only fit and the value used as input to generate the alternative  $t\bar{t}$  @hvq+PS samples. The blue points correspond to the samples computed using the full simulation of the ATLAS detector, while the red points represent the samples produced using the fast simulation of the detector. The cyan line represents the average discrepancy derived from all the samples, which is compatible with zero within the uncertainties.

#### Expected precision of the $m_t^{\text{MC}}$ measurement and the parton level differential cross section: All uncertainties.

In order to assess the expected level of precision for the measurement of  $m_t^{\text{MC}}$  and the unfolded parton level differential distribution, the profile maximum likelihood fit is performed using the full statistical model on the nominal Asimov dataset. The full statistical model includes the statistical uncertainty, as well as all the systematic uncertainties described in Section 8.2.2. This test also allows the study of the behaviour of the statistical model, enabling the optimization of the model without unblinding the analysis by looking at recorded data.

The resulting post-fit distributions for the Asimov fit with  $m_t^{\text{MC}} = 172.5 \text{ GeV}$  are shown in Figure 8.7. In these plots, it can be observed that the post-fit uncertainties are smaller than the pre-fit uncertainties, which is a consequence of

the post-fit constraint (profiling) of some of the NPs included in the statistical model, such as some of the systematic uncertainties and the top quark MC mass NP. The resulting pull distributions for this fit are shown in Figures 8.8 and 8.9, which show the mean values of the post-fit NPs (pulls) and their associated post-fit uncertainties. For the  $\gamma$  NPs, the post-fit mean values are shown in Figure 8.10.

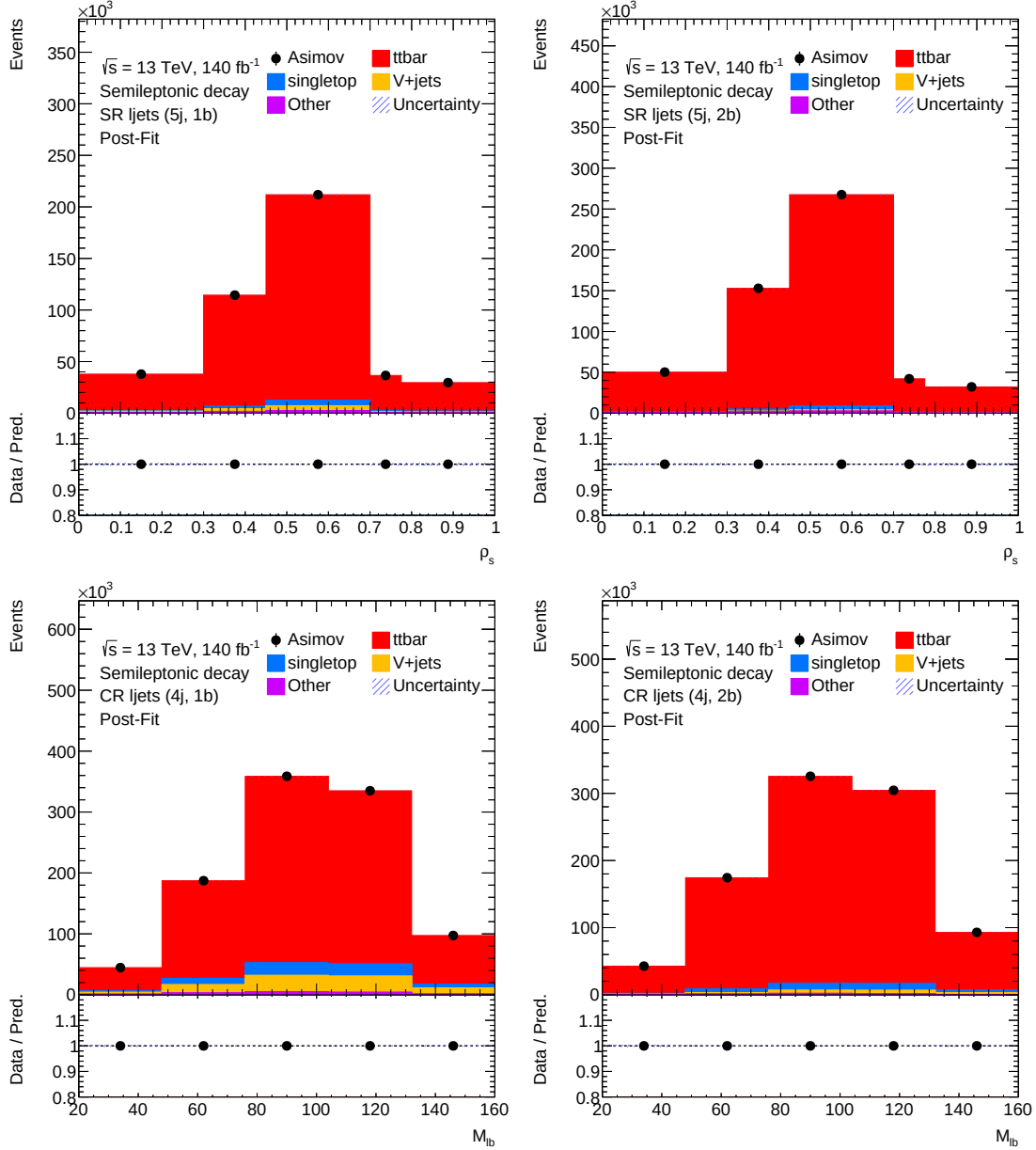


Figure 8.7: Comparison between the Asimov dataset and the post-fit MC predictions for the two signal regions (top) and the two control regions (bottom) considered in the analysis.

The FSR systematic uncertainty associated with the  $t\bar{t}$  sample is found to have

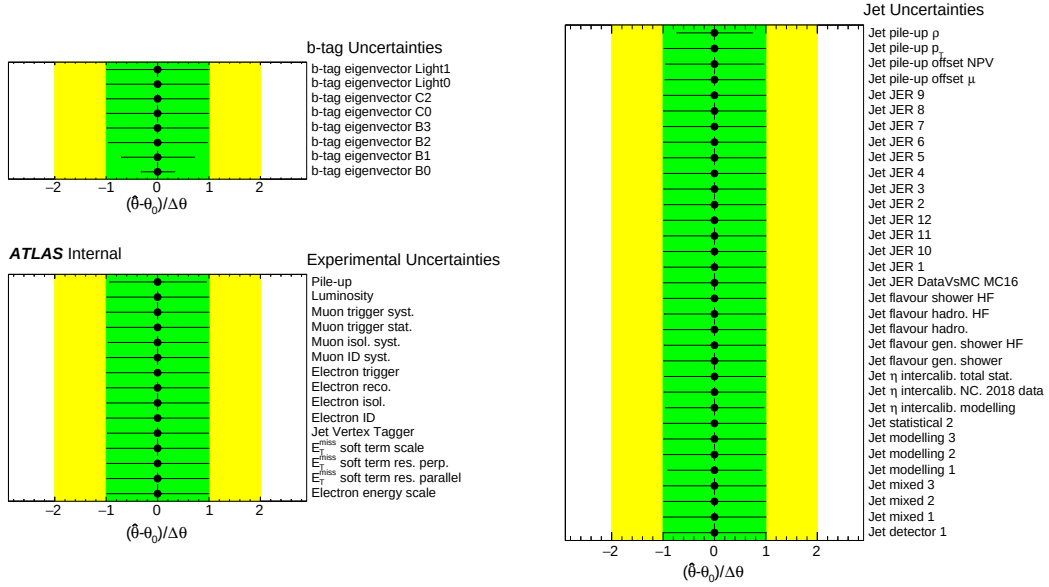


Figure 8.8: The pull plots for the NPs associated with the experimental systematic uncertainties in the fit of the Asimov dataset. The green and yellow bands represent the pre-fit uncertainties at one and two standard deviations, respectively. The black dots correspond to the post-fit mean values of the NP, while the black lines represent the post-fit NP uncertainties.

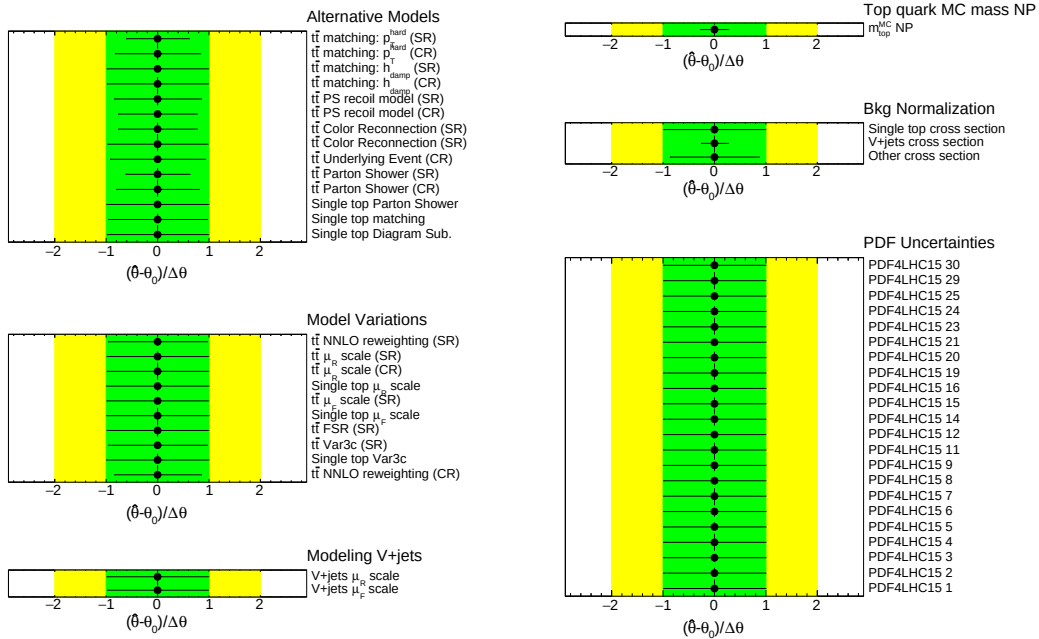


Figure 8.9: Similar to Figure 8.8 but for the NPs associated with the systematic modeling uncertainties.

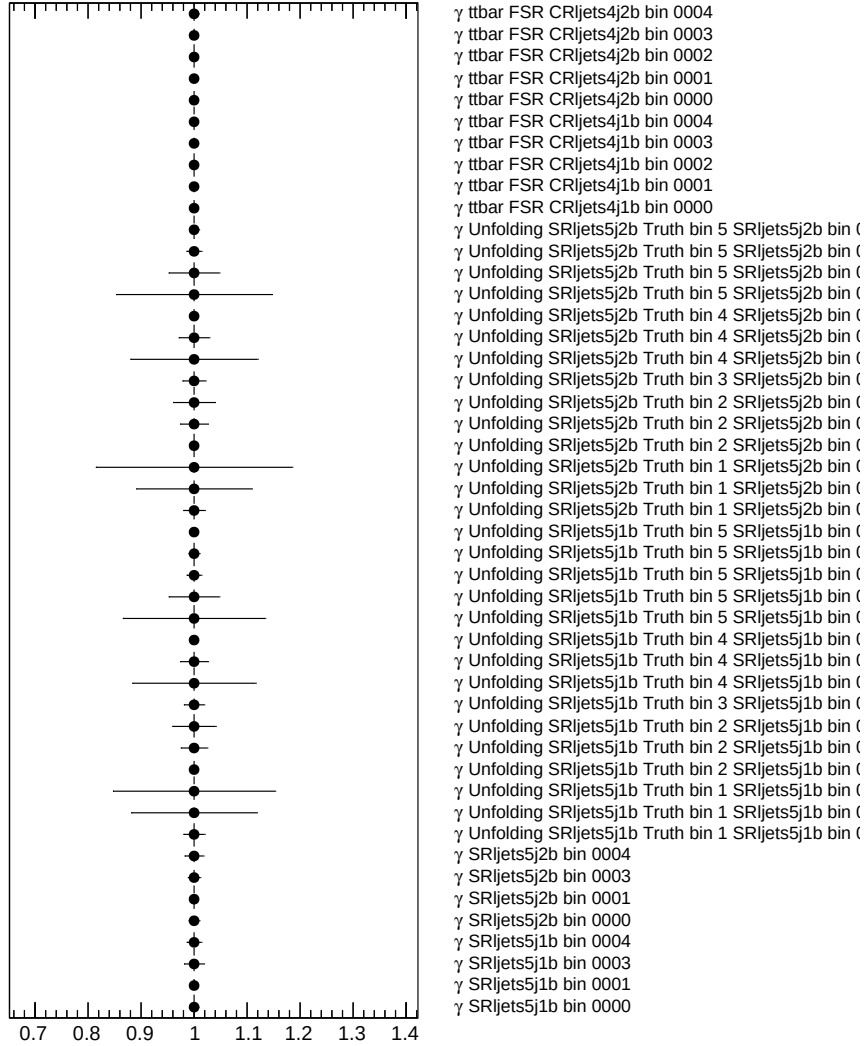


Figure 8.10: List of the post-fit values for the  $\gamma$  NPs. These NPs include the ones associated with the MC statistical uncertainty of each bin in each region, as well as the NPs originated from the bin-by-bin decorrelation of “ $t\bar{t}$  FSR (CR)” uncertainty.

a significant effect on the  $M_{lb}$  distributions, which would lead to a  $\sim 60\%$  constraint in the NP associated with this systematic in the CRs. In order to alleviate this constraint, a bin-by-bin decorrelation approach is adopted for this systematic, which is technically implemented by introducing an independent NP to model the effect of this systematic in each bin of the distribution. This implementation is equivalent to the way the *gamma* MC statistical uncertainties are introduced into the model, hence the associated NPs are present in the  $\gamma$  NPs plot in Figure 8.10. The introduction of this set of NPs not only avoids the overconstraint of this NP, but also moderates the overall constraining power of the fit, contributing to the relaxation of other minor constraints observed in the fit.

No pulls are observed in the Asimov fit, while some of the NPs are constrained in the fit. These include one of b-tag eigenvector B0, the V+jets cross section, and the NP associated to the top quark MC mass.

The constraint in the *b*-tagging uncertainty can be attributed to the dedicated calibration used to define the up and down variations. This calibration was developed using a subset of the dataset, covering the period from 2015 to 2017 ( $80 \text{ fb}^{-1}$ ), and used dileptonic  $t\bar{t}$  events. In contrast, the present analysis uses the full Run 2 dataset ( $140 \text{ fb}^{-1}$ ) and is carried out using semileptonic  $t\bar{t}$  events. These two factors lead to a larger data sample, which can explain the observation of constraints in the NP associated with the flavour tagging. Other auxiliary measurements used to define the up and down variations for some experimental systematics are also evaluated using only a part of the Run 2 dataset, however, the statistical model is not very sensitive to their effects hence they are not constrained.

Considering the conservative pre-fit uncertainty of 50% associated with the V+jets cross section, it is not unexpected that it is constrained in the fit. This constraint originates from the large sample size and the significant contribution of this background in the regions with one *b*-tagged jet. As a result, the NP associated to this uncertainty is constrained to 26%, resulting in a post-fit uncertainty of 13% for the cross section of the V+jets processes.

Since the NP associated to the top quark MC mass parameter is introduced as a free NP into the statistical model, it lacks a constraint term, enabling the post-fit value to be interpreted as a measurement of this parameter. The post-fit value extracted from the fit for this NP is  $0.000^{+0.270}_{-0.276}$ . As the up/down variations for this NP are produced with a 1.5 GeV difference from the nominal value of

172.5 GeV, the associated expected level of precision for the determination of  $m_t^{\text{MC}}$  from the profile likelihood fit is:

$$\Delta m_t^{\text{MC}}(\text{total}) \simeq 0.41 \text{ GeV} \quad , \quad (8.12)$$

A similar level of precision is expected when performing the profile maximum likelihood fit over recorded data once the unblinding of the analysis is approved.

The post-fit values of the parameters of interest in the statistical model and their total associated uncertainty from the fit are shown in Figure 8.11. This list includes the normalization factors associated with the bin contents of the normalized parton level  $\rho_s$  distribution (except for the first bin), as well as the total  $t\bar{t}$  normalization factor for both the signal regions and control regions. Since the main goal of the profile maximum likelihood fit is the extraction of the  $\rho_s$  parton level normalized differential distribution, the effect of each individual systematic uncertainty in the extraction of the associated normalization factors are shown in the ranking plots in Figure 8.12.

The nuisance parameter ranking plots are obtained by repeating the maximum likelihood fit a total of four times for each nuisance parameter. In each of these fits, the NP value is fixed to the pre-fit value  $\pm$  the pre-fit uncertainty or to the post-fit value  $\pm$  the post-fit uncertainty. Then, the impact of each systematic on the corresponding POI is estimated by the difference of the POI obtained in each of these four fits, and the POI value obtained in the nominal fit.



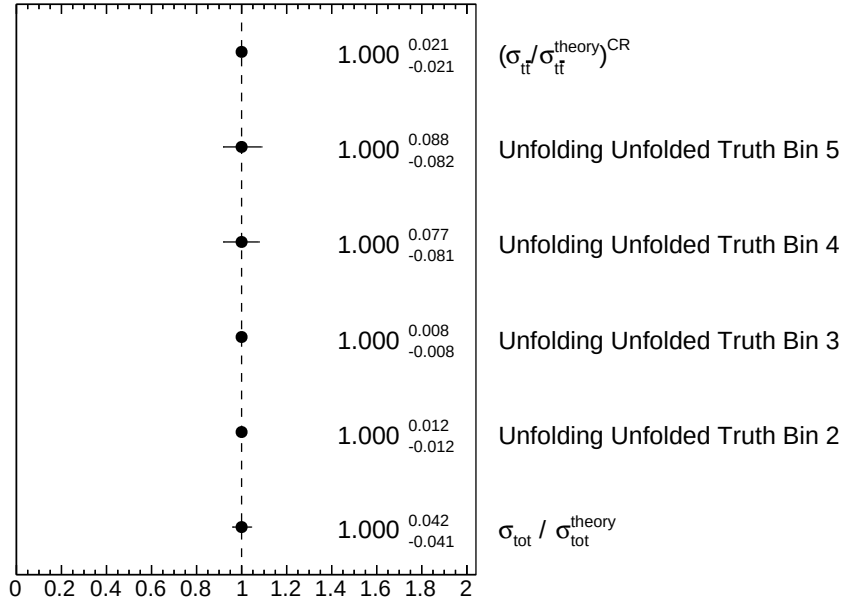


Figure 8.11: POIs in the statistical model and their associated uncertainties obtained from the Asimov Stat.+Syst. maximum likelihood fit. The *Unfolding Unfolded Truth Bin  $k$*  POIs denote the  $\mu_{t\bar{t}+\text{jet}}^{\text{rel},k}$  normalization factors,  $\sigma_{\text{tot}}/\sigma_{\text{tot}}^{\text{theory}}$  denotes the  $\mu_{t\bar{t}+\text{jet}}^{\text{tot}}$  normalization factor, and  $(\sigma_{\text{tot}}/\sigma_{\text{tot}}^{\text{theory}})^{\text{CR}}$  denotes the  $\mu_{t\bar{t}}^{\text{CR}}$  normalization factor, as expressed in Equations 8.8 and 8.9.

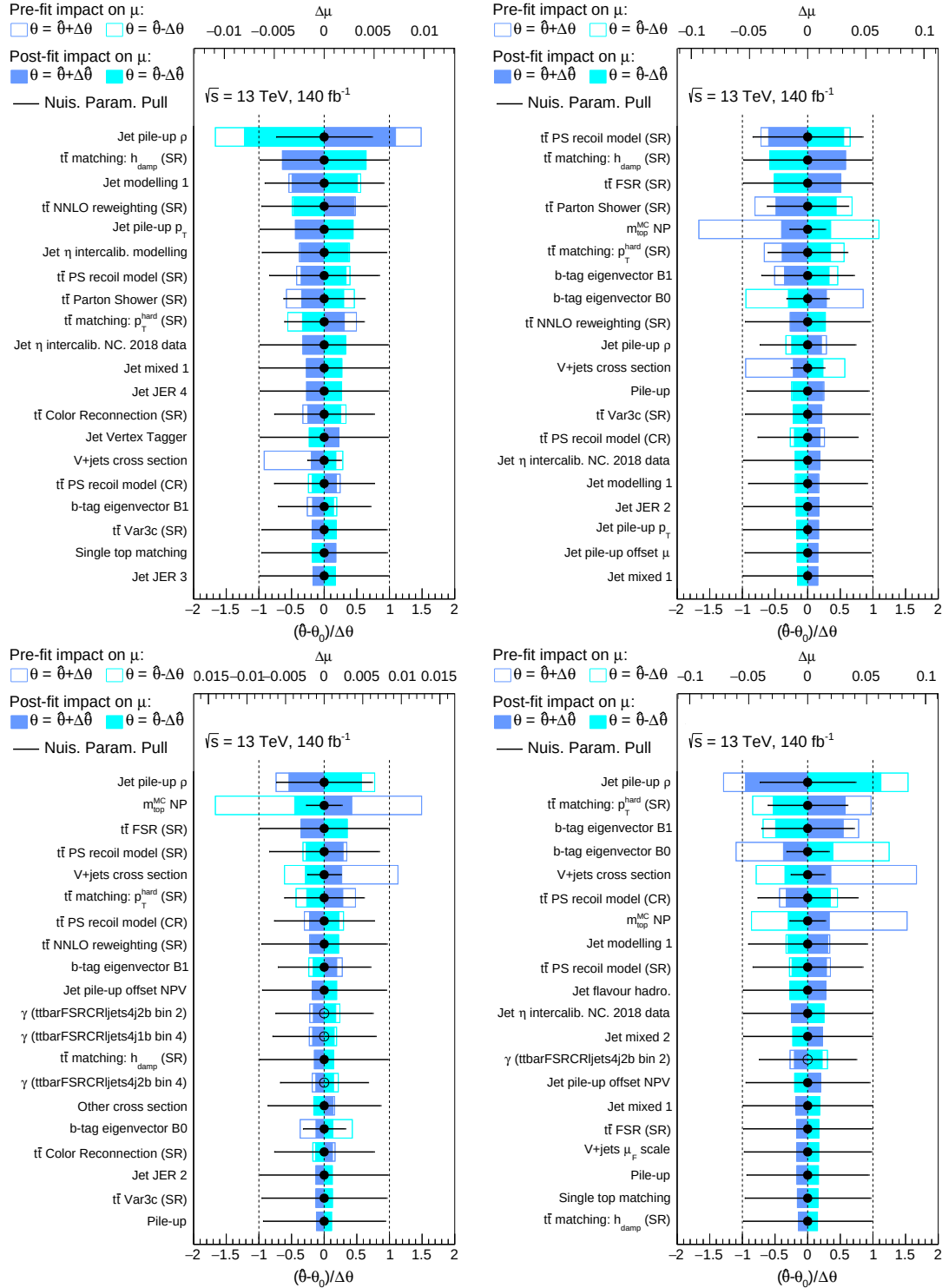


Figure 8.12: Ranking plot of the normalization factors associated with the bin content of the  $\rho_s$  normalized parton level distribution for the second (top-left), third (top-right), fourth (bottom-left), and fifth (bottom-right) bins. Only the 20 highest-ranking NPs for each POI are shown. The empty boxes represent the pre-fit effect of the NP on the POI, while the full boxes represent the post-fit effects. The black points accompanied by error bars represent the pulls of the NPs and their associated post-fit constrain.

The dominant uncertainties driving the precision of the measurement of the  $\mu_{t\bar{t}+\text{jet}}^{\text{rel},k}$  normalization factors are the JES pile-up  $\rho$  experimental systematic uncertainty, as well as the  $t\bar{t}$  Parton Shower,  $t\bar{t}$  matching:  $p_{\text{T}}^{\text{hard}}$ , and the  $t\bar{t}$  PS recoil model, among other modeling systematic uncertainties.

The JES pile-up  $\rho$  accounts for the uncertainty stemming from the pile-up contribution to the  $p_{\text{T}}$  of the jets in the event. As the analysis is conducted in the semileptonic channel of the  $t\bar{t}$  +jet system, which is characterized by a high jet multiplicity ( $N_{\text{jet}} \geq 5$ ), it is reasonable to expect that the dominant experimental systematic uncertainties are those associated with jet-related effects. In fact, other experimental systematics listed in the ranking plot, such as Jet modelling 1 and Jet  $\eta$  intercalibration modeling are also related to jets.

The matching uncertainty, represented by the  $p_{\text{T}}^{\text{hard}}$  NP, has a significant impact on the additional parton radiation from the  $t\bar{t}$  system. Consequently, it is unsurprising that it has a significant effect in the extraction of these normalization factors, which correspond to  $t\bar{t}$  +jet events. Similarly, the  $h_{\text{damp}}$  and the FSR uncertainties, which also have a significant effect on the additional radiation of the  $t\bar{t}$  system, feature prominently in the ranking plot of some of the normalization factors.

The  $t\bar{t}$  PS recoil model, which was significant in a previous top quark MC mass measurement from the ATLAS collaboration [81], also manifests as a significant uncertainty in the analysis.

Finally, the unfolded  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  distribution at parton level, obtained from the  $\mu_k^{t\bar{t}+\text{jet}}$  normalization factors derived from the fit to the nominal Asimov dataset, is presented in Figure 8.13. This figure also includes the total covariance matrix associated with this distribution, which accounts for the effects of the statistical, as well as all the systematic uncertainties affecting the analysis.

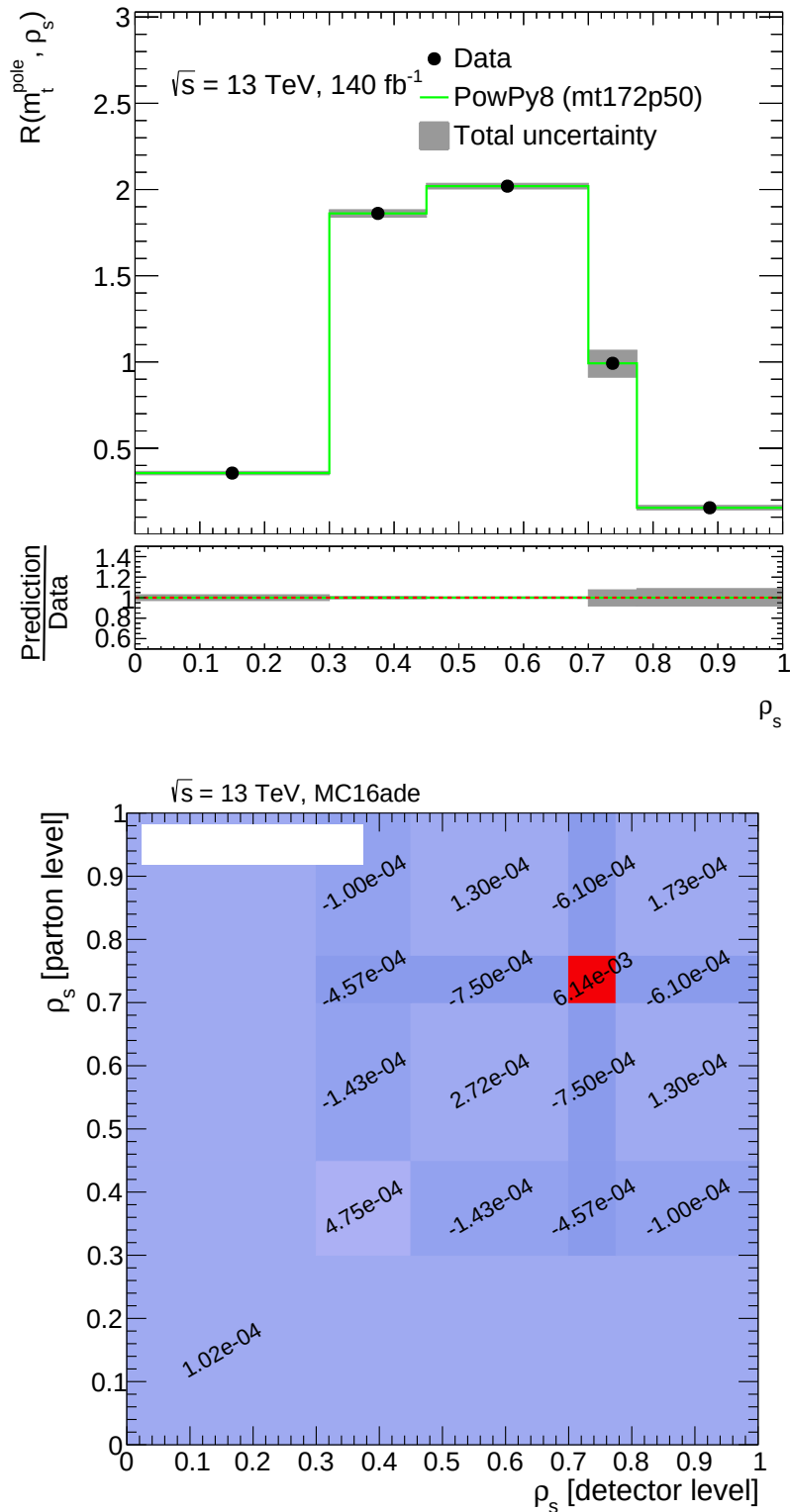


Figure 8.13: Top: Normalized parton level unfolded distribution of the Asimov dataset. The gray band represents the total uncertainty associated with each bin content. Bottom: Covariance matrix between the various bins in the normalized unfolded distribution. While the matrix is complete for the last four bins, as the first bin is expressed as a function of the others, only the diagonal element is being filled.

# Chapter 9

## Extraction of the top quark pole mass

This chapter describes the extraction of the top quark mass parameter of the SM Lagrangian in the on-shell renormalization scheme, the top quark pole mass,  $m_t^{\text{pole}}$ . This chapter is structured as follows: In Section 9.1, the value of the  $m_t^{\text{pole}}$  and its associated fit uncertainty are extracted from the  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  unfolded distribution by means of a  $\chi^2$  fit to the  $t\bar{t} + \text{jet@NLO}$  fixed-order theory predictions for the  $\mathcal{R}$  observable [95]. Section 9.2 describes the procedure followed to estimate the uncertainties associated with the computation of the theory predictions. Finally, Section 9.3 presents the expected precision of  $m_t^{\text{pole}}$  considering all sources of uncertainties.

Since the analysis remains blinded, the central value of  $m_t^{\text{pole}}$  and the fit uncertainty are obtained from the  $\chi^2$  fit performed on the  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  unfolded distribution, which originates from the nominal Asimov dataset as described in Section 8.4. Consequently, the results presented in this chapter correspond to the expected level of precision in the measurement of  $m_t^{\text{pole}}$ . The final result, derived from the recorded ATLAS data, is under approval, hence, it can not be included in this thesis until the approval process is completed.

## 9.1 Top quark pole mass extracted from the nominal Asimov dataset and its associated fit uncertainty

In this section, the top quark pole mass value ( $m_t^{\text{pole}}$ ) is extracted from the unfolded Asimov data distribution of the  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  observable obtained in Chapter 8. This extraction is carried out through a  $\chi^2$  fit of this distribution to the  $t\bar{t} + \text{jet@NLO}$  fixed-order theory predictions. These predictions are computed using the **Powheg-Box-v2**  $t\bar{t}J$  process [95], with the **CT18NLO** (LHAPDF-ID=14400) PDF set [214] as the nominal PDF choice. Alternative theory predictions computed using other PDF sets, such as NNPDF3.0 (LHAPDF-ID=303000) [215], PDF4LHC21 (93300) [216], and ABMP16NLO (43110) [217], have also been generated.

In the  $\chi^2$  method<sup>1</sup>, the extracted  $m_t^{\text{pole}}$  value is the one that minimizes the following expression:

$$\chi^2 = \sum_{i,j} \left[ \mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}} - \mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}}) \right]_i [V^{-1}]_{ij} \left[ \mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}} - \mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}}) \right]_j, \quad (9.1)$$

where  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  represents the unfolded data distribution,  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  is a parametrization of the  $t\bar{t} + \text{jet@NLO}$  fixed-order theory predictions for the binned distribution, and  $V_{ij}^{-1}$  represents each of the elements of the inverse of the total covariance matrix obtained from the unfolding.

Since the  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  observable is normalized, the content of one bin can always be expressed in terms of the contents of the other bins. Therefore, for the computation of the  $\chi^2$  value, one of the bins has to be excluded from the summation in Equation 9.1. In this analysis, the nominal choice is to exclude the first bin of the distribution ( $0 < \rho < 0.3$ ). However, as the bins are correlated and share the same information, the fit result is independent of the specific choice of the bin that is excluded from the calculation.

The analytical form describing the dependence of  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  with respect to the top quark pole mass is not known. To approximate this dependence,

<sup>1</sup>Also known as *least squares method*.

a set of theory calculations is generated, which includes the nominal calculation computed assuming  $m_t^{\text{pole}} = 172.5$  GeV, as well as a series of additional calculations with various values of  $m_t^{\text{pole}}$ , ranging from 166 to 179 GeV in 1 GeV increments. These calculations are used to construct the parametrization of the content of each bin in the distribution with respect to the top quark pole mass value. This parametrization is derived using the following second-order polynomial function:

$$\left[\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})\right]_i = a_i + b_i(m_t^{\text{pole}} - 170 \text{ GeV}) + c_i(m_t^{\text{pole}} - 170 \text{ GeV})^2, \quad (9.2)$$

where  $i$  is an index that represents each of the bins in the distribution, while  $a_i$ ,  $b_i$ , and  $c_i$  are the coefficients of the second-order polynomial function. The values of top quark mass extracted using higher-order polynomials produce results that are compatible with the one derived from the second-order parametrization.

For each of the bins used in the nominal binning choice of this analysis, the resulting parametrizations are shown in Figure 9.1.

The estimation of the uncertainty associated with the parametrization of the bin content dependence with respect to  $m_t^{\text{pole}}$  is described in detail in Appendix G.1. The effect is found within the statistical uncertainty of the theory predictions, thus no additional uncertainty is added to the final top quark pole mass determination.

Since the  $V_{ij}$  covariance matrix is obtained through the profiled maximum likelihood fit, it includes the statistical uncertainty associated with the measurement, as well as the contribution of all the systematic uncertainties described in Section 8.2. The combination of these sources of uncertainties is referred to as the fit uncertainty, and it is extracted from the mass shift that results in a variation of the  $\chi^2$  function by one unit with respect to its minimum value,  $\Delta\chi^2 = 1$ . As the covariance matrix is symmetric, the fit uncertainty is also expected to be symmetric.

Using the  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  parametrizations depicted in Figure 9.1, along with the unfolded Asimov distribution and the total covariance matrix obtained from the PLU unfolding (Figure 8.13), the resulting  $\chi^2$  distribution from Equation 9.1 with respect to the top quark pole mass is shown in Figure 9.2.

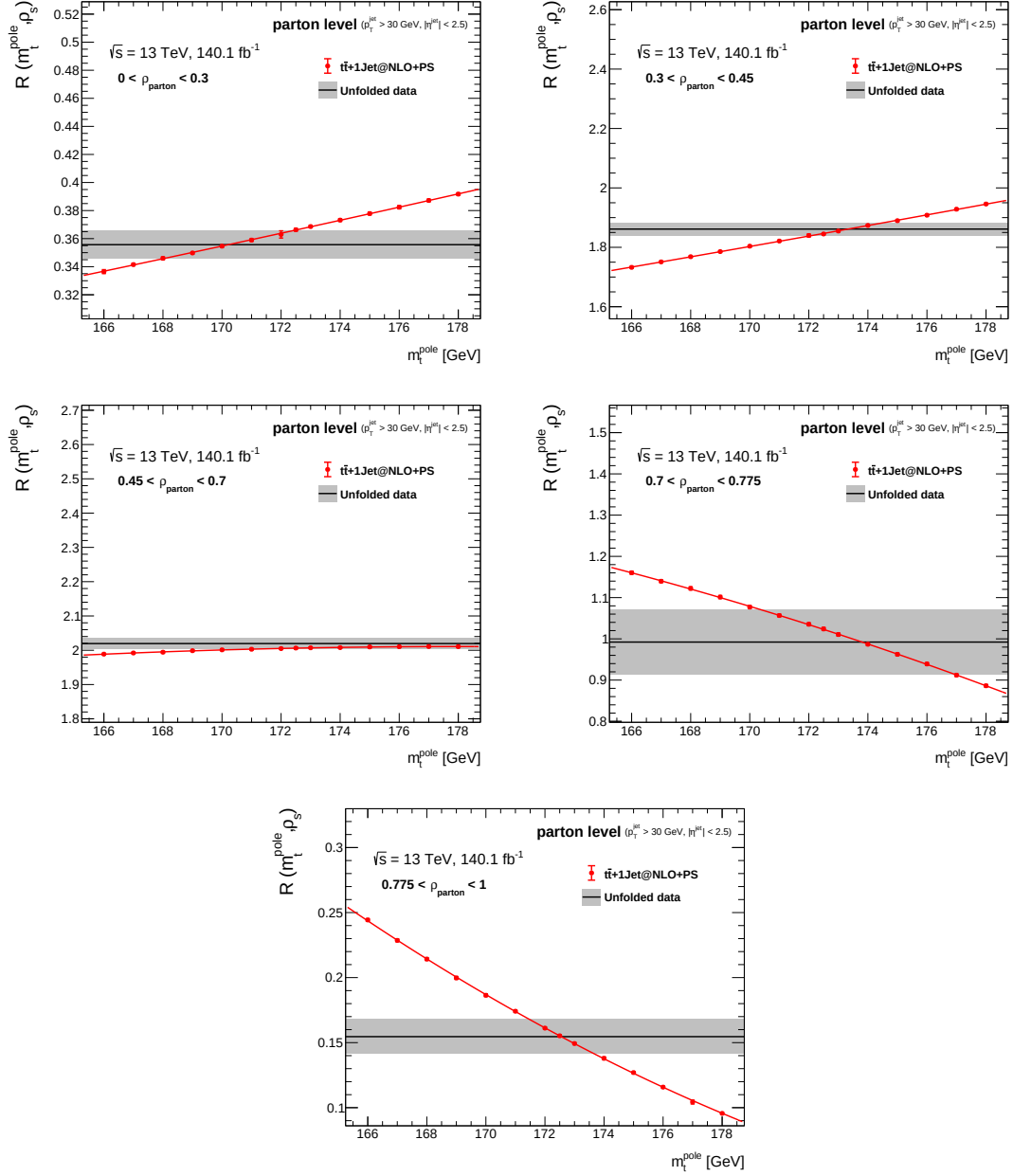


Figure 9.1: Parametrization of  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  for each of the  $i$  bins of the distribution. The black line represents the bin content of the unfolded Asimov distribution obtained from the PLU method, with the grey band representing the associated uncertainty extracted from the total covariance matrix.



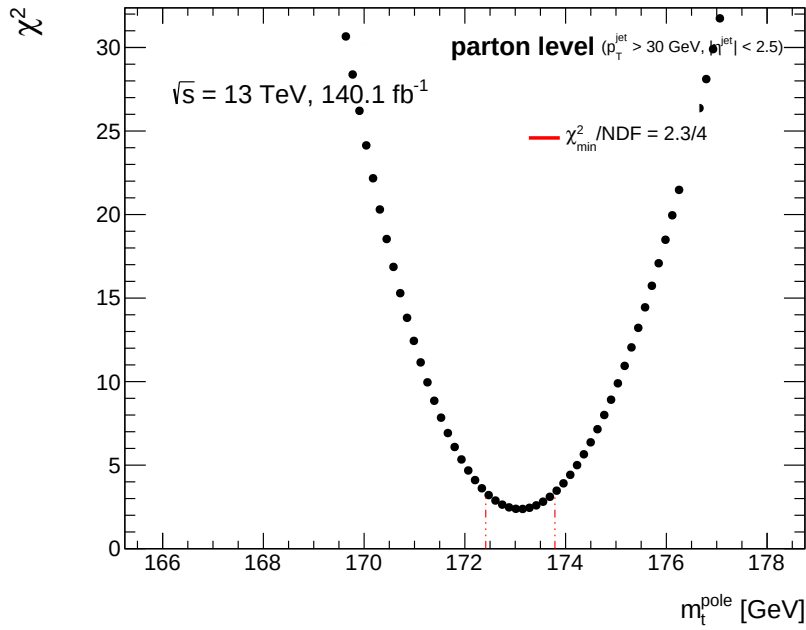


Figure 9.2:  $\chi^2$  distribution versus  $m_t^{\text{pole}}$  obtained from the comparison of the  $\mathcal{R}_{\text{Asimov}}^{t\bar{t}+\text{jet}}$  distribution to the  $t\bar{t} + \text{jet}$  NNLO fixed-order predictions using the CT18NNLO PDF set (Equation 9.1). The vertical dashed lines represent the  $\Delta\chi^2 = 1$  variations with respect to its minimum value, which corresponds to the fit uncertainty of the measurement.

The minimum value of the  $\chi^2$  distribution extracted from the fit to the Asimov distribution and its associated fit uncertainty is:

$$173.09 \pm 0.69 \text{ (fit) GeV.} \quad (9.3)$$

To estimate the statistical component of the fit uncertainty, the  $\chi^2$  fit is repeated using the unfolded Asimov parton level distribution obtained from the stat. only profile maximum likelihood fit. The resulting uncertainty from this fit estimates the statistical component of the fit uncertainty as  $\Delta m_t^{\text{pole}}(\text{stat.}) = 0.122 \text{ GeV}$ . This estimate of the statistical uncertainty accounts for less than 16% of the total fit uncertainty, highlighting that in the extraction of the top quark pole mass, the total systematic uncertainty is dominant over the statistical component.

In addition to the fit uncertainty originated from the data statistical and systematic uncertainties described in Section 8.2, it is necessary to consider the impact of the theory uncertainties associated with the  $t\bar{t} + \text{jet@NLO}$  fixed-order calculations. This theoretical uncertainty is typically divided into two components: The uncertainty associated with the PDF set and  $\alpha_S$  used in the calculations, and the uncertainty associated with the variations of the  $\mu_R$  and  $\mu_F$  scales. The estimation of the PDF+ $\alpha_S$  and the scale uncertainties in the theoretical calculations are described in the following section.

## 9.2 Theory uncertainties

### PDF and $\alpha_S$ uncertainties

The CT18NLO PDF set [218] in the five-flavor scheme is employed as the nominal PDF set in the computation of the  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  theory predictions. In this section, a detailed description of the procedure followed to estimate the PDF and  $\alpha_S$  uncertainties associated with the nominal theoretical calculations computed using the CT18NLO PDF set is provided. The estimation of these uncertainties using the alternative theoretical predictions computed with the NNPDF3.0 [215], PDF4LHC21 [216], and ABMP16NLO [217] is provided in Appendix G.3.

The uncertainties that originated from the use of the CT18NLO PDF set

in the computation of the theory predictions are propagated throughout the analysis by considering the variations of the PDF eigenvectors. The CT18NLO PDF set consists of a total of 59 members, which include the central value and the positive and negative variations associated with the 29 eigenvectors that constitute the PDF parameter space. In addition to the PDF eigenvector variations, the CT18NLO PDF set also incorporates two additional variations, which correspond to the variation of the value of  $\alpha_s(M_Z)$  within its uncertainty. Both the eigenvectors and  $\alpha_s$  variations are provided at a confidence level (CL) boundary of 90%, which differs from the usual 68% CL limit ( $1\sigma$ ).

For each member of the PDF set, a  $\mathcal{R}$  distribution is computed, and a value of  $m_t^{\text{pole}}$  is extracted by fitting this distribution using the templates depicted in Figure 9.1. The top quark pole mass variations associated with each of the PDF set members are combined following the recommended procedure outlined in Ref. [219, 220]. The total PDF uncertainty is obtained using the following equation:

$$\begin{aligned}\Delta^+ m_t^{\text{pole}}(\text{PDF}) &= \sqrt{\sum_{i=1}^{N_a} \left[ \max((m_t^{\text{pole}})_i^{(+)} - (m_t^{\text{pole}})_0, (m_t^{\text{pole}})_i^{(-)} - (m_t^{\text{pole}})_0, 0) \right]^2} \\ \Delta^- m_t^{\text{pole}}(\text{PDF}) &= \sqrt{\sum_{i=1}^{N_a} \left[ \max((m_t^{\text{pole}})_0 - (m_t^{\text{pole}})_i^{(+)}, (m_t^{\text{pole}})_0 - (m_t^{\text{pole}})_i^{(-)}, 0) \right]^2},\end{aligned}\tag{9.4}$$

where  $(m_t^{\text{pole}})_0$  represents the top quark pole mass value extracted from the 0-th member of the PDF set, which corresponds to the PDF central value.  $(m_t^{\text{pole}})_i^{(\pm)}$  denotes the top quark pole mass value extracted from the positive and negative variations of the  $i$ -th PDF eigenvector. The dimension of the eigenvector PDF parameter space is denoted by  $N_a$ , and for CT18NLO, it is  $N_a = 24$ .

In a similar manner, the  $\alpha_s$  variations included in the PDF members are used to calculate the corresponding  $\Delta m_t^{\text{pole}}(\alpha_s)$  uncertainty. This uncertainty is added in quadrature to the PDF uncertainty to obtain the total  $\Delta m_t^{\text{pole}}(\text{PDF} + \alpha_s)$  uncertainty.

As the eigenvector and  $\alpha_s$  variations provided by the CT18NLO authors correspond to a 90% confidence level interval, the uncertainty obtained from Equation 9.4 is scaled down to the 68% confidence level interval by dividing the

corresponding uncertainty at 90% CL by 1.645, as recommended by the authors.

The variation on the top quark pole mass value obtained using each of the PDF eigenvector's positive and negative variations and the  $\alpha_S$  variations are shown in Figure 9.3, along with the total uncertainty band extracted at a 90% and 68% confidence levels. The total  $\Delta m_t^{\text{pole}}(\text{PDF} + \alpha_S)$  uncertainty extracted using the CT18NLO PDF set corresponds to:

$$\Delta m_t^{\text{pole}}(\text{PDF} + \alpha_S) = {}^{+0.34}_{-0.21} \text{ GeV} \quad (9.5)$$

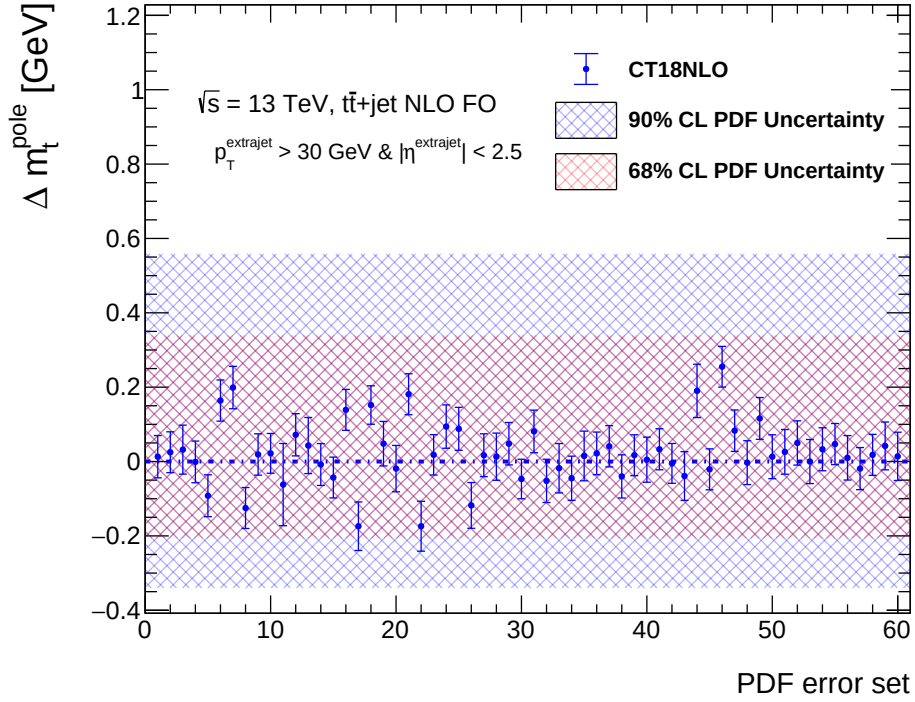


Figure 9.3: The top quark pole mass variation associated with each of the members of the CT18NLO PDF set, including the two  $\alpha_S$  variations. The blue band corresponds to the total  $\Delta m_t^{\text{pole}}(\text{PDF} + \alpha_S)$  uncertainty at a 90% CL, while the red band corresponds to this uncertainty at a 68% CL.

## Scale uncertainties

The theory predictions for the  $\mathcal{R}$  observable are calculated at NLO in QCD. To estimate the uncertainty arising from the missing higher-order corrections in the perturbative calculations, a set of theory predictions with varied values of the renormalization scale ( $\mu_R$ ) and factorization scale ( $\mu_F$ ) are produced. The renormalization and factorization scales are non-physical parameters that should vanish when considering all orders in the perturbation theory. Therefore, their non-zero effect in the calculations can be used to estimate the effects of the uncalculated higher-order contributions.

The renormalization scale is a parameter introduced in the calculations to avoid the ultraviolet divergences that arise from the loops of virtual particles in the Feynman diagrams that represent the scattering amplitudes contributing to the desired process (further details in Section 1.4.2).

On the other hand, the factorization scale is introduced into the calculations when considering the factorization theorem in the collision of two hadrons, such as the colliding protons in the LHC. In this collision, the infrared and collinear divergencies arising in the calculations are absorbed into the parton distribution functions (PDFs) of each colliding proton, and the factorization scale determines the threshold above which the perturbative calculations are valid.

The renormalization and factorization scales in the nominal  $t\bar{t} + \text{jet@NLO}$  fixed-order theory calculation are chosen to have the same value and to dynamically set to  $H_T^B/2$ , as recommended in Ref. [90, 221]. The choice of equal factorization and renormalization scales simplifies the calculations and avoids logarithmic terms that depend on the ratio of the scales and which could invalidate the perturbation theory.  $H_T^B$  is calculated from the scalar sum of the top and anti-top transverse masses plus the transverse momentum of the additional jet:

$$H_T^B = \sqrt{(p_T^{t,B})^2 + m_t^2} + \sqrt{(p_T^{\bar{t},B})^2 + m_t^2} + p_T^{j,B} \quad , \quad (9.6)$$

where the  $B$  superscript denotes that the calculation is performed using the four-momenta of the outgoing particles in the Born phase-space of the POWHEG framework.

The prescription followed to estimate the scale uncertainties is described in

detail in Ref. [90]. It consists of varying the renormalization and factorization scales in the theory calculations independently by a factor of two up and down, avoiding the extreme combinations in which  $\frac{\mu_R}{\mu_F} = \frac{1}{4}, 4$ . This procedure is known as *the seven-point variation*, and the corresponding scale uncertainty is estimated by taking the maximum and minimum difference with respect to the nominal  $m_t^{\text{pole}}$  value.

The variation in the top quark pole mass values obtained from each of the seven combinations of the  $\mu_R$  and  $\mu_F$  scales are depicted in Figure 9.4, along with the envelope of these variations which is identified as the 68% confidence level interval associated with the estimation of this uncertainty. Therefore, the total scale uncertainty extracted using the CT18NLO PDF set corresponds to:

$$\Delta m_t^{\text{pole}}(\text{scale}) = {}^{+0.43}_{-0.31} \text{ GeV} \quad (9.7)$$

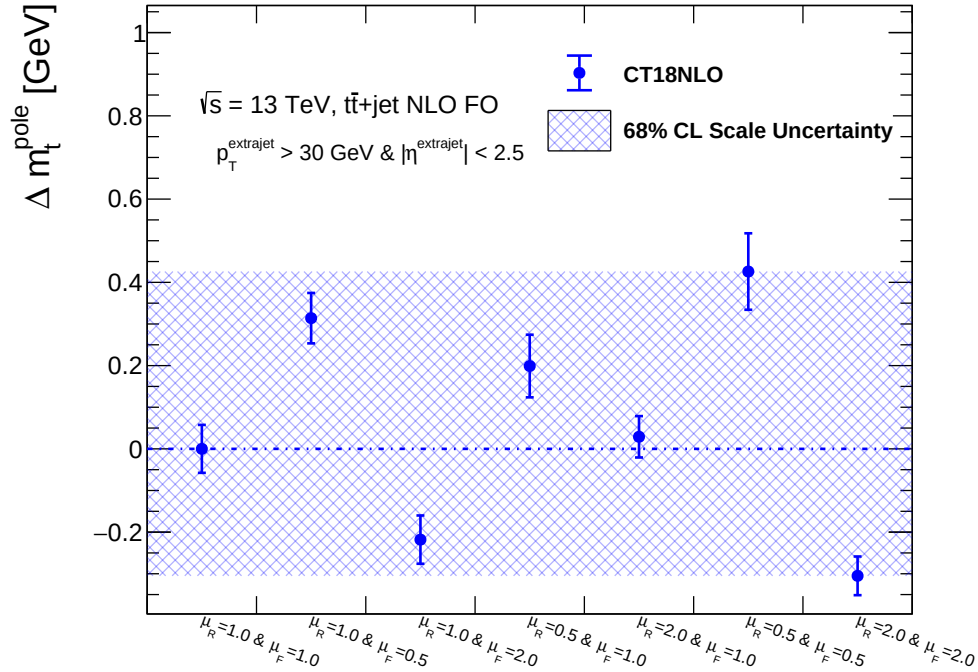


Figure 9.4: The top quark pole mass variation associated with each of the seven combinations of the  $\mu_R$  and  $\mu_F$  scales. The blue band corresponds to the total  $\Delta m_t^{\text{pole}}(\text{scale})$  uncertainty at a 68% CL interval.

## 9.3 Measurement of the top quark pole mass: Expected precision

This section presents the value of the top quark pole mass extracted from the  $\mathcal{R}_{\text{Asimov}}^{t\bar{t}+\text{jet}}$  unfolded distribution along with its total uncertainty, which combines both the fit and the theory uncertainties, obtained as described in Sections 9.1 and 9.2. The corresponding value of  $m_t^{\text{pole}}$  has been extracted using various PDF sets for the calculation of the theory predictions and their associated uncertainties. The resulting top quark pole mass extracted from the Asimov dataset for the nominal PDF set, CT18NLO, as well as for the alternative PDF sets NNPDF3.0 [215], PDF4LHC21 [216], and ABMP16NLO [217], are:

**CT18NLO:**

$$m_t^{\text{pole}} = 173.09 \pm 0.69 (\text{fit})_{-0.21}^{+0.34} (\text{PDF} + \alpha_S)_{-0.31}^{+0.43} (\text{scale}) \text{ GeV} \quad , \quad (9.8)$$

**NNPDF3.0:**

$$m_t^{\text{pole}} = 172.93 \pm 0.69 (\text{fit}) \pm 0.45 (\text{PDF} + \alpha_S)_{-0.50}^{+0.37} (\text{scale}) \text{ GeV} \quad , \quad (9.9)$$

**PDF4LHC21:**

$$m_t^{\text{pole}} = 173.07 \pm 0.70 (\text{fit})_{-0.29}^{+0.31} (\text{PDF} + \alpha_S)_{-0.47}^{+0.37} (\text{scale}) \text{ GeV} \quad , \quad (9.10)$$

**ABMP16NLO:**

$$m_t^{\text{pole}} = 172.84 \pm 0.67 (\text{fit})_{-0.17}^{+0.22} (\text{PDF} + \alpha_S)_{-0.29}^{+0.32} (\text{scale}) \text{ GeV}. \quad (9.11)$$

The results obtained from fitting the unfolded Asimov dataset distribution with theory predictions generated using different PDF sets are compatible within the  $\text{PDF} + \alpha_S$  theory uncertainties. Nevertheless, the highest precision is obtained when using the predictions produced with the CT18NLO and the ABMP16NLO PDF sets.





# Chapter 10

## Summary and conclusions

The top quark is the most massive elementary particle in the SM, which makes it play an important role in this theory and many of its extensions. As a free parameter of the SM, the top quark mass cannot be derived from first principles and has to be determined experimentally. Physics analyses that seek to determine the top quark mass can be classified into two categories, depending on the strategy adopted to measure this parameter: direct measurements and indirect measurements.

Direct measurements are based on the reconstruction of the kinematic properties of the final-state decay products of the top quark, from which observables sensitive to its mass are derived. While these methods have reached uncertainties in the top quark mass of  $\mathcal{O}(500)$  MeV, they rely on MC generators to describe non-perturbative QCD effects. Consequently, the value extracted from these measurements for the top quark MC mass parameter in the generator,  $m_t^{\text{MC}}$ , cannot be directly interpreted as the top quark mass parameter in the SM Lagrangian. One of the observables used to determine  $m_t^{\text{MC}}$  is the  $M_{lb}$  observable, which is defined as the invariant mass of the lepton and the  $b$ -jet associated with a leptonically decaying top quark.

Indirect measurements are based on observables that are sensitive to the top quark mass, but for which it is possible to calculate the associated distributions in a well-defined renormalization scheme. These measurements can be directly interpreted as the top quark mass parameter in the SM Lagrangian. In the on-shell renormalization scheme, these methods have achieved uncertainties of  $\mathcal{O}(1)$  GeV in the measurement of the so-called top quark pole mass,  $m_t^{\text{pole}}$ . One of such

observables used to determine  $m_t^{\text{pole}}$  is the  $\mathcal{R}(\rho_s)$  observable, which is defined in  $t\bar{t}$  +jet topologies as:

$$\mathcal{R}(\rho_s) = \frac{1}{\sigma_{t\bar{t}+\text{jet}}} \frac{d\sigma_{t\bar{t}+\text{jet}}}{d\rho_s}, \quad \rho_s = \frac{2m_0}{\sqrt{s_{t\bar{t}+\text{jet}}}} \quad (10.1)$$

This thesis presents the current development status of a top quark pole mass measurement using semileptonically decaying top quark pair events produced in association with at least one energetic jet ( $t\bar{t}$  +jet). Additionally, the top quark mass parameter in the MC ( $m_t^{\text{MC}}$ ) is also measured using top quark pair events produced without additional jets ( $t\bar{t}$ ). This analysis is performed using the  $pp$  collision data at 13 TeV collected by the ATLAS experiment at the LHC during Run 2 (2015-2018), which corresponds to an integrated luminosity of  $140 \text{ fb}^{-1}$ . As the final results using the recorded collision data are not yet approved for unblinding by the ATLAS collaboration, the results presented in this thesis are reported using a simulated dataset. Therefore, they correspond to the expected sensitivity of the analysis rather than the actual measured value.

The analysis starts with the identification of events with signatures that are compatible with originating from a  $t\bar{t}$  or  $t\bar{t}$  +jet event decaying semileptonically. To do so, events at the detector containing object candidates for a lepton ( $e$  or  $\mu$ ), 4 or more jets with at least one passing the  $b$ -tagging DL1r algorithm at 70% WP, and a significant amount of missing transverse energy, are selected. In the events compatible with originating from a  $t\bar{t}$  +jet process, the variable of interest is  $\rho_s$ , while for events that are only compatible with originating from a  $t\bar{t}$  process, and not  $t\bar{t}$  +jet, which corresponds with events with exactly four jets, the variable of interest is  $M_{lb}$ .

The reconstruction of the  $t\bar{t}$  +jet system and the lepton+ $b$ -jet system in  $t\bar{t}$  events is performed using a machine learning model developed within the SPA-NET framework. The performance of this machine learning model in the reconstruction of these event topologies outperformed any of the alternative kinematic-based reconstruction algorithms tested. This is one of the first times a ML model constructed within the SPA-NET framework is going to be applied to recorded data, and due to its unparalleled performance, it is a promising candidate to become the preferred method for reconstructing top quark events in forthcoming analyses.

Once the  $\rho_s$  and the  $M_{lb}$  variables are reconstructed, the events are divided into four orthogonal analysis regions based on their jet and  $b$ -tagged jet multiplicities and a set of final event selection requirements are imposed to enhance the fraction of correctly matched events in each of the regions.

Using these four regions, a profiled maximum likelihood fit is performed to extract  $m_t^{\text{MC}}$  and unfold the detector level  $\rho_s$  distribution to parton level, thereby extracting the  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  distribution. The expected level of precision for the determination of the top quark MC mass parameter is:

$$\Delta m_t^{\text{MC}}(\text{total}) \simeq 0.41 \text{ GeV} \quad (10.2)$$

where the uncertainty includes both the statistical and the systematic modeling uncertainties. A similar level of precision is expected when performing the fit over recorded data. The projected level of precision is highly competitive, being similar to the precision achieved in various analyses conducted by the ATLAS and CMS collaborations in the semileptonic decay channel [222, 223].

The unfolded  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  parton level distribution obtained from the profile likelihood fit is used to extract the top quark pole mass. This is achieved through a  $\chi^2$  fit, where the  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  distribution is compared with a series of  $t\bar{t} + \text{jet@NLO}$  fixed-order theory predictions generated using different values of  $m_t^{\text{pole}}$ , ranging from 166 to 179 GeV. Four distinct collections of theory predictions are computed using the parton density functions (PDF) sets CT18NLO, NNPDF3.0, PDF4LHC21, and ABMP16NLO. The resulting top quark pole mass extracted from the Asimov dataset generated with  $m_t^{\text{MC}} = 172.50 \text{ GeV}$ , and using the theory predictions computed with the two PDF sets that yield the highest level of precision are:

$$\begin{aligned} m_t^{\text{pole}} &= 173.09 \pm 0.69 \text{ (fit)}_{-0.21}^{+0.34} \text{ (PDF} + \alpha_s)_{-0.31}^{+0.43} \text{ (scale) GeV} \\ &= 173.09_{-0.78}^{+0.88} \text{ GeV} \quad , \end{aligned} \quad (10.3)$$

when using the CT18NLO PDF set, and

$$\begin{aligned}
m_t^{\text{pole}} &= 172.84 \pm 0.67 \text{ (fit)}_{-0.17}^{+0.22} \text{ (PDF} + \alpha_s)_{-0.29}^{+0.32} \text{ (scale) GeV} \\
&= 172.84_{-0.75}^{+0.77} \text{ GeV} \quad ,
\end{aligned}
\tag{10.4}$$

when using the ABMP16NLO PDF set.

The fit uncertainty includes both the statistical and all the systematic uncertainties, while the theory uncertainty is divided into two components: the uncertainty associated with the PDF set and  $\alpha_s$  value used in the calculations, and the uncertainty associated with the variations of the  $\mu_R$  and  $\mu_F$  scales in the calculations. The expected level of precision in the measurement of  $m_t^{\text{pole}}$  extracted from the  $\chi^2$  fit to the unfolded Asimov  $\mathcal{R}$  distribution is dominated by the fit uncertainty. The main contributions to this uncertainty originate from jet-related experimental systematic uncertainties and the modeling systematic uncertainties of the  $t\bar{t}/t\bar{t} + \text{jet}$  process.

Compared to previous  $m_t^{\text{pole}}$  measurements performed using the  $\mathcal{R}$  observable [7, 93, 94], the methodology described in this thesis has the potential to achieve the most precise determination of the top quark pole mass in  $t\bar{t} + \text{jet}$  event topologies, once it is applied over the recorded ATLAS dataset. In comparison with the 8 TeV measurement performed by the ATLAS collaboration in the semileptonic decay channel [7], the present analysis exhibits a reduction in statistical, systematic, and theory uncertainties.

The improvement in the systematic uncertainty is primarily attributed to two factors: Firstly, the improved reconstruction of the  $t\bar{t} + \text{jet}$  system performed by the SPA-NET ML model. Secondly, the implementation of the profile likelihood technique, which allows the use of multiple signal regions in the analysis and the inclusion of control regions to measure  $m_t^{\text{MC}}$ , mitigating the effect of this parameter during the unfolding.

The improvement in the theory uncertainties is primarily attributed to the use of the dynamic scales instead of a fixed scale in the calculation of the  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  theory distributions, as the use of the dynamical scale highly reduces the effects of the scale variations [90, 221].

## Prospects for future analyses

Since the level of precision expected from the analysis presented in this thesis is dominated by the jet-related experimental systematic uncertainties and the modeling systematic uncertainties of the  $t\bar{t}/t\bar{t} + \text{jet}$  process, possible improvements could be obtained from reducing these sources of uncertainties.

The jet-related experimental systematic uncertainties can be reduced by combining the semileptonic decay channel of the top pair system with the dileptonic decay channel. Since the reconstruction of the  $\rho_s$  variable in the dileptonic decay channel only requires  $n_{\text{jets}} \geq 3$ , instead of  $n_{\text{jets}} \geq 5$  necessary in the semileptonic channel, it is expected that the reconstruction of this variable would be less affected by jet uncertainties in the dileptonic channel.

These two decay channels can be combined using the profile likelihood statistical model constructed for the current analysis. The combination would consist of adding the distributions of  $\rho_s$  and  $M_{lb}$  reconstructed in the dileptonic channel as additional signal and control regions in the statistical model. Subsequently, the analysis would be carried out as in the case presented in this thesis.

In order to reduce the impact of the systematic modeling uncertainties, a more refined approach to handle them can be adopted. For instance, a potential approach to improve the parton shower, hadronization, and fragmentation modeling uncertainty is by tuning the  $t\bar{t}$  HERWIG 7 sample using the ATLAS 13 TeV data. Alternatively, this uncertainty could be estimated by varying the parameters that govern the fragmentation functions in PYTHIA 8 within their uncertainties.

The impact of the subdominant theory uncertainties can be reduced through various strategies. Firstly, the calculation of the  $t\bar{t} + \text{jet}$  process at NNLO has the potential to decrease the scale uncertainties. Secondly, improvements in the precision of the PDF sets and a more precise measurement of  $\alpha_s$  would reduce their associated uncertainties. Lastly, it's essential to include a rigorous treatment of the cross section enhancement at the production threshold of the  $t\bar{t}$  pair due to the formation of a pseudo-bound-state between these two quarks, as these corrections are currently absent in the theory calculations [224, 225].

Finally, considering that the contribution of the statistical uncertainty to the total uncertainty is minor, the expected increase in the recorded luminosity by

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the ATLAS detector would not inherently result in a significant reduction in the uncertainty of the measurements.

# Appendix A

## Custom boosted $W/Z$ jet tagger for the large- $R$ jet in-situ analysis

The large- $R$  jets originated from the hadronic decay of a heavy resonance have a different distribution of energy inside the jet than the ones originated from a single quark or gluon. This difference is reflected in some jet substructure variables that can then be used to construct tagging algorithms to distinguish large- $R$  jets with respect to their origin. The nominal large- $R$  jet taggers for  $W/Z$  bosons used by the ATLAS collaboration can not be applied in this analysis because they have a big dependence on the jet mass that would bias the jet mass distribution, invalidating any JMS and JMR measurements extracted from it. To avoid this bias, a custom tagger for large- $R$  jets coming from an hadronically decaying  $W/Z$  boson has been developed for the forward folding analysis of Section 4.8.3. Several jet substructure variables have been tested for the construction of this tagger. The variables that have been observed to provide the biggest discriminant power between the  $W/Z$ +jets signal and the multijet background, without introducing a significant bias in the jet mass distribution, are  $D_2$  [226] and the number of tracks associated with the jet,  $N_{\text{trk}}$ .

The  $D_2$  variable is constructed from the ratio of two Energy Correlation Functions<sup>1</sup> and it is designed to distinguish between one- and two-prong jets<sup>2</sup>.  $D_2$  takes small values for two-prong jets and large values for one-prong jets. In

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<sup>1</sup>The Energy Correlation Functions (ECFs) are calculated from the angular energy correlation between all the particles inside a jet. There are different ECFs depending on the power of the angular dependence.

<sup>2</sup>*Prongs* refers to the number of partons that are captured within the jet.

the context of the in-situ analysis of this thesis, this variable has a high tagging power since the large- $R$  jets originating from boosted  $W/Z$  bosons are more likely to have a two-prong structure than the QCD jets from the multijet background. A cut based tagging algorithm designed to identify boosted  $W$  bosons using the  $D_2$  variable was proposed in Ref. [144]. The algorithm imposes a cut in the  $D_2$  variable that increases with the  $p_T$  of the jet in order to keep a constant signal efficiency across the full  $p_T$  range. The algorithm provides two different working points called *Medium* and *Tight*, with a 50% and 25% signal efficiency, respectively. For the nominal selection of this analysis the *Medium* working point is used whereas the *Tight* working point is used to estimate the uncertainty associated with this choice. In the  $p_T$  interval between 500 GeV and 1.2 TeV, the  $D_2$  cut of the *Medium* and *Tight* working points vary from 1.2 to 1.6 and from 0.9 to 1.2, respectively.

The number of tracks inside a jet ( $N_{\text{trk}}$ ) is the second jet substructure variable used to construct the custom  $W/Z$  jet tagger used in the forward folding analysis. Since the multijet background contains a significant contribution of gluon jets and the multiplicity of charged hadrons inside a gluon initiated jet is, on average, higher than the one for a quark initiated jet with the same  $p_T$  [149], the  $N_{\text{trk}}$  variable is expected to have a significant discriminant power between the signal and the background. In addition, the discrimination power of this variable increases after the  $D_2$  cut is applied [227]. It would be desirable to use a fix  $N_{\text{trk}}$  cut for all the events in the sample, but the  $N_{\text{trk}}$  distribution has been found to have a significantly lower average value for the events in the 2015+2016 data taking periods than for 2017 one. This difference is due to the increase in the average number of collisions per bunch crossing (pile-up) in 2017 period respect to the previous years. To take this effects into account, two different nominal values for the  $N_{\text{trk}}$  cut are set for the two periods. The nominal values are chosen to minimize the impact of the difference in the pile-up conditions on the cut, and two up/down variations are chosen to cover for the uncertainty associated to this choice. For the 2015+2016, period the events are required to have  $N_{\text{trk}} < 25_{-2}^{+3}$ , while for the 2017 period they are required to have  $N_{\text{trk}} < 30_{-3}^{+5}$ .

The custom  $W/Z$  jet tagger is then constructed by applying the cuts in the  $D_2$  and  $N_{\text{trk}}$  variables described above. The normalized distributions of  $D_2$  for the  $W/Z$ +jets signal and the multijet background after the basic event requirements, but without applying any cut in  $N_{\text{trk}}$ , are shown in Figure A.1. This Figure shows the discriminant power of the  $D_2$ . No dependence on the data taking period is



observed. Figure A.2 shows the normalized distributions of  $N_{\text{trk}}$  for the  $W/Z$ +jets signal and the multijet background after the basic event requirements and the *Medium* working point cut in the  $D_2$  variable have been imposed. As expected, this variable also has a significant discriminant power between the signal and the background. The dependence of the  $N_{\text{trk}}$  distribution with respect of the data taking period is clearly visible in this figure. Other variables such as the subjetiness  $\tau_{21}$  were also tested for constructing the  $W/Z$  jet tagger, but despite its large discriminant power, it introduced a bias in the jet mass, so it was not included in the final version of the tagger.

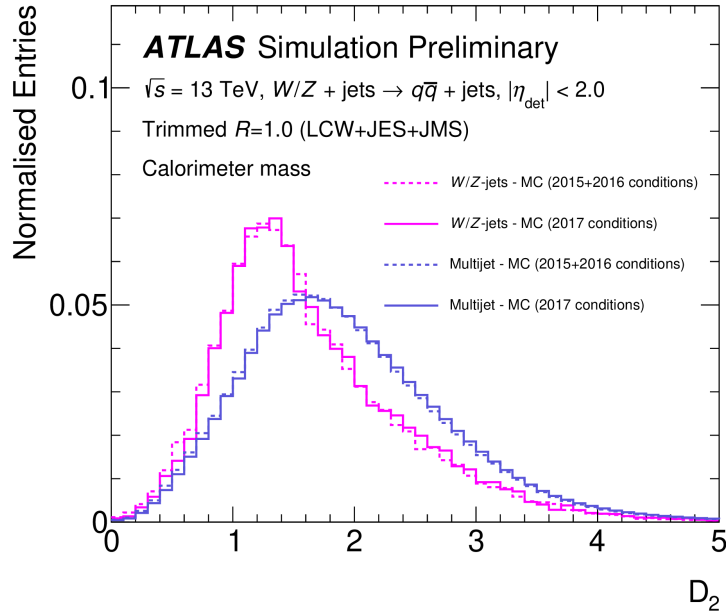


Figure A.1: The  $D_2$  distribution for the  $W/Z$ +jets signal and the multijet background after the basic preselection of the in-situ analysis of Section 4.8.3 is applied.

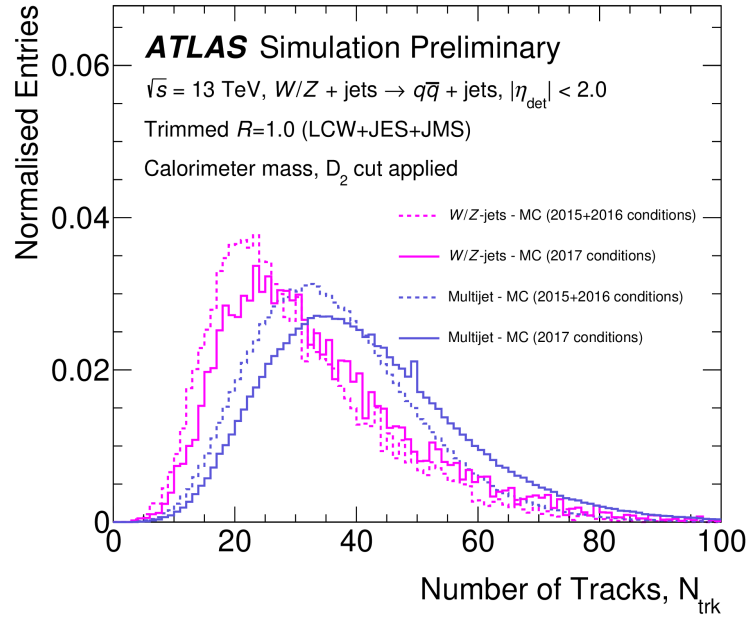


Figure A.2: The  $N_{\text{trk}}$  distribution for the  $W/Z$ +jets signal and the multijet background after the basic preselection and the  $D_2$  *Medium* working point cut are applied.

## Appendix B

# Breakdown of the JMS and JMR uncertainties of the large- $R$ jet in-situ analysis

This appendix contains the breakdown of the total uncertainty associated to the JMS and JMR measurements for calorimeter jets obtained using  $W/Z$ +jets events, the blue data points in Figure 4.12 of Section 4.8.3. The statistical uncertainty associated to the overall procedure is estimated by creating pseudo-data distributions obtained by varying independently each bin of the measured mass distributions within their statistical uncertainties (pseudo-experiments).

There are five different sources of systematic uncertainties considered in this analysis named as: modeling, detector, normalization,  $D_2$ , and  $N_{\text{trk}}$ . The modeling uncertainty is estimated by repeating the fit procedure using HERWIG++ 2.7.1 instead of SHERPA for the  $W/Z$ +jets signal modeling, and then using SHERPA instead of PYTHIA 8 for the background modeling. The absolute difference between the measured JMS/JMR when using the alternative samples and the nominal ones is symmetrized, added in quadrature for the two independent variations (signal and background), and taken as the model uncertainty. The detector uncertainty is evaluated by varying the jet energy response (JES/JER) within their uncertainties and then repeating the fit for the resulting distributions. The  $D_2$  and  $N_{\text{trk}}$  uncertainties are estimated as explained in Appendix A, they cover the uncertainties related to the custom  $W/Z$  jet tagger. The so called *normalization* uncertainty is considered to cover the relative normalization of the

$W/Z$ +jets signal respect to the background. This uncertainty is estimated by varying the  $W/Z$ +jets cross section within their uncertainties ( $\sim 24\%$  for  $W/Z$ +jet events with at least one jet [228]) and then repeating the fit.

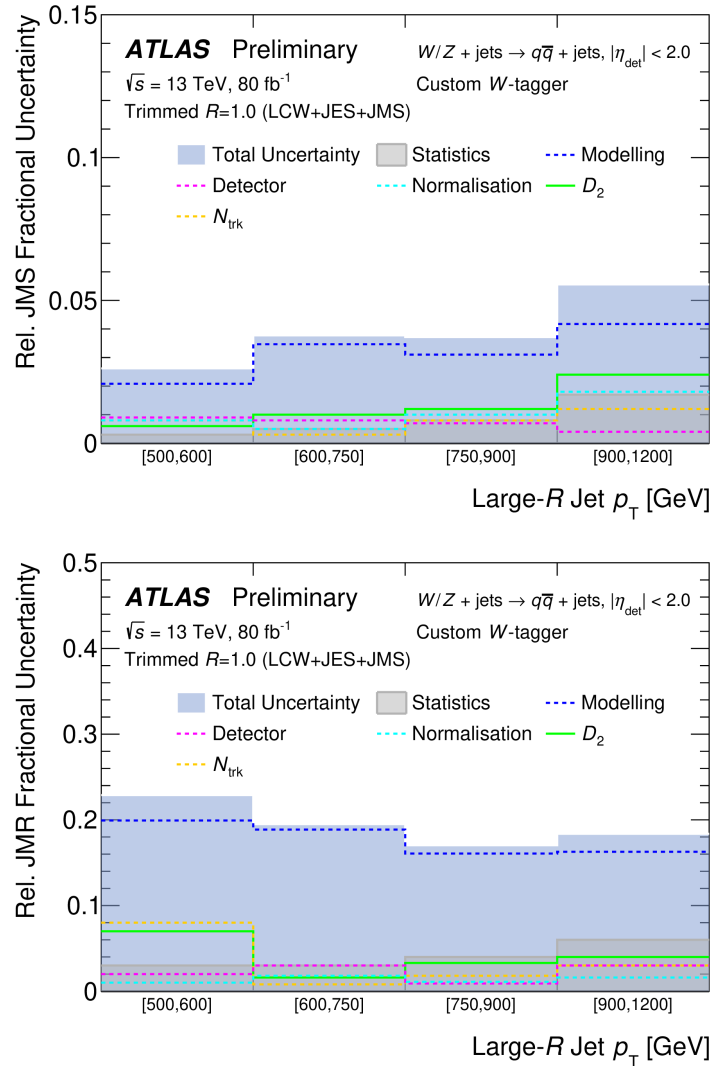


Figure B.1: Breakdown of the uncertainties associated to the jet mass scale and resolution for calorimeter jets obtained using  $W/Z$ +jets events (blue points in Figure 4.12). A similar pattern is observed for track-assisted mass jets.

# Appendix C

## Alternative $t\bar{t}$ +jet event reconstruction

This appendix describes two alternative event reconstruction algorithms for the semileptonic decaying  $t\bar{t}$ +jet system. This appendix is organized as follows: Section C.1 describes the reconstruction algorithm used in the ATLAS 7 and 8 TeV measurements of the top quark pole mass using the  $\rho_s$  observable. Section C.2 describes one of the most commonly used methods for the reconstruction of a semileptonic decaying  $t\bar{t}$  system, the KLFITTER algorithm. At last, Section C.3 contains a study performed to optimize the performance of the KLFITTER algorithm by applying a cut in the  $-\ln L$  of this reconstruction.

### C.1 $t\bar{t}$ +jet system reconstruction from the 7 and 8 TeV analyses

The algorithm used in the 7 and 8 TeV analyses [7, 93] to reconstruct the  $t\bar{t}$ +jet system performs the full reconstruction of the four-momenta of the two top candidates in the event. To do so, the algorithm reconstructs and associates the decay products of each top quark, the  $b$ -jets, and the  $W$  bosons. Only events with exactly two  $b$ -tagged jets are considered in this reconstruction.

In the semileptonic decay of a  $t\bar{t}$  system, one of the  $W$  bosons decays leptonically into a lepton and a neutrino ( $W \rightarrow l\nu$ ). The leptonic  $W$  boson candidate is reconstructed by combining the selected charged lepton and the

reconstructed neutrino. The component along the beam axis of the neutrino momentum,  $p_z^\nu$ , is unknown. To reconstruct it, a constrain on the mass of the  $W$  boson is assumed, which leads to the following equation:

$$(M_W^{leptonic})^2 = m_l^2 + 2(E_l E_\nu - \vec{p}_l \vec{p}_\nu) = (M_W^{PDG})^2 \quad (\text{C.1})$$

where  $l$  indicates the charged lepton,  $\nu$  indicates the neutrino and  $M_W^{PDG}$  is the value of the  $W$  boson mass reported by the particle data group (PDG) [4]. In this nomenclature, the four-momentum of a particle  $a$  is written as  $p_a = (E_a, \vec{p}_a)$ . Equation C.1 is a second-order equation for the  $p_z^\nu$  component. Depending on the value of the radicand in the determinant of this equation, up to two solutions can exist for  $p_z^\nu$ . If the radicant is positive, two leptonic  $W$  boson candidates are obtained with this procedure, and the solution with the lower value of  $p_z^\nu$  is selected. If the radical is negative, instead, the magnitude  $E_T^{\text{miss}}$  is adjusted to get a null radicand, and only one leptonic  $W$  boson is reconstructed.

The second  $W$  boson coming from the decay of the  $t\bar{t}$  system decays hadronically into a pair of quarks ( $W \rightarrow q\bar{q}$ ). To reconstruct the hadronically decaying  $W$  boson, all the different permutations of two not  $b$ -tagged jets are considered. For each pair of jets  $(i, j)$ , its invariant mass,  $m_{ij}$ , and its angular distance,  $\Delta R_{ij} = \sqrt{\Delta\phi(i, j)^2 + \Delta\eta(i, j)^2}$ , are calculated. Then, to reduce the combinatorial background (events with miss-matched jets-to-partons), minimize the effects of jet energy corrections on light jets, and improve the mapping of reconstructed hadronic  $W$  boson candidates to truth level  $W$  bosons, only pairs that satisfy the following criteria are selected:

- $0.9 < \alpha < 1.25$ , with  $\alpha = \frac{M_W^{PDG}}{m_{ij}}$
- $\Delta k_T^{ij} = \min(p_T^i, p_T^j) \cdot \Delta R_{ij} < 90 \text{ GeV}$

These criteria significantly reduce the amount of wrong jet pairing in the reconstruction, ensuring that the  $W$  boson candidate is reasonably well reconstructed. Then, the  $\alpha$  factor is used to correct the four-momenta of the light jets that come from the  $W$  decay. This ensures that the hadronic  $W$  boson

candidate has the proper mass, as defined in the PDG.

Among all the remaining possible combinations of hadronic and leptonic  $W$  boson candidates, the one that minimizes the criteria in Equation C.2 is selected. This selects the combination where the two reconstructed top quark candidates have the smallest difference between their kinematical masses. This is not a direct constrain in the top quark mass, and as discussed in Ref. [93], it does not introduce any bias in the extracted top quark mass.

$$\beta' = \frac{M_{t_{lep}} - M_{t_{had}}}{M_{t_{lep}} + M_{t_{had}}} \quad (\text{C.2})$$

The additional extra jet, which is needed to reconstruct the  $t\bar{t}$  +jet system, is selected from all the remaining jets that have not been used to reconstruct the top quark candidates. The discarded jets include the two light jets associated with the hadronically decaying  $W$  boson and the two  $b$ -tagged jets in the event. Among the remaining jets, the one with the leading  $p_T$  is chosen. The event is accepted if the additional jet satisfies the conditions:

- $p_T^{extrajet} > 30 \text{ GeV}$
- $|\eta^{extrajet}| < 2.5$

At last, to reject background events and enhance the purity of the sample, the following requirement is applied:

$$\frac{M_{t_{lep}}}{M_{t_{had}}} > 0.9 \quad (\text{C.3})$$

The reconstruction described in this section is only used for regions with five or more jets, from which exactly two of them are  $b$ -tagged. The resulting  $\rho_s$  distribution obtained after the reconstruction and the cuts in the  $\alpha$  and  $\beta$  variables defined in this section are applied is shown in Figure C.1. A good Data/MC agreement is observed in this and all other control plot variables, including the kinematic variables of the reconstructed  $t\bar{t}$  system.

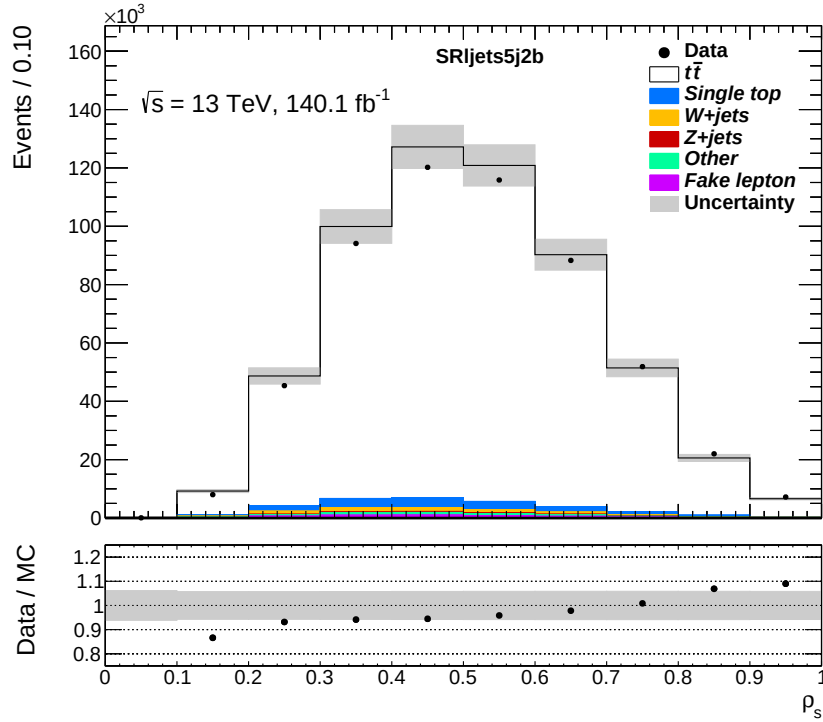


Figure C.1: Data/prediction agreement for the  $\rho_s$  observable in the  $t\bar{t}$  +jet system using the reconstruction algorithm employed in the 7 and 8 TeV analysis.

In Figure 7.10 of Section 7.4, the resolution of  $\rho_s$  obtained using this reconstruction is compared with the one obtained using KLFITTER and the SPA-NET ML model. As the SPA-NET ML model is the best-performing algorithm, this reconstruction is only used as a cross-check.

## C.2 $t\bar{t}$ +jet system reconstruction using the KLFitter algorithm

KLFITTER is a likelihood-based reconstruction algorithm where the four-vectors of the measured objects in an event are used to fit them to the kinematical properties of a given model signature [191]. In the case of a semileptonic decaying  $t\bar{t}$  system, it can be used to select the jet-to-parton assignment and to perform the full event reconstruction. In this event topology, the likelihood takes the following form:



$$\begin{aligned} \mathcal{L} = & \text{BW}(m_{q_1 q_2 q_3} | m_t, \Gamma_t) \cdot \text{BW}(m_{q_1 q_2} | m_W, \Gamma_W) \cdot \text{BW}(m_{q_4 \ell \nu} | m_t, \Gamma_t) \cdot \text{BW}(m_{\ell \nu} | m_W, \Gamma_W) \cdot \\ & \cdot \prod_{i=1}^4 W_{\text{jet}}(E_i^{\text{meas}} | E_i) \cdot W_{\ell}(E_{\ell}^{\text{meas}} | E_{\ell}) \cdot W_{\text{miss}}(E_x^{\text{miss}} | p_x^{\nu}) \cdot W_{\text{miss}}(E_y^{\text{miss}} | p_y^{\nu}) \end{aligned} \quad (\text{C.4})$$

The objects used in Equation C.4 are marked with indices  $q_i$  for each of the  $i$  quarks of the  $t\bar{t}$  decay,  $\ell$  for the charged lepton,  $\nu$  for the neutrino and,  $E_x^{\text{miss}}(E_y^{\text{miss}})$  for the  $x(y)$  measured component of the missing transverse energy. The  $W_x(E_x^{\text{meas}} | E_x)$  terms represent transfer functions for the measured object  $x$ . These functions are probability distributions that model the detector effects and allow the energies of the objects to float within the detector resolution. They map the response of calibrated reconstructed objects onto that of the true associated particles. They are derived from MC and depend on the object type and the  $\eta$ -region. The  $\text{BW}(m_{ij(k)} | m_P, \Gamma_P)$  terms represents Breit-Wigner functions for the particle  $P$ . These functions are probability distributions used to model the resonances of unstable particles. They provide constraints based on the  $W$  boson mass and width ( $m_W, \Gamma_W$ ) and, optionally, on the top-quark mass and width ( $m_t, \Gamma_t$ ).

In Equation C.4, the mass and width of the  $W$  boson are set to the PDG values,  $m_W = 80.4$  GeV and  $\Gamma_W = 2.1$  GeV. The top quark mass is left as a free parameter of the model, and the top quark decay width is fixed to the LO SM prediction corresponding to the fitted top mass. As this reconstruction does not assume a prior value of the top quark mass, it does not introduce any bias in the extraction of this parameter.

From all the possible permutations of the jets, the ones where a  $b$ -tagged jet is associated with a jet of the  $W$  boson hadronic decay are vetoed. Then, for the remaining permutations, the configuration of the parameters that minimize the negative log-likelihood  $-\ln L$  is calculated. The permutation with the lowest  $-\ln L$  is selected as the best permutation and used in the analysis.

The additional extra jet, which is needed to reconstruct the  $t\bar{t}$  +jet system, is selected from all the remaining jets that have not been used in the reconstruction of the top quark candidates. Among the remaining jets, the one with the leading  $p_T$  is chosen. The event is accepted if the additional jet satisfies the conditions:

- $p_T^{\text{extrajet}} > 30$  GeV

- $|\eta^{\text{extrajet}}| < 2.5$

At last, the condition in Equation C.5 is applied to reject events with a large value of  $-\ln L$ . This cut improves the jet-to-parton matching and the resolution in the  $\rho_s$  observable. A dedicated study to optimize this cut can be found in Section C.3.

$$-\ln L < 46 \tag{C.5}$$

The reconstruction algorithm described in this section can be applied to all control and signal regions in the analysis, CRLjets4j1b, CRLjets4j2b, SRLjets5j1b and SRLjets5j2b. The resulting  $\rho_s$  and  $M_{lb}$  distribution obtained before and after the cuts in  $-\ln L$  are shown in Figures C.2 and C.3. These distributions are shown only for the signal and control regions with exactly two  $b$ -tagged jets, SRLjets5j2b and CRLjets4j2b. A good Data/MC agreement is observed in this and in all other control plot variables, including the kinematic variables of the reconstructed  $t\bar{t}$  system.

In Figure 7.10 of Section 7.4, the resolution of  $\rho_s$  obtained using this reconstruction is compared with the one obtained using the 8 TeV reconstruction algorithm and the SPA-NET ML model. As the SPA-NET ML model is the best-performing algorithm, this reconstruction is only used as a cross-check.

### C.3 Optimization of the $-\ln L$ cut in the KLFitter reconstruction

In this section, the selection in the case of performing the reconstruction of the  $t\bar{t}$  system using the KLFITTER algorithm described in the previous section is optimized with respect to the likelihood of the reconstruction.

To reconstruct the  $t\bar{t}$  system, the KLFITTER algorithm has to identify the jets corresponding to each of the partons of the top decays. To evaluate the performance in this task, the generator-level information from the MC simulation is used to perform the matching of each parton-level object with its corresponding jet at detector level (if it exists). The generator-level matching is performed with

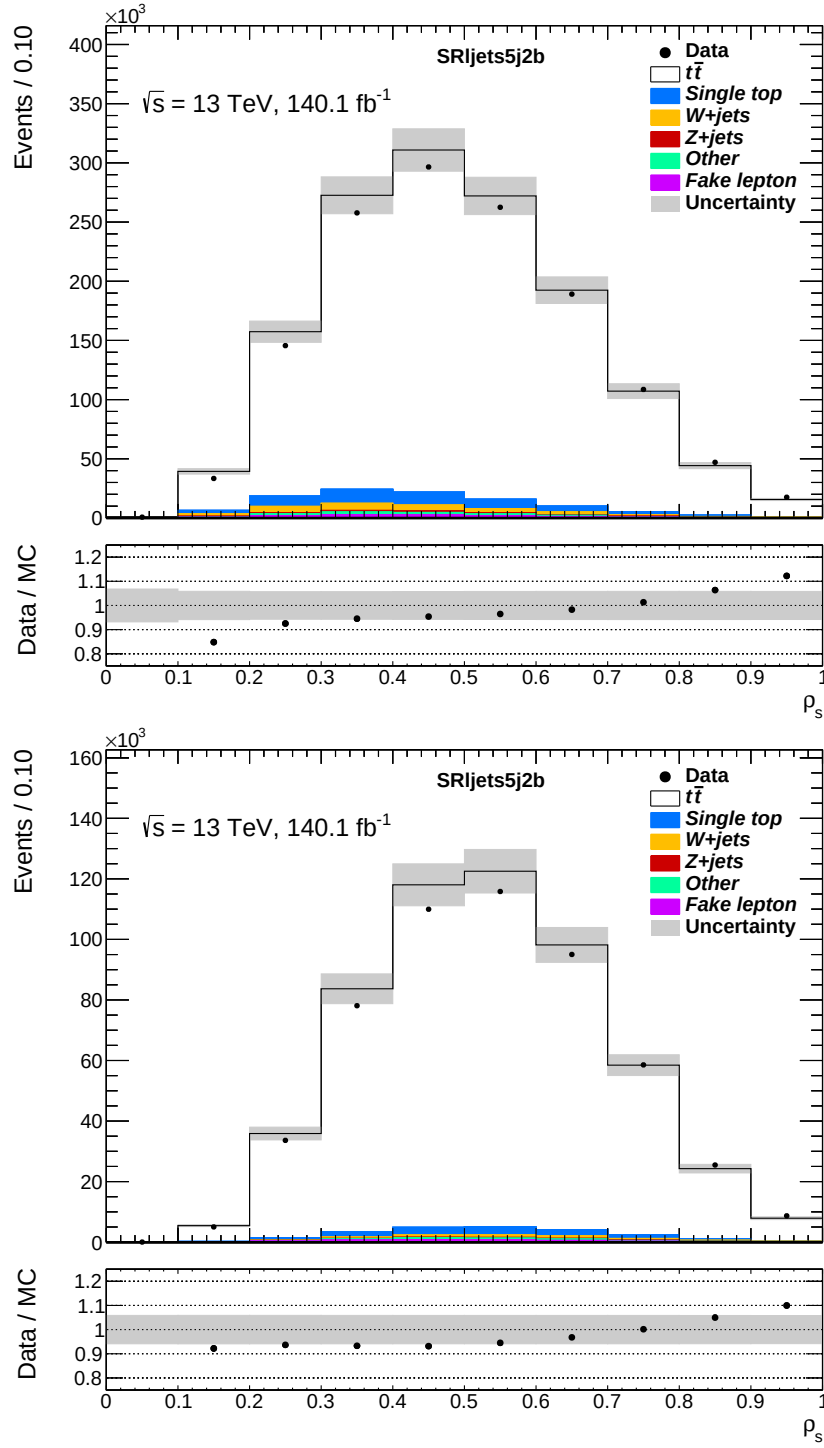


Figure C.2: Data/prediction agreement for the  $\rho_s$  observable in the SRljets5j2b region reconstructed using the KLFITTER algorithm. The top plot shows the distribution before any cut in  $-\ln L$  is applied, while the bottom plot shows the distribution after applying the final event selection, which requires  $-\ln L < 46$ .

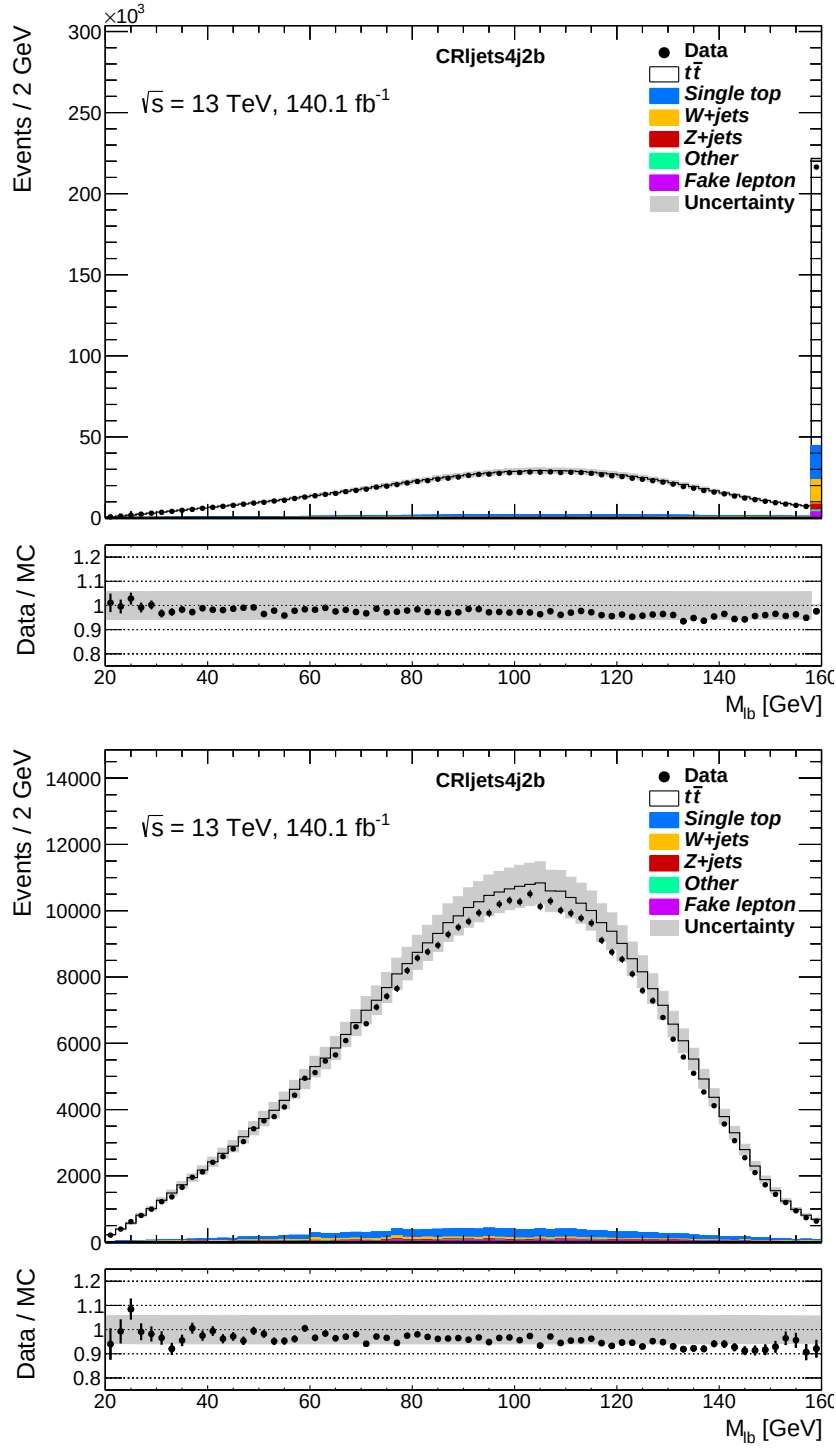


Figure C.3: Similar to Figure C.2, but for the  $M_{lb}$  variable in the CRIjets4j2b. The final event selection includes the requirement  $20 < M_{lb} < 160$ .

the geometrical criterion of  $\Delta R(\text{parton}, \text{jet}) < 0.4$ . The reconstructed events are then classified into three different categories, as in the case of the study of the

performance of the SPA-NET ML model. These categories are *correctly matched*, *incorrectly matched*, and *unmatchable* events.

The performance of the reconstruction algorithm can be assessed in terms of the fraction of events found in each category. For the nominal POWHEG +PYTHIA  $t\bar{t}$  sample, the distribution of each of these event categories with respect to the  $\ln L$  obtained with the KLFITTER  $t\bar{t}$  system reconstruction are shown in Figure C.4. This distribution is shown only for the signal regions studied in the analysis. However, the performance over the control regions is very similar. The exclusive selection with  $\rho_{parton} > 0.7$  is studied to evaluate the performance of the event reconstruction algorithms in the most sensitive region of the  $\rho$  to the top-quark mass.

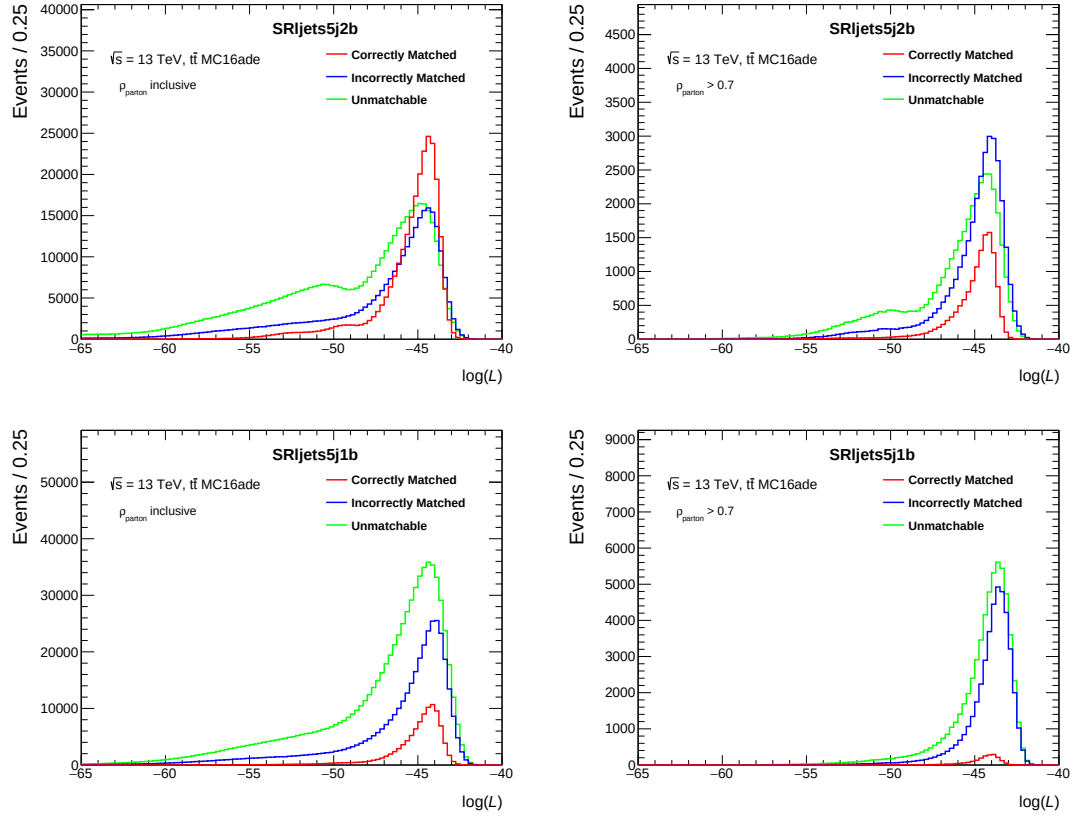


Figure C.4: Distributions of events categorized as *correctly matched*, *incorrectly matched*, and *unmatchable* for the  $\ln L$  variable provided by the KLFITTER algorithm used to reconstruct the  $t\bar{t}$  system.

The results shown in these distributions indicate that the KLFITTER reconstruction algorithm performs relatively well in the 2  $b$ -tagged jet regions,

but performs poorly in the 1  $b$ -tagged jet regions. Moreover, the distributions show that the  $\ln L$  variable has a big discriminating power between the different event categories; thus, an optimized cut in this variable can increase the fraction of *correctly matched* in the sample. After careful consideration, the final choice is to apply a cut in  $\ln L > -46$ . This requirement offers a good balance as it significantly reduces the fraction of *unmatchable* events, while keeping a substantial portion of *correctly matched* events.

## Appendix D

# Complementary information and studies about the SPA-Net model used to reconstruct the $t\bar{t}$ and $t\bar{t}+\text{jet}$ systems

This appendix contains complementary information about the Symmetry Preserving Neuronal Network (SPA-NET) used in Section 7.3 to reconstruct the  $t\bar{t} + \text{jet}$  system and the  $M_{lb}$  variable. This Appendix is organized as follows: In Section D.1, the architecture of the transformer encoder, the core of the attention mechanism in SPA-NET, is presented and described. The specific information about the configuration of the SPA-NET network, such as the details about the low-level structure (number of dimensions, layers, etc), is given in Section D.2. Section D.3 explores the concept of overtraining and the methods employed to prevent it in the ML model developed within this analysis. At last, Section D.2 presents a collection of tables that show the specific numerical results that assess the performance of the ML model in the reconstruction of the  $t\bar{t} + \text{jet}$  system and the  $M_{lb}$  observable across the different signal and control regions considered in the analysis.

## D.1 Architecture of the transformer encoder

The transformer encoder is *half* of a more complex model, the Transformer, a ML architecture formed by a transformer encoder and a transformer decoder that was introduced for the first time by the **Google Brain** team in Reference [229]. The Transformer was originally designed for processing language translation, but as seen in this thesis, its use has been extended to many fields, such as particle physics. The model architecture of the Transformer is shown in Figure D.1, where the encoder and the decoder are represented by the left and right halves, respectively.

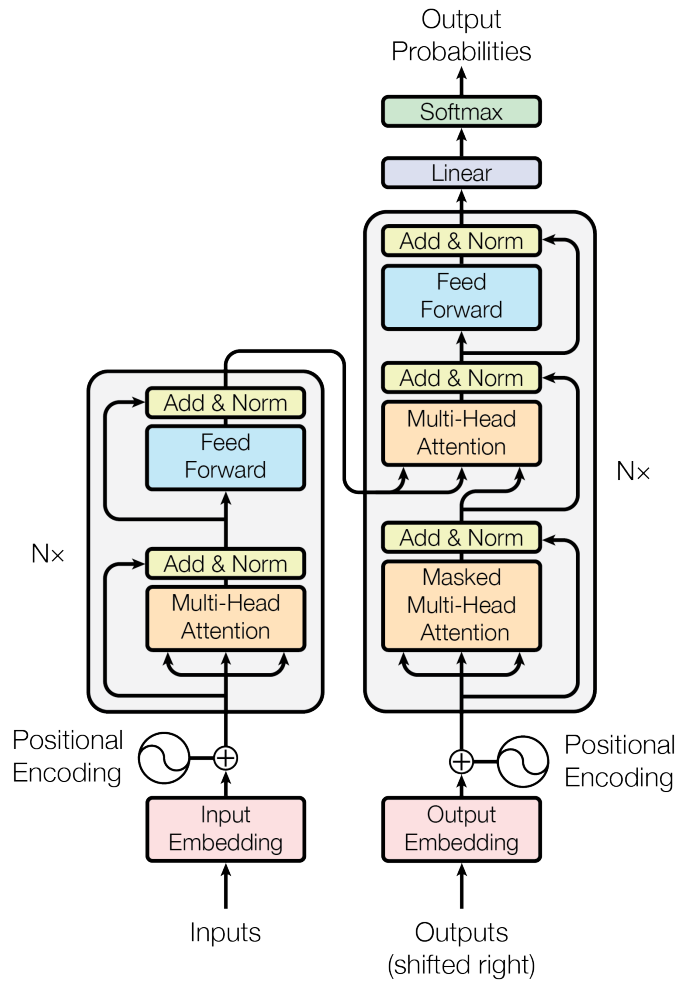


Figure D.1: Model architecture of the Transformer. The left-half of the architecture represents the transformer encoder, whereas the right-half represents the transformer decoder [229].

As discussed in Section 7.3.1, the Transformers generate an output relying only on an attention mechanism, and not on recurrence and convolution. The attention



mechanism is introduced into the Transformer by the Multi-head architecture shown in Figure D.2.

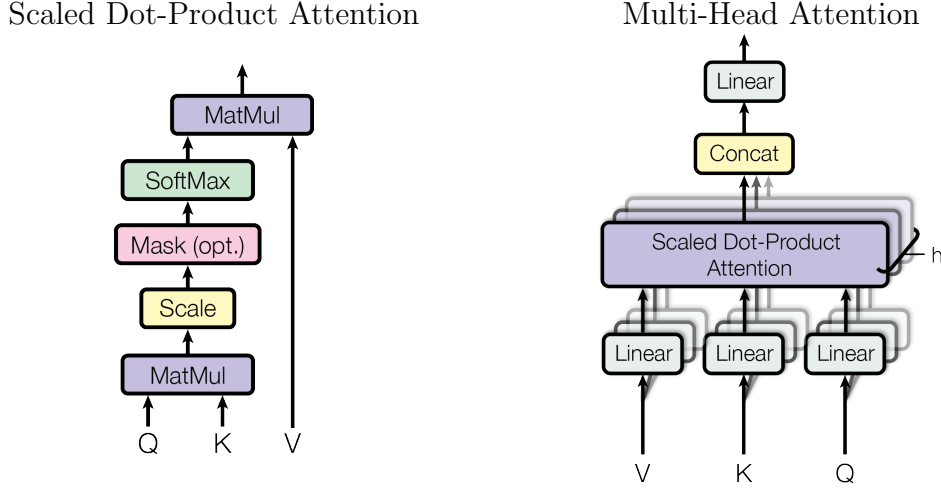


Figure D.2: The Multi-Head Attention architecture (right) is formed by several attention heads running in parallel. Each of these heads uses the Scale Dot-Product Attention (left) to calculate the attention by scaling the value (V) by a function that compares the compatibility between the query (Q) and the corresponding key (K) [229].

## D.2 Hyper-parameters of the SPA-Net model

The hyper-parameters of the  $t\bar{t}$  +jet SPA-NET model include setting the low level characteristics of the network such as the dimension of the transformer, the number of attention heads, the number of regression layers, etc. A full list of the choice of the hyper-parameters can be found in Table D.1.

## D.3 Overtraining study for the SPA-Net model

When a neuronal network has a large number of free parameters, it becomes flexible enough to learn how to describe many of the particularities of the dataset. However, this flexibility may lead the model to learn some trends in the training dataset that are unique and not generalizable to the whole dataset. This overfitting of the network parameters is known as *overtraining*, and it results in an excellent performance over the training dataset. Still, it causes the network

Table D.1: Specific configuration of the SPA-NET used to reconstruct the  $t\bar{t} + \text{jet}$  system.

| Network parameter                   | Value     | Network parameter          | Value |
|-------------------------------------|-----------|----------------------------|-------|
| dropout:                            | 0.1       | num_branch_encoder_layers: | 3     |
| hidden_dim:                         | 64        | num_dataloader_workers:    | 16    |
| initial_embedding_dim:              | 16        | num_detector_layers:       | 2     |
| initial_embedding_skip_connections: | 1         | num_embedding_layers:      | 10    |
| kl_loss_scale:                      | 0.0       | num_encoder_layers:        | 8     |
| l2_penalty:                         | 0.0002    | num_gpu:                   | 4     |
| learning_rate:                      | 0.0015    | num_jet_encoder_layers:    | 2     |
| learning_rate_cycles:               | 1         | num_regression_layers:     | 4     |
| learning_rate_warmup_epochs:        | 1.0       | optimizer:                 | AdamW |
| limit_to_num_jets:                  | 0         | partial_events:            | 1     |
| linear_activation:                  | gelu      | position_embedding_dim:    | 32    |
| linear_block_type:                  | GRU       | regression_loss_scale:     | 1.0   |
| linear_prelu_activation:            | true      | skip_connections:          | 1     |
| mask_sequence_vectors:              | 1         | split_symmetric_attention: | 1     |
| masking:                            | Filling   | train_validation_split:    | 0.95  |
| normalization:                      | LayerNorm | transformer_activation:    | gelu  |
| normalize_features:                 | 1         | transformer_dim:           | 64    |
| num_attention_heads:                | 4         | transformer_dim_scale:     | 2.0   |
| num_branch_embedding_layers:        | 3         | transformer_type:          | Gated |

to perform worse on unseen data (data not used for the training). Some of the most common techniques used to prevent overtraining in ML models are:

- **Regularization:** A weight penalty term is added into the loss function to limit the complexity of the model.
- **Dropout:** During each training iteration, some randomly selected neurons are dropped, causing to effectively train in different networks, which has the net overall effect of reducing the overfitting when considering all the neurons in the model.
- **Early stopping:** The training of the network is stopped before it becomes overtrained, just before the performance over the validation dataset starts to degrade with further training.

In the case of the SPA-NET implementation for the  $t\bar{t} + \text{jet}$  system, a dropout rate of 10% is used to deal with overtraining. The training is performed till it reaches the maximum in the validation accuracy and it starts to show signs of saturation. In Figure D.3, the validation accuracy for the  $t\bar{t} + \text{jet}$  SPA-NET

network is compared with the curve produced by a clearly overtrained network, which is produced by fitting a SPA-NET model to reconstruct the  $t\bar{t}$  all-hadronic decay using the  $\sim 2\text{M}$  events dataset provided by the SPA-NET authors [190].

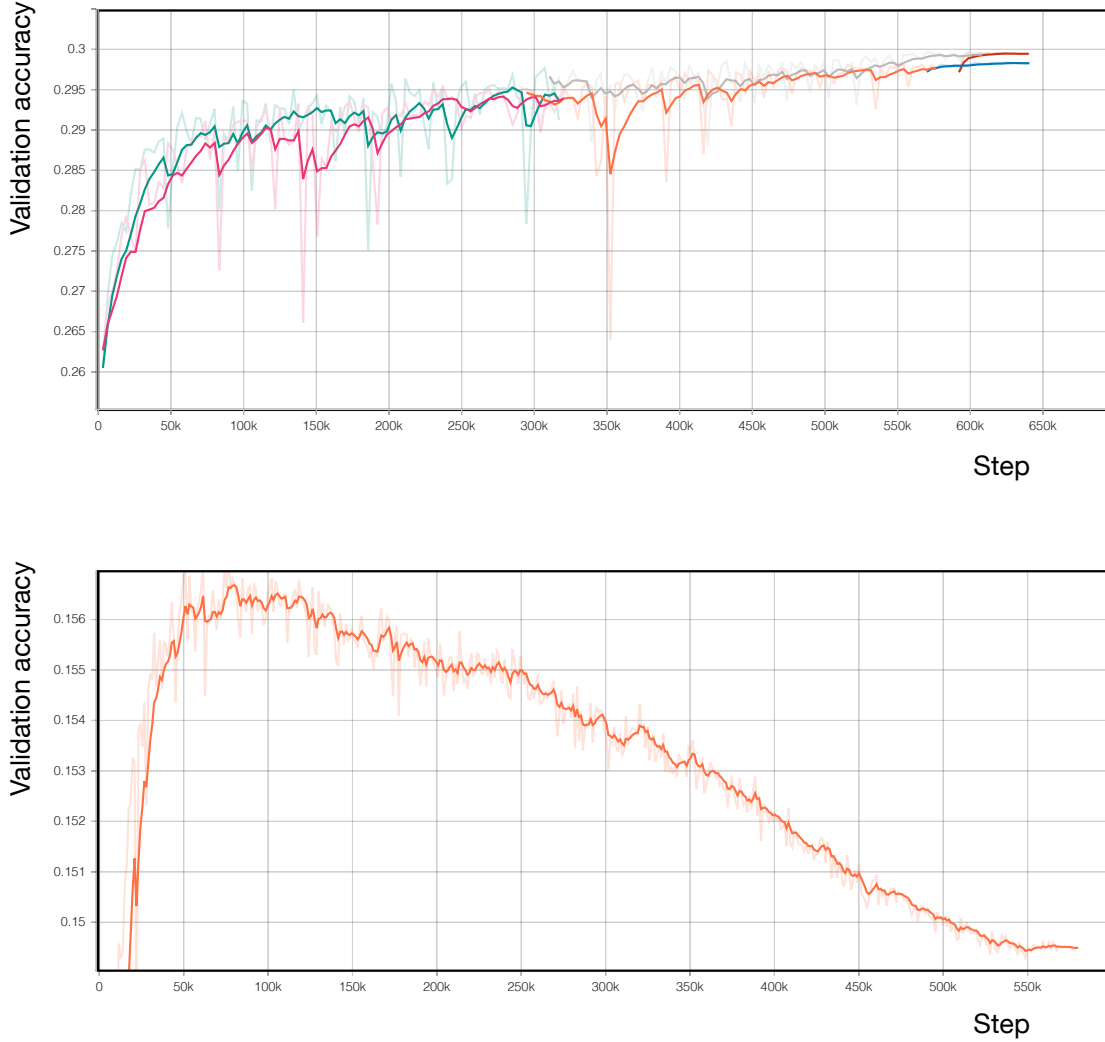


Figure D.3: Top: The validation accuracy curve for the SPA-NET implementation to reconstruct the  $t\bar{t}$  +jet system (Figure 7.5 of section Y). Bottom: Validation accuracy curve for a simple SPA-NET model trained to reconstruct the  $t\bar{t}$  all-hadronic decay using the  $\sim 2\text{M}$  events dataset provided by the SPA-NET authors [190]. The training is performed until a clear overtraining trend is observed for comparison purposes.

The evolution of the validation curve vs. the training step number follows a clear trend. In the beginning, the validation accuracy increases rapidly as the network learns the main properties of the dataset. Then, the increase slows down until it reaches a maximum value around which it fluctuates and stagnates. At last, the network starts to become overtrained, and the performance

over the validation dataset starts to drop. However, the use of the dropout technique in the  $t\bar{t} + \text{jet}$  SPA-NET model prevents the overtraining of the model. The training is performed for 200 epochs until no further improvement in the network's performance on the validation dataset is observed and the fluctuations are mitigated.

## D.4 SPA-Net model matching efficiencies, $\rho_s$ resolution, and $M_{lb}$ resolution for all the signal and control regions in the analysis

In this section, the matching efficiencies, the  $\rho_s$  resolution, and the  $M_{lb}$  resolution are studied for all the signal and control regions of the analysis. These magnitudes are evaluated for the following algorithms:

- SPA-NET reconstruction before the final selection cuts
- SPA-NET reconstruction after the final event selection, which includes requirements in the detection and assignment probabilities variables. These requirements enhance the fraction of matchable events in the sample.
- The reconstruction algorithm used in the 8 TeV analysis (Appendix C.1).
  - Only implemented for the signal region with exactly two  $b$ -tagged jets.
- KLFitter algorithm (Appendix C.2)
- KLFitter algorithm after the  $\ln L$  cut used to enhance the fraction of matchable events in the sample (Appendix C.3).

The performance of each reconstruction algorithm for all signal regions is shown in Table D.2, while Table D.3 shows the performance of these algorithms for all the control regions. The SPA-NET reconstruction algorithm, especially after the final event selection cuts are imposed, outperforms all the alternative reconstruction algorithms studied in this analysis. As a result, it is selected as the preferred algorithm to reconstruct the  $\rho_s$  and  $M_{lb}$  variables before executing the profile maximum likelihood fit described in Chapter 8.



Table D.3: Performance of the SPA-NET reconstruction of the  $M_{lb}$  variable compared with the alternative event reconstructions described in Appendix C. The assessment is conducted for the two control regions considered in the analysis, CRljets4j2b and CRljets4j1b.

| Region      | Algorithm                              | Correctly Matched<br>$b_{lep}$ | Incorrectly Matched<br>$b_{lep}$ | UnMatched<br>$b_{lep}$ | Event<br>Fraction | $M_{lb}$ res.<br>[GeV] |
|-------------|----------------------------------------|--------------------------------|----------------------------------|------------------------|-------------------|------------------------|
| CRljets4j2b | KLFITTER                               | 59.1%                          | 19.8%                            | 20.9%                  | 100%              | 16.13                  |
|             | KLFITTER<br>( $\log(L) > -46$ )        | 75.5%                          | 16.2%                            | 8.20%                  | 35.4%             | 13.63                  |
|             | SPA-NET                                | 69.1%                          | 8.78%                            | 22.0%                  | 100%              | 13.95                  |
|             | SPA-NET<br>(det. & assign. prob. cuts) | 83.6%                          | 5.06%                            | 11.2%                  | 69.7%             | 12.72                  |
| CRljets4j1b | KLFITTER                               | 42.6%                          | 25.8%                            | 31.4%                  | 100%              | 19.43                  |
|             | KLFITTER<br>( $\log(L) > -46$ )        | 52.0%                          | 25.2%                            | 22.7%                  | 47.1%             | 17.84                  |
|             | SPA-NET                                | 56.2%                          | 11.0%                            | 32.7%                  | 100%              | 16.96                  |
|             | SPA-NET<br>(det. & assign. prob. cuts) | 77.8%                          | 6.01%                            | 16.1%                  | 52.5%             | 13.86                  |

## D.5 Additional SPA-Net performance plots and distributions

This section provides a collection of supplementary performance plots and distributions for the SPA-NET reconstruction model. These plots include the  $\rho_s$  resolution for the SRLjets5j1b region (Figure D.4), the SPA-NET predicted detection probability and assignment probability for the CRljets4j1b and SRLjets5j1b regions (Figure D.6 and D.5), the  $\rho_s$  and  $M_{lb}$  distributions before the final event selection requirements (Figure D.7), and the  $\rho_s$  and  $M_{lb}$  distributions after the final event selection for the SRLjets5j1b and CRljets4j1b regions (Figure D.8 and D.9).

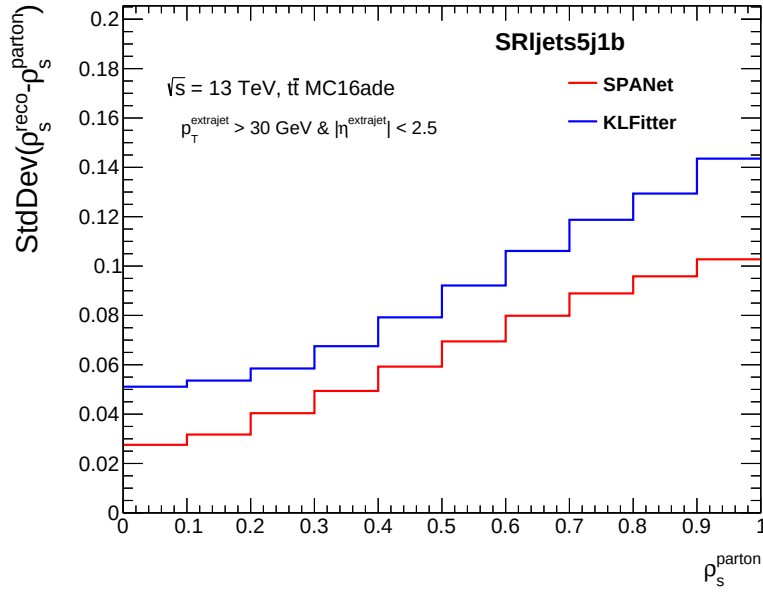


Figure D.4: Similar to Figure 7.10 but for the signal region with exactly one  $b$ -tagged jet, SRLjets5j1b.

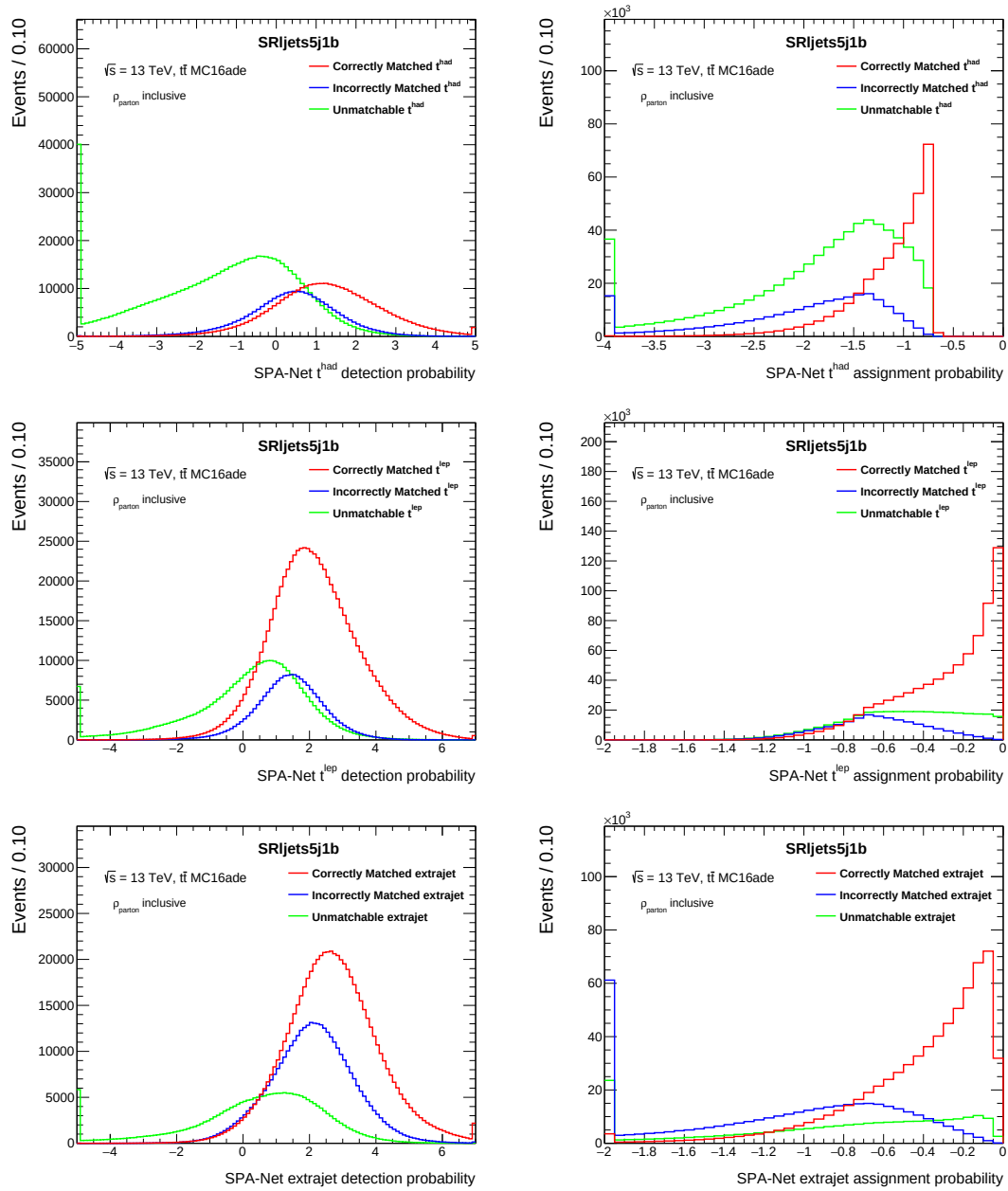


Figure D.5: Similar to Figure 7.8 but for the signal region with exactly one  $b$ -tagged jet, SRljets5j1b.



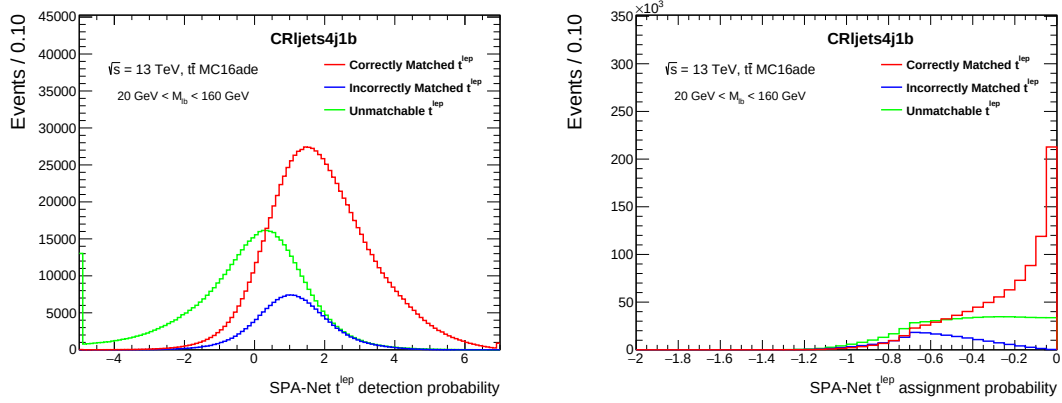


Figure D.6: Similar to Figure 7.12 but for the control region with exactly one  $b$ -tagged jet, CRLjets4j1b.

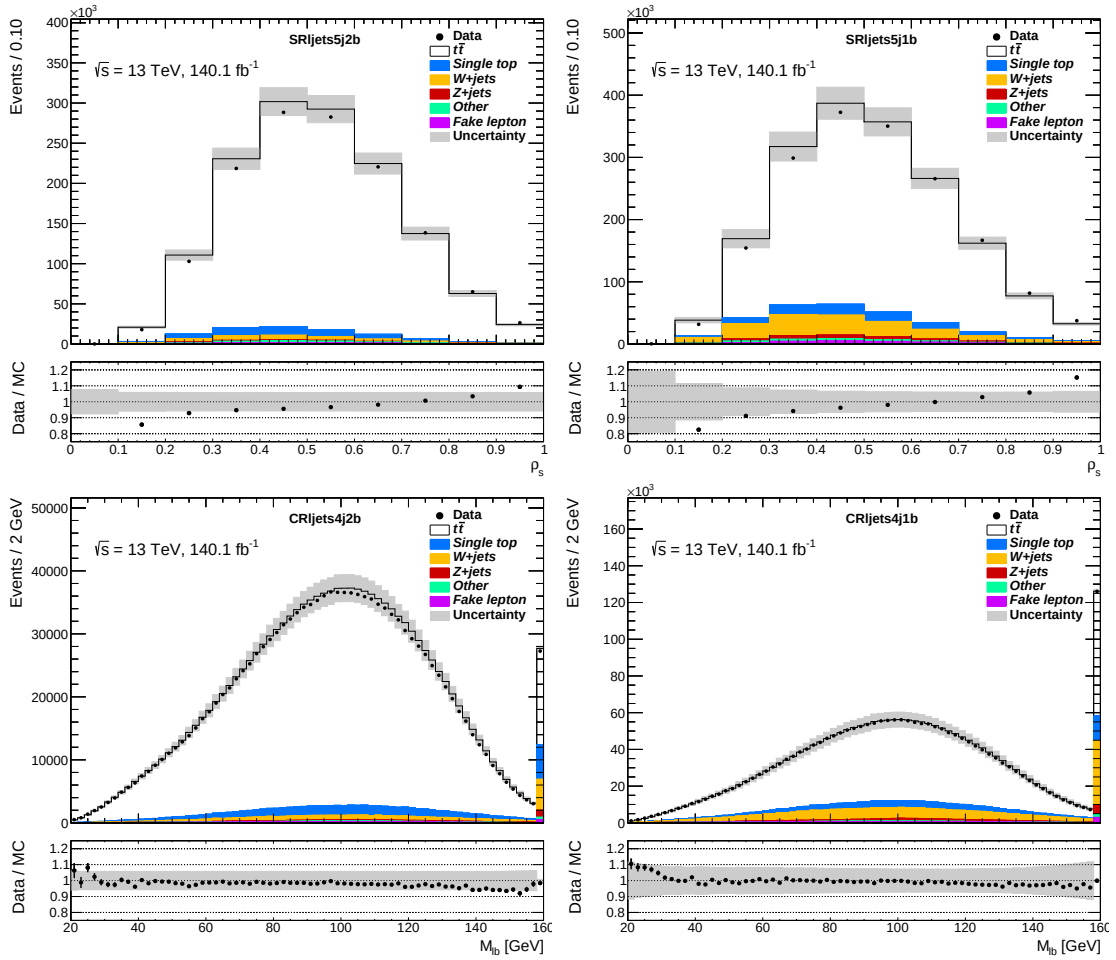


Figure D.7: Data/prediction agreement for the  $\rho_s$  and  $M_{lb}$  variables reconstructed using the SPA-NET ML model in the various signal and control regions considered in the analysis before applying the final selection requirements.

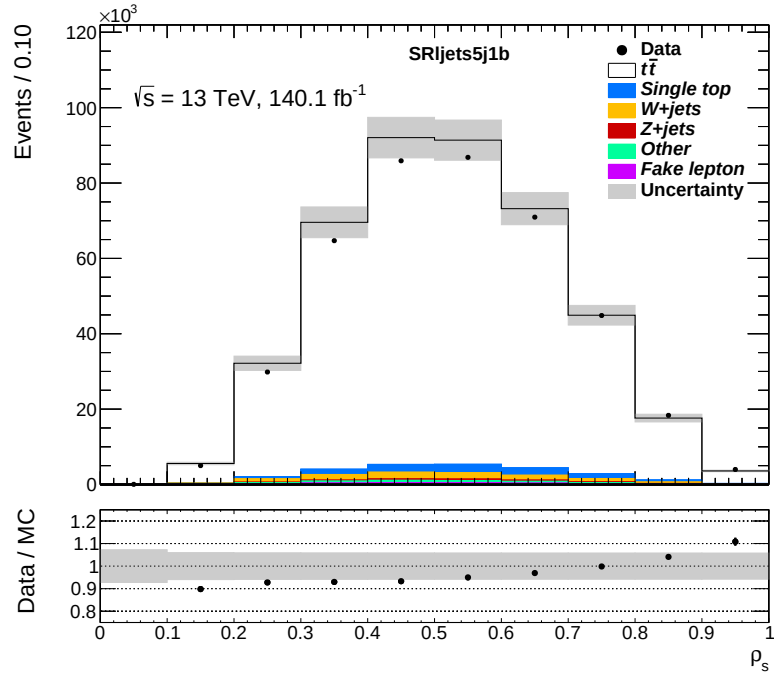


Figure D.8: Data/prediction agreement for the  $\rho_s$  observable in the  $t\bar{t}$  + jet system using the SPA-NET reconstruction after the final selection cuts on the *detection probabilities* of each parton level particle are imposed.

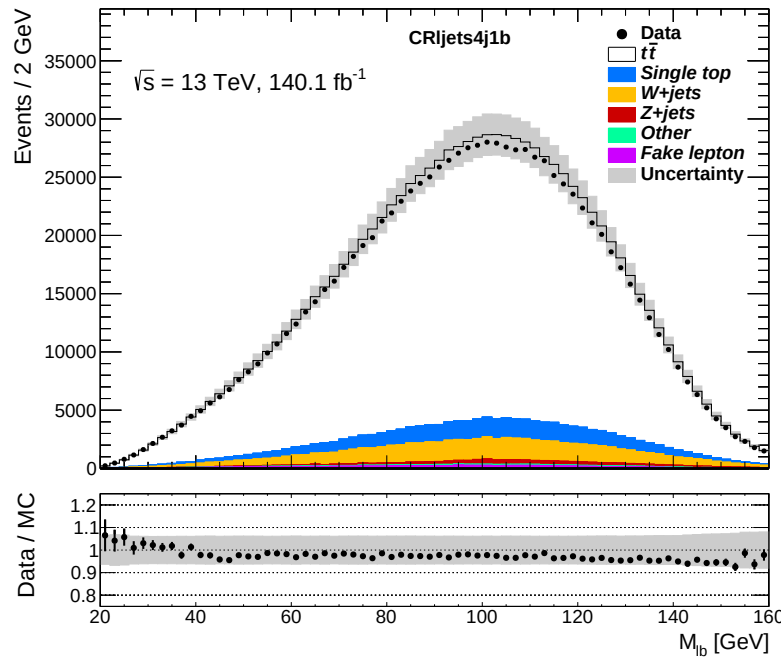


Figure D.9: Data/prediction agreement for the  $M_{lb}$  observable in the  $t\bar{t}$  system using the SPA-NET reconstruction after the final selection cuts on the *detection* and *assignment* probabilities of the leptonically decaying top are imposed.

# Appendix E

## Event yields and control plots after the final event selection

This appendix provides the event yields for all the signal and control regions considered in this analysis after the final event selection as shown in Table E.1. Additionally, several control plot distributions corresponding to reconstructed objects are shown in Figure E.1. Overall, a good agreement between data and the SM prediction is observed for all the studied variables.

Table E.1: Event yields for each of the signal and control regions considered in the analysis after the final event selection.

|                      | SRljets5j2b    | SRljets5j1b    | CRljets4j2b    | CRljets4j1b    |
|----------------------|----------------|----------------|----------------|----------------|
| $t\bar{t}$           | 527635 (96.8%) | 404464 (94.0%) | 888653 (94.5%) | 869234 (85.0%) |
| Single Top           | 8876 (1.6%)    | 10146.9 (2.4%) | 30733.7 (3.3%) | 59666.4 (5.8%) |
| $W$ +jets            | 2469.7 (0.5%)  | 8618.7 (2.0%)  | 11609.1 (1.2%) | 68183 (6.7%)   |
| $Z$ +jets            | 659.6 (0.1%)   | 1889 (0.4%)    | 2801.2 (0.3%)  | 11686.1 (1.1%) |
| Diboson+ $t\bar{t}X$ | 3075.5 (0.6%)  | 2900.5 (0.7%)  | 1651.2 (0.2%)  | 3763.2 (0.4%)  |
| Fake leptons         | 2158.8 (0.4%)  | 2122.5 (0.5%)  | 4435.8 (0.5%)  | 10285 (1.0%)   |
| Total pred.          | 544874.6       | 430141.6       | 939884         | 1022817.7      |
| Data                 | 512613         | 410424         | 902377         | 993491         |
| Data/Prediction      | 0.941          | 0.954          | 0.960          | 0.971          |

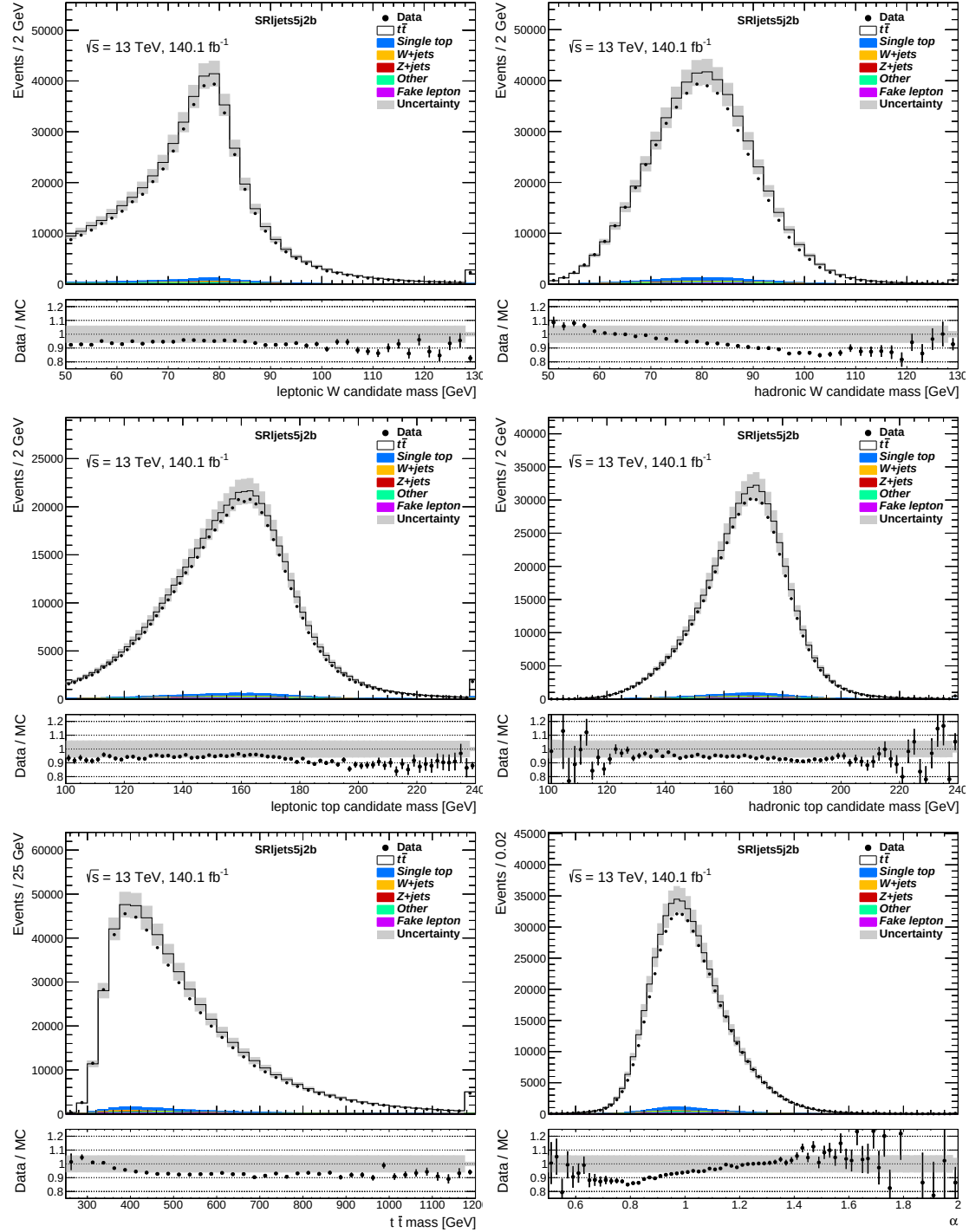


Figure E.1: Additional control plot distributions for the SPA-NET reconstruction in the SRljets5j2b signal region.

# Appendix F

## Complementary information about the profile likelihood fit

This appendix contains complementary information about the profile maximum likelihood fit used to extract the top quark MC mass parameter,  $m_t^{\text{MC}}$ , and the normalized parton level distribution  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$ . This appendix is organized as follows: In Section [F.1](#) the efficiency factor, acceptance factor, and migration matrix for the SRljets5j1b region are presented. Section [F.2](#) contains the ranking plot for the  $\gamma$  NPs. At last, Section [F.3](#) shows the correlation matrix for all the POI and NP in the fit.

### F.1 Efficiency factor, acceptance factor, and migration matrix for the SRljets5j1b region

For the nominal  $t\bar{t}$  POWHEG +PYTHIA 8 sample, the efficiency factor, migration matrix, and acceptance factor for the SRljets5j1b signal region are depicted in Figure [F.1](#). These quantities have been obtained using the final  $\rho_s$  binning used in the analysis. Additionally, Figure [F.2](#) presents the folded distributions associated with each bin of the  $\rho_s$  parton level distribution.

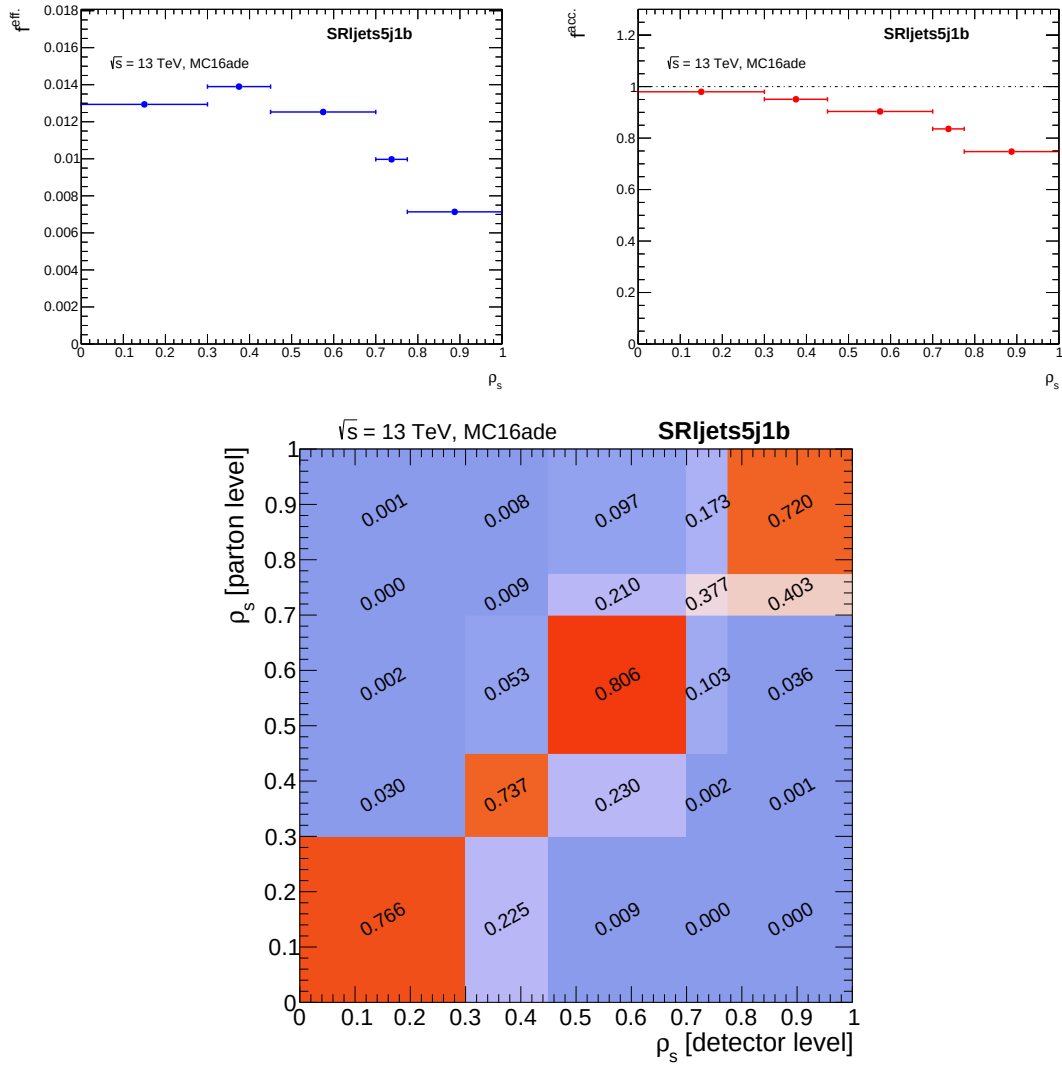


Figure F.1: Efficiency factor (top-left), acceptance factor (top-right), and migration matrix (bottom) used for the folding of the nominal  $t\bar{t}$  sample from parton to detector level. These factors and migration matrix are computed for the SRljets5j1b signal region.

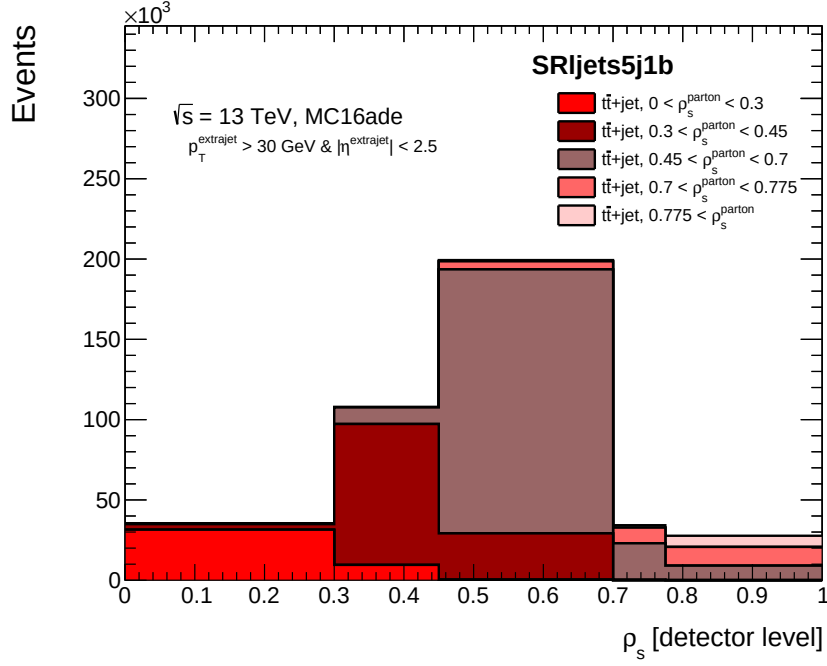


Figure F.2:  $\rho_s$  detector level distribution for the SRljets5j1b signal region obtained by folding the parton level distribution with the corresponding response matrix. Each bin in the parton level distribution contributes to multiple bins at detector level.

## F.2 Ranking plot for the $\gamma$ NPs in the profile maximum likelihood fit

The  $\gamma$  NPs in the statistical model are introduced to estimate the MC statistical uncertainty. Additionally, the effect of the “ $t\bar{t}$  FSR (CR)” uncertainty is decorrelated bin-by-bin using a  $\gamma$  NP for each of the bins in the distributions. This is done to reduce the constraints present in the NPs. The resulting Ranking plot for the  $\gamma$  NPs for the normalization factors associated with the bin content of the  $\rho_s$  normalized parton level distribution are shown in Figure F.3.

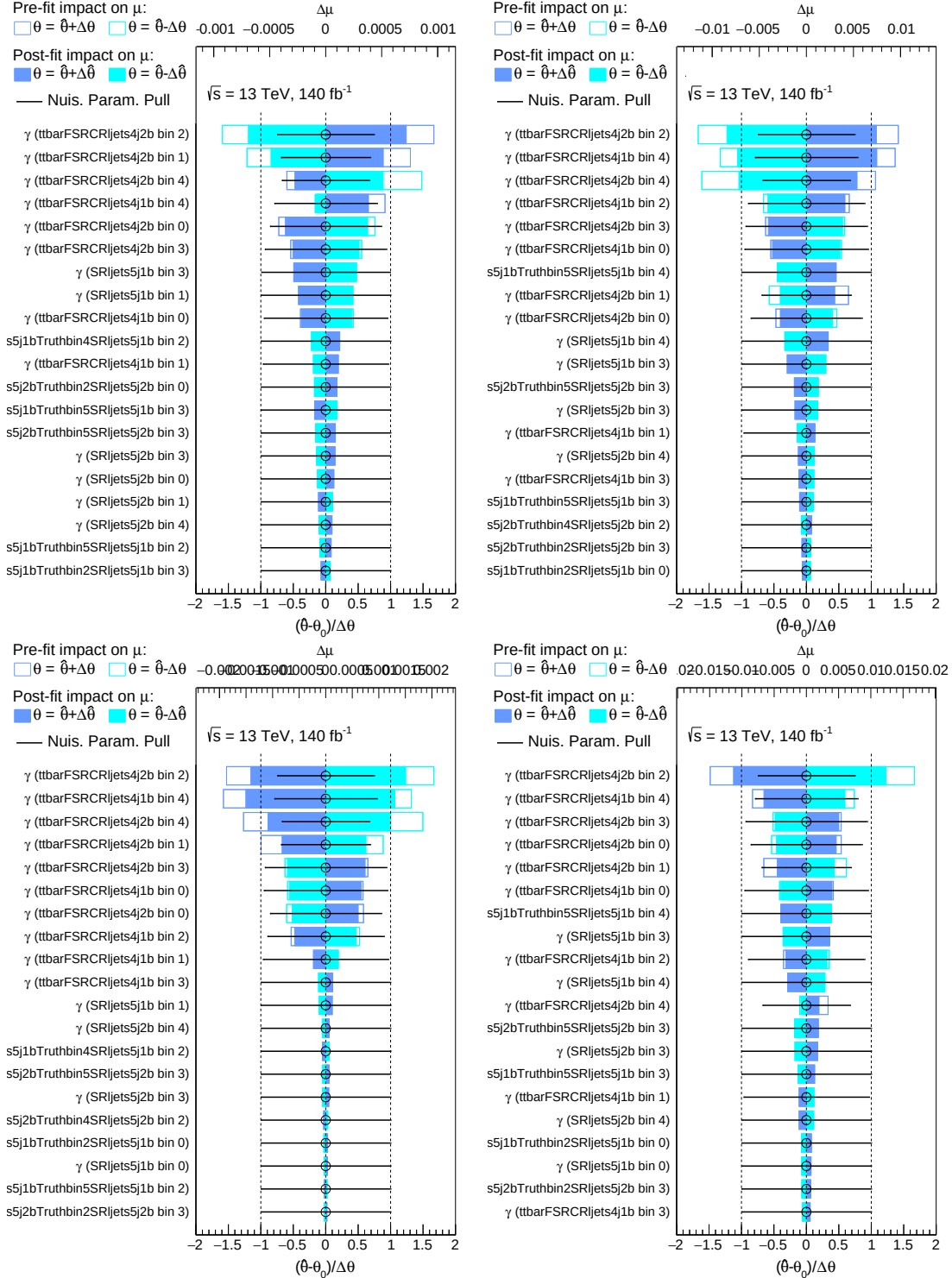


Figure F.3: Ranking plot for the  $\gamma$  NPs of the normalization factors associated with the bin content of the  $\rho_s$  normalized parton level distribution for the second (top-left), third (top-right), fourth (bottom-left), and fifth (bottom-right) bins. Similar to Figure 8.12.







# Appendix G

## Complementary studies about the top quark pole mass fit

This appendix contains complementary studies on the  $\chi^2$  fit used to extract the top quark pole mass at parton level. The sections in this appendix are organized as follows: In Section G.1, the uncertainty associated with the parametrization of the theory predictions into the  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  function is evaluated. Section G.2 contains a study to validate the fit at parton level, ensuring no bias in the extracted value of the top quark mass. Section G.3 contains the plots associated with the top quark mass fit using alternative PDF sets to calculate the theory predictions. At last, Section G.4 contains the results for the top quark pole mass extraction using alternative binning configurations.

### G.1 Uncertainty arising from the parametrization of $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$

One of the components required to compute the  $\chi^2$  fit described in Equation 9.1 is the  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  function. However, since the analytical dependence of the  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}$  distribution as a function of  $m_t^{\text{pole}}$  is unknown, this function is approximated using a second-order parametrization. This parametrization is constructed from a set of nine  $t\bar{t} + \text{jet@NLO}$  samples, which are generated assuming various values of the top quark pole mass. These parametrizations are calculated following Equation 9.2, and they are shown in Figure 9.1.

If the set of second-order parametrizations shown in Figure 9.1 would perfectly describe the theory  $\mathcal{R}$  distributions, the extracted top quark pole mass value obtained from fitting each of the theory samples should precisely match the value used in the generation of each of these samples. However, due to the imperfect parametrizations, there are discrepancies between these two top quark pole mass values.

In Figure G.1, the difference between the fitted and the top quark pole mass value used in the generation are shown for each of the  $t\bar{t} + \text{jet@NLO}$  theory calculations with the CT18NLO PDF set. The blue band represents the envelope of these differences, which covers any misparametrization effects. In principle, an uncertainty associated with the misparametrization of  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  could be added as  $\Delta m_t^{\text{pole}}(\text{param.})_{\text{CT18NLO}} = {}^{+0.04}_{-0.04}$  GeV. Nevertheless, this would be an overconservative approach, since the misparametrization of these mass points is contained within the statistical uncertainty associated with the corresponding theory samples. Therefore, no additional uncertainty associated with the misparametrization is added to the final  $m_t^{\text{pole}}$  measurement.

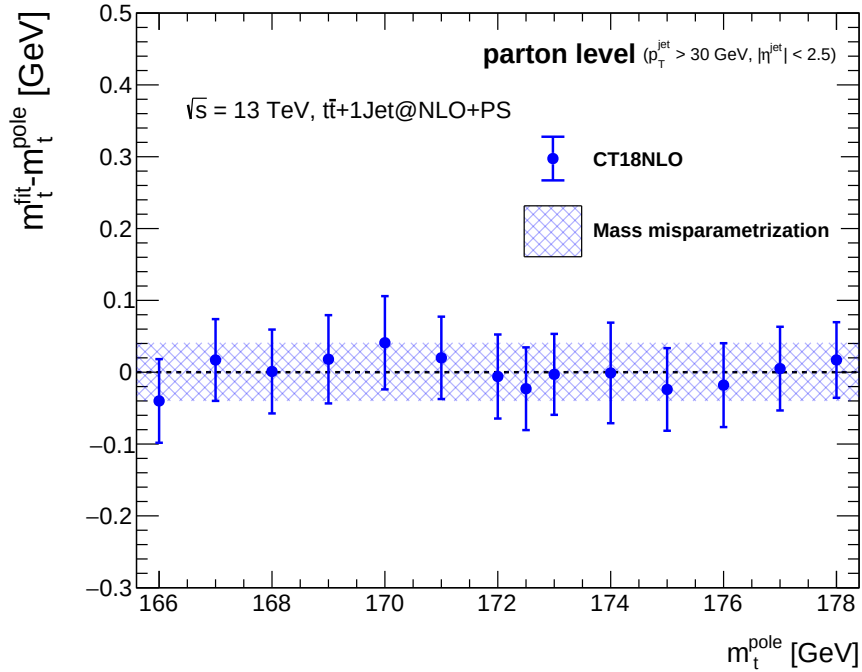


Figure G.1: Difference between the top quark pole mass extracted from the  $\chi^2$  fit and the value used in the generation for each of the  $t\bar{t} + \text{jet@NLO}$  theory calculations with the CT18NLO PDF set. The blue band represents the envelope of these differences, which covers any misparametrization effects.

## G.2 Fit validation: Top quark MC mass extraction at parton level

In the present analysis, it is important to acknowledge that the extracted value of the top quark mass at parton level, obtained from the  $\chi^2$  fit in Equation 9.1, may be influenced by the assumed value of the top quark MC mass in the nominal hvq+PS  $t\bar{t}$  sample,  $m_t^{\text{MC}} = 172.5$  GeV (Chapter 6.2.1).

This potential bias in the extracted mass value could be introduced in two distinct steps of the analysis: during the training of the SPA-NET neuronal network used to reconstruct the  $t\bar{t}$  +jet system and the  $M_{lb}$  variable in Section 7.3, or during the unfolding of the detector level  $\rho_s$  distribution to parton level in Section 8.4.

- In the reconstruction of the  $t\bar{t}$  +jet system and the  $M_{lb}$  variable, the potential bias may arise from the training process of the SPA-NET model. This training is performed using the nominal hvq+PS  $t\bar{t}$  sample with  $m_t^{\text{MC}} = 172.5$  GeV, which means that the model might learn and adopt characteristics specific to this particular sample. While it is important to investigate this possibility, the function of the model is to predict the correct jet-to-parton association and regress the neutrino  $p_T$  and  $\eta$  and, since each of these variables has a low sensitivity to the top quark mass, the network is not expected to be biased towards any specific value of this parameter.
- In the unfolding of the  $\rho_s$  distribution from detector to parton level, the potential bias may arise from the use of the nominal response matrix to generate the folded distributions for each parton level bin, as this response matrix is derived from the hvq+PS  $t\bar{t}$  sample with  $m_t^{\text{MC}} = 172.5$  GeV. However, the introduction of the top quark MC mass as a free nuisance parameter in the statistical model defined in Section 8.3 should help mitigate, if not completely eliminate, this bias.

To assess the presence of any bias in the analysis, the entire procedure is repeated for each of the ATLAS  $t\bar{t}$  samples generated with various values of the top quark MC mass (additional information about these samples can be found in Section 6.2.2). For each alternative sample, a pseudo-Asimov data sample is created. These samples are reconstructed and unfolded using the nominal

SPA-NET and PLU models, respectively, but only considering the statistical uncertainty and the post-fit uncertainty associated with the  $m_t^{\text{MC}}$  free nuisance parameter of the PLU model. Finally, the unfolded pseudo-Asimov distributions obtained from each sample and corrected to parton level are fitted using a modified version of the  $\chi^2$  fit in Equation 9.1, which is adapted for the extraction of  $m_t^{\text{MC}}$  at parton level:

$$\chi^2 = \sum_{i,j} \left[ \mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}} - \mathcal{R}_{\text{hvq+PS}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}}) \right] [V^{-1}]_{ij} \left[ \mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}} - \mathcal{R}_{\text{hvq+PS}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}}) \right]_j, \quad (\text{G.1})$$

where the  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  parametrization of Equation 9.1 is replaced by  $\mathcal{R}_{\text{hvq+PS}}^{t\bar{t}+\text{jet}}(m_t^{\text{MC}})$ . This parametrization in terms of the MC top quark mass is computed with the same methodology as the ones in Figure 9.1, but using the hvq+PS parton level distributions to obtain the second-order polynomials.

The values of the parton level unfolded normalized distributions associated with each Asimov data set are shown in Table G.1, which has the same structure as Table 8.4 in Section 8.3. The difference between the top quark MC mass values extracted at parton level from the fit in Equation G.1 and the input values used in the generation of each alternative Asimov  $t\bar{t}$  hvq+PS samples are shown in Figure G.2. The results confirm that, within the statistical and  $m_t^{\text{MC}}$  nuisance parameter uncertainties, there is no discernible bias in the extracted top quark mass used in the simulation of the  $t\bar{t}$  samples.

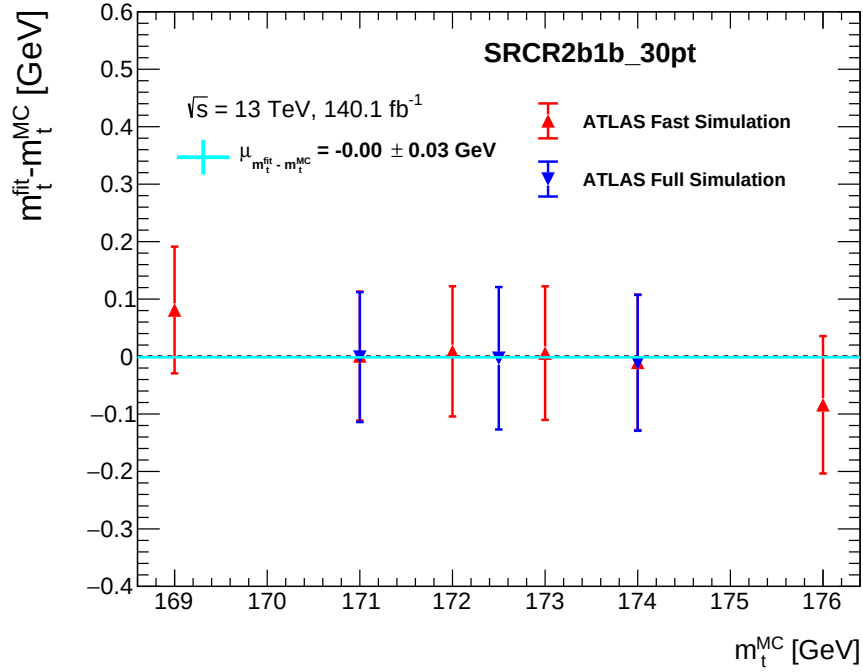


Figure G.2: Difference between the top quark MC mass extracted from the  $\chi^2$  fit at parton level and the value used as input in the generation of the alternative  $t\bar{t}$  @h $\nu$ q+PS samples. The blue points correspond to the samples computed using the full simulation of the ATLAS detector, while the red points represent the samples computed using the fast simulation of the detector. The PLU model used for the correction of the fast simulated samples to parton level uses the response matrix for the nominal sample with this modeling of the detection response. The cyan line represents the average discrepancy derived from all the samples, which is compatible with zero within the uncertainties.

Table G.1: Summary of the bin contents of the parton level  $\mathcal{R}_{\text{unfold}}^{t\bar{t}+\text{jet}}$  distributions extracted from the Asimov datasets produced with various values of  $m_t^{\text{MC}}$ .

| Input $m_t^{\text{MC}}$ [GeV] | Detector sim. | Fit setting | $\mathcal{R}_{\text{unfold}}^{t\bar{t}+\text{jet}}$ bin content |                     |                     |                     |                     |
|-------------------------------|---------------|-------------|-----------------------------------------------------------------|---------------------|---------------------|---------------------|---------------------|
|                               |               |             | 1 <sup>st</sup>                                                 | 2 <sup>nd</sup>     | 3 <sup>rd</sup>     | 4 <sup>th</sup>     | 5 <sup>th</sup>     |
| 169.00                        | ATLFASTII     | Stat.       | $0.3390 \pm 0.0014$                                             | $1.8072 \pm 0.0045$ | $2.0087 \pm 0.0035$ | $1.0902 \pm 0.0186$ | $0.1924 \pm 0.0053$ |
| 171.00                        | ATLFASTII     | Stat.       | $0.3488 \pm 0.0014$                                             | $1.8346 \pm 0.0046$ | $2.0175 \pm 0.0035$ | $1.0279 \pm 0.0191$ | $0.1720 \pm 0.0055$ |
| 172.00                        | ATLFASTII     | Stat.       | $0.3541 \pm 0.0014$                                             | $1.8498 \pm 0.0047$ | $2.0205 \pm 0.0036$ | $1.0005 \pm 0.0193$ | $0.1607 \pm 0.0056$ |
| 172.50                        | ATLFASTII     | Stat.       | $0.3557 \pm 0.0014$                                             | $1.8614 \pm 0.0047$ | $2.0195 \pm 0.0036$ | $0.9922 \pm 0.0194$ | $0.1546 \pm 0.0057$ |
| 173.00                        | ATLFASTII     | Stat.       | $0.3593 \pm 0.0014$                                             | $1.8666 \pm 0.0048$ | $2.0211 \pm 0.0036$ | $0.9858 \pm 0.0195$ | $0.1468 \pm 0.0058$ |
| 174.00                        | ATLFASTII     | Stat.       | $0.3625 \pm 0.0015$                                             | $1.8887 \pm 0.0049$ | $2.0206 \pm 0.0036$ | $0.9557 \pm 0.0198$ | $0.1383 \pm 0.0059$ |
| 176.00                        | ATLFASTII     | Stat.       | $0.3701 \pm 0.0015$                                             | $1.9346 \pm 0.0050$ | $2.0128 \pm 0.0037$ | $0.9541 \pm 0.0202$ | $0.1068 \pm 0.0062$ |
| 171.00                        | Full sim.     | Stat.       | $0.3487 \pm 0.0014$                                             | $1.8347 \pm 0.0047$ | $2.0176 \pm 0.0036$ | $1.0278 \pm 0.0191$ | $0.1720 \pm 0.0055$ |
| 174.00                        | Full sim.     | Stat.       | $0.3625 \pm 0.0015$                                             | $1.8886 \pm 0.0049$ | $2.0206 \pm 0.0036$ | $0.9561 \pm 0.0196$ | $0.1382 \pm 0.0058$ |
| 171.00                        | Full sim.     | Stat.+Syst. | $0.3491 \pm 0.0099$                                             | $1.8352 \pm 0.0218$ | $2.0166 \pm 0.0165$ | $1.0293 \pm 0.0774$ | $0.1717 \pm 0.0129$ |
| 174.00                        | Full sim.     | Stat.+Syst. | $0.3624 \pm 0.0102$                                             | $1.8887 \pm 0.0205$ | $2.0210 \pm 0.0159$ | $0.9551 \pm 0.0786$ | $0.1382 \pm 0.0128$ |
| 172.50                        | Full sim.     | Stat.       | $0.3557 \pm 0.0014$                                             | $1.8614 \pm 0.0048$ | $2.0195 \pm 0.0036$ | $0.9922 \pm 0.0194$ | $0.1546 \pm 0.0057$ |
| 172.50                        | Full sim.     | Stat.+Syst. | $0.3557 \pm 0.0101$                                             | $1.8614 \pm 0.0215$ | $2.0195 \pm 0.0166$ | $0.9922 \pm 0.0760$ | $0.1546 \pm 0.0137$ |



Table G.2: Summary of the  $\chi^2$  fitting procedure tests using the unfolded  $\mathcal{R}$  distribution obtained from the statistics only and the full systematics model for the Asimov datasets produced with various values of  $m_t^{\text{MC}}$ . A good agreement between the input and the fitted values is observed.

| Input $m_t^{\text{MC}}$ [GeV] | Detector sim. | Fit setting | Fitted $m_t^{\text{MC}}$ [GeV] |
|-------------------------------|---------------|-------------|--------------------------------|
| 169.00                        | ATLFASTII     | Stat.       | $169.08 \pm 0.11$              |
| 171.00                        | ATLFASTII     | Stat.       | $171.00 \pm 0.11$              |
| 172.00                        | ATLFASTII     | Stat.       | $172.01 \pm 0.11$              |
| 173.00                        | ATLFASTII     | Stat.       | $173.01 \pm 0.12$              |
| 174.00                        | ATLFASTII     | Stat.       | $173.99 \pm 0.12$              |
| 176.00                        | ATLFASTII     | Stat.       | $175.92 \pm 0.12$              |
| 171.00                        | Full sim.     | Stat.       | $171.00 \pm 0.11$              |
| 174.00                        | Full sim.     | Stat.       | $173.99 \pm 0.12$              |
| 171.00                        | Full sim.     | Stat.+Syst. | $170.99 \pm 0.71$              |
| 174.00                        | Full sim.     | Stat.+Syst. | $174.02 \pm 0.70$              |
| 172.50                        | Full sim.     | Stat.       | $172.50 \pm 0.11$              |
| 172.50                        | Full sim.     | Stat.+Syst. | $172.50 \pm 0.72$              |

### G.3 Extraction of the top quark pole mass using various theory predictions computed with different PDF sets

In this section, the unfolded  $\mathcal{R}$  distribution obtained from the Asimov PLU fit in Section 8.4 is fitted using various PDF sets to compute the theory predictions for the observable. The PDF sets tested in this appendix are NNPDF3.0 [215], PDF4LHC21 [216], and ABMP16NLO [217]. The total expected uncertainty obtained using the different PDF sets is similar to the one obtained using the nominal CT18NLO PDF set [214]. In the following, the  $\chi^2$  distributions and the plots used to estimate the theory uncertainties associated with the determination of  $m_t^{\text{pole}}$  are shown for each set of theory calculations.

#### NNPDF3.0

For the NNPDF3.0 PDF set, the dimension of the eigenvector PDF parameter space is  $N_a = 100$ . As in the case of the CT18NLO PDF set, for each member of the PDF set, a  $\mathcal{R}$  distribution is computed, and a value of  $m_t^{\text{pole}}$  is extracted. Then, as NNPDF3.0 is a hessian PDF set, the total PDF uncertainty is calculated using the following equation:

$$\Delta m_t^{\text{pole}}(\text{PDF}) = \sqrt{\sum_{i=1}^{N_a} \left[ (m_t^{\text{pole}})_i - (m_t^{\text{pole}})_0 \right]^2} \quad , \quad (\text{G.2})$$

The  $m_t^{\text{pole}}$  values obtained from the  $\mathcal{R}$  distributions associated with the  $\alpha_s$  variations are also added in quadrature using this equation. The scale uncertainties are estimated in the same manner as in the case of the CT18NLO PDF set (Section 9.2). The resulting  $\chi^2$  distribution from the fit, as well as the plots illustrating the PDF and the scale uncertainties for the NNPDF3.0 PDF set, are shown in Figure G.3. The resulting top quark pole mass extracted from the Asimov dataset for the NNPDF3.0 PDF set is:

$$m_t^{\text{pole}} = 172.93 \pm 0.69 (\text{fit}) \pm 0.45 (\text{PDF} + \alpha_s)_{-0.50}^{+0.37} (\text{scale}) \text{ GeV}. \quad (\text{G.3})$$

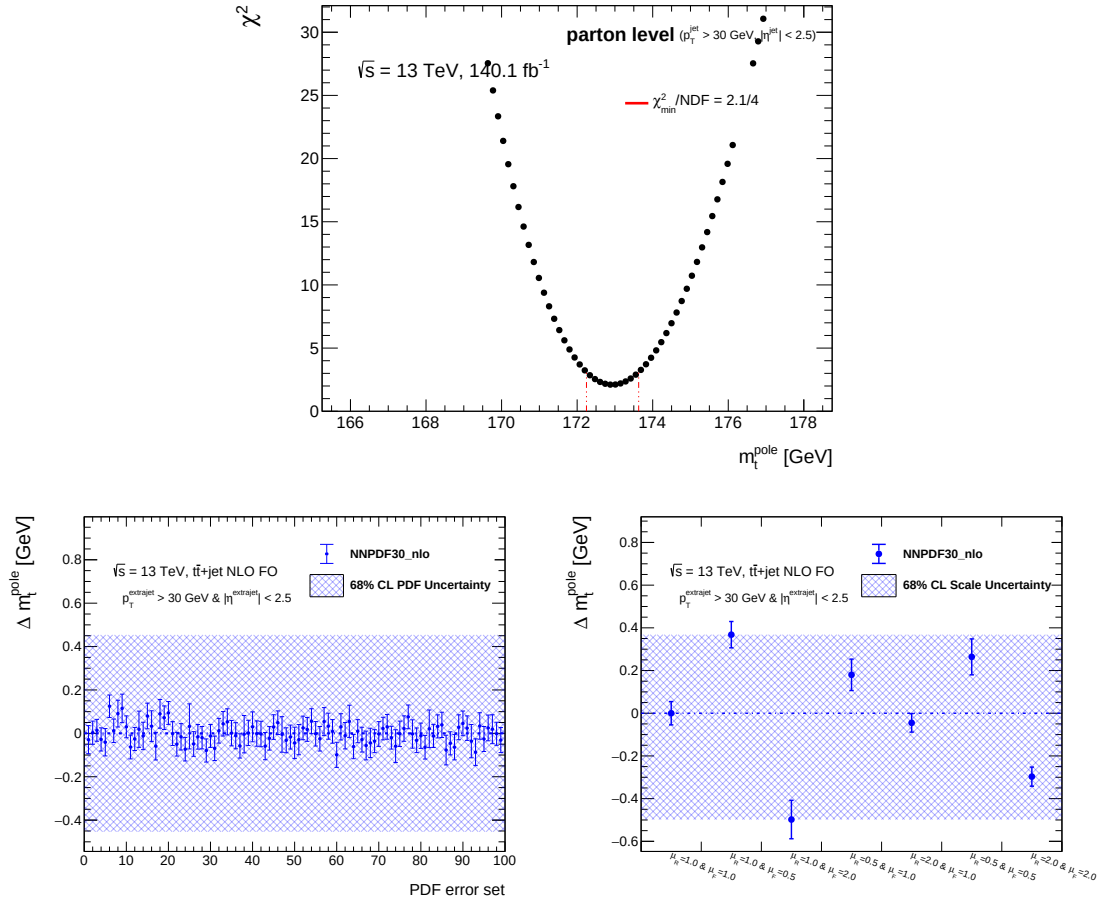


Figure G.3: Top:  $\chi^2$  distribution of the fit to the Asimov dataset using the theory predictions computed with the NNPDF3.0 PDF set. Bottom: PDF and scale uncertainties for the extraction of  $m_t^{\text{pole}}$  derived using the NNPDF3.0 PDF set.

## PDF4LHC21

For the PDF4LHC21 PDF set, the dimension of the eigenvector PDF parameter space is  $N_a = 41$ , plus the two additional  $\alpha_s$  variations. The PDF4LHC21 PDF set is also hessian hence the total PDF uncertainty is calculated using Equation G.3, as in the case of NNPDF3.0. However, the uncertainty associated with the  $\alpha_s$  variations is added considering the direction of the mass shift, using Equation 9.4 from Section 9.2 The resulting  $\chi^2$  distribution from the fit, as well as the plots illustrating the PDF and the scale uncertainties for the PDF4LHC21 PDF set, are shown in Figure G.3. The resulting top quark pole mass extracted from the Asimov dataset for the PDF4LHC21 PDF set is:

$$m_t^{\text{pole}} = 173.07 \pm 0.697 \text{ (fit)}_{-0.29}^{+0.31} \text{ (PDF} + \alpha_S)_{-0.47}^{+0.37} \text{ (scale) GeV.} \quad (\text{G.4})$$

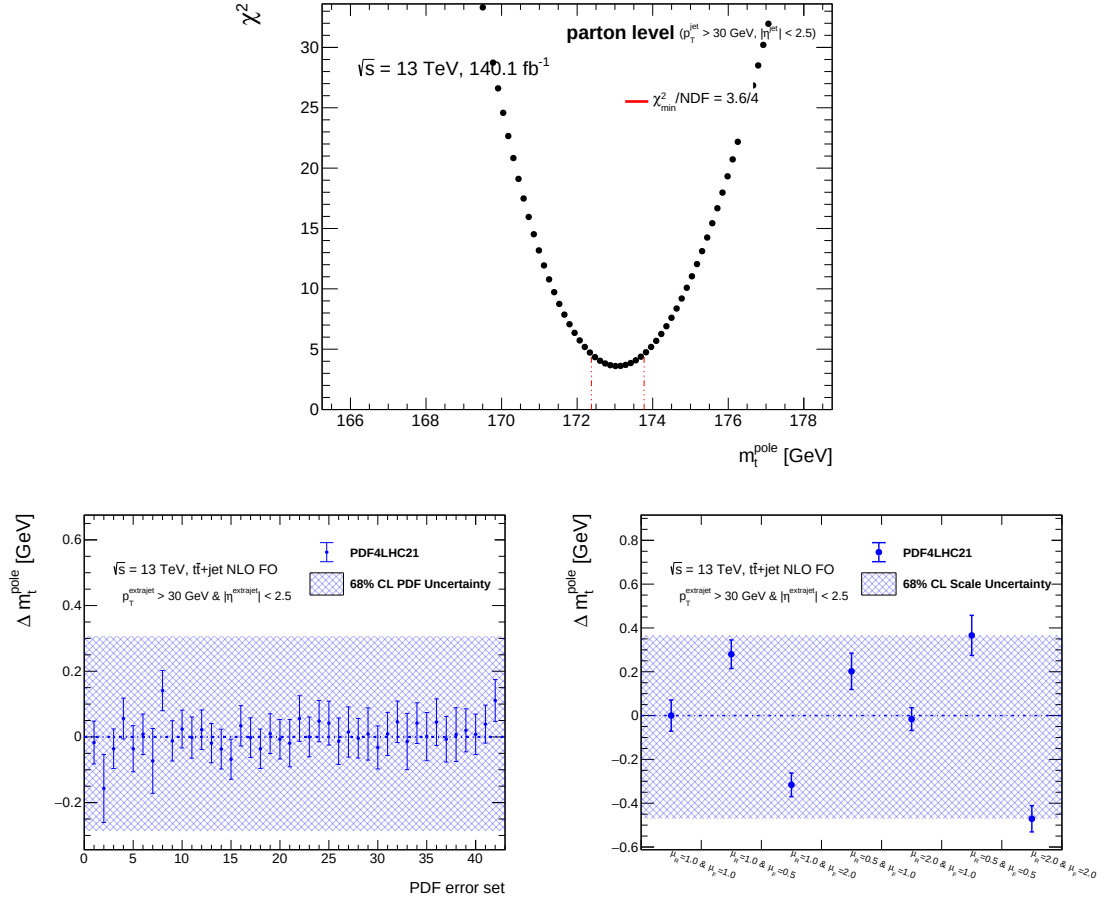


Figure G.4: Top:  $\chi^2$  distribution of the fit to the Asimov dataset using the theory predictions computed with the PDF4LHC21 PDF set. Bottom: PDF and scale uncertainties for the extraction of  $m_t^{\text{pole}}$  derived using the PDF4LHC21 PDF set.

## ABMP16NLO

For the ABMP16NLO PDF set, the dimension of the eigenvector PDF parameter space is  $N_a = 30$ , plus the two additional  $\alpha_S$  variations. The estimation of the uncertainties for this PDF set is performed as in the case of PDF4LHC21, as this is also a hessian PDF set. The resulting  $\chi^2$  distribution from the fit, as well as the plots illustrating the PDF and the scale uncertainties for the ABMP16NLO

PDF set, are shown in Figure G.5. The resulting top quark pole mass extracted from the Asimov dataset for the ABMP16NLO PDF set is:

$$m_t^{\text{pole}} = 172.84 \pm 0.67 \text{ (fit)}_{-0.17}^{+0.22} \text{ (PDF} + \alpha_S)_{-0.29}^{+0.32} \text{ (scale) GeV.} \quad (\text{G.5})$$

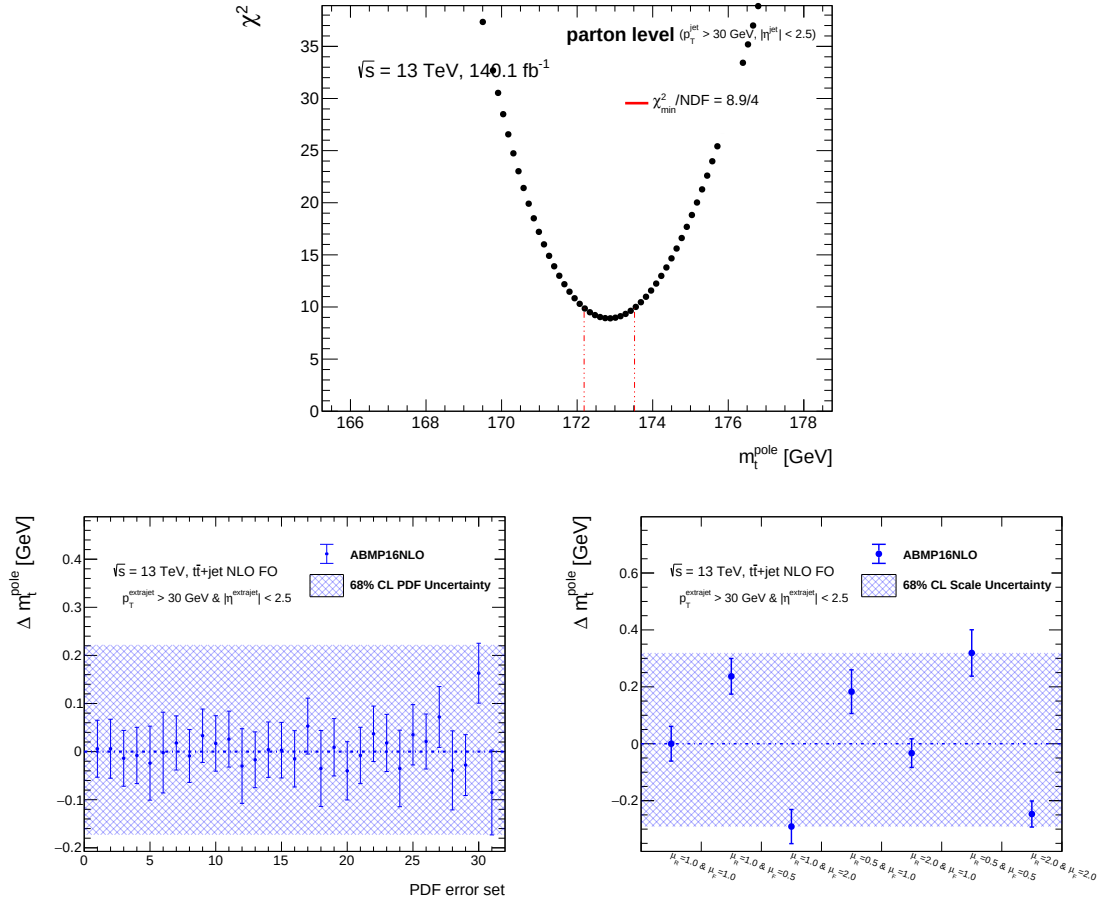


Figure G.5: Top:  $\chi^2$  distribution of the fit to the Asimov dataset using the theory predictions computed with the ABMP16NLO PDF set. Bottom: PDF and scale uncertainties for the extraction of  $m_t^{\text{pole}}$  derived using the ABMP16NLO PDF set.

## G.4 Extraction of the top quark pole mass using alternative binnings for the $\mathcal{R}$ observable

This subsection contains a cross-check of the expected precision in the measurement of  $m_t^{\text{pole}}$  using two alternative binnings for the  $\mathcal{R}$  observable.

### $\mathcal{R}$ distribution with four bins

The full Asimov analysis is performed using the  $\mathcal{R}$  observable binned following the bin edges:  $\rho_s = \{0, 0.3, 0.45, 0.7, 1\}$ . This binning is the same binning employed by the CMS collaboration in the measurement of the top quark mass using the  $\mathcal{R}$  observable in the dileptonic final state of the  $t\bar{t}$  +jet system at 13 TeV [94].

The resulting distribution and its associated total covariance matrix from the profiled maximum likelihood fit when using this binning are depicted in Figure G.6. Additionally, Figure G.6 presents the  $\chi^2$  distribution resulting from the fit and, as well as the plots illustrating the PDF and the scale uncertainties for the CT18NLL0 PDF set. The resulting top quark pole mass extracted from the Asimov dataset for this binning configuration is:

$$m_t^{\text{pole}} = 172.49 \pm 1.16 (\text{fit})_{-0.25}^{+0.48} (\text{PDF} + \alpha_s)_{-0.44}^{+0.54} (\text{scale}) \text{ GeV} \quad , \quad (\text{G.6})$$

The result obtained using the four-bin configuration is compatible with the result obtained using the nominal five-bin configuration used in the analysis. However, as this bin only has a single bin in the  $\rho_s > 0.7$  region, the sensitivity of the top quark mass of the observable is reduced, leading to the reduction in the precision of the mass determination.

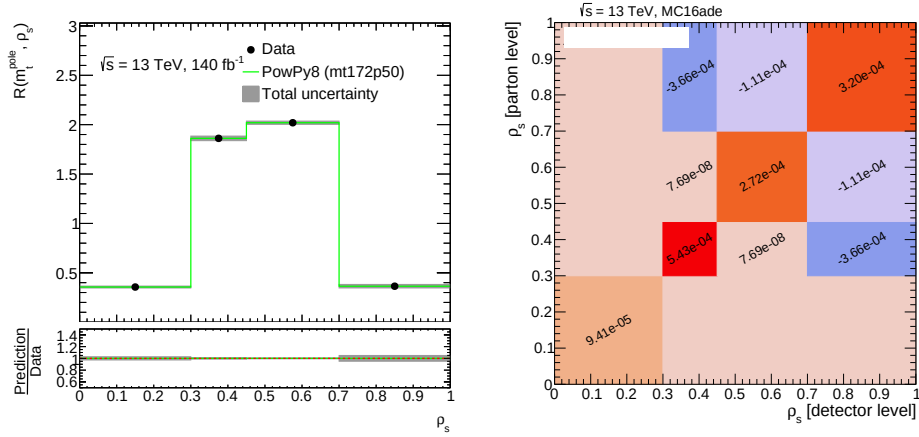


Figure G.6: Top: Normalized parton level unfolded distribution of the Asimov dataset when using the  $\mathcal{R}$  distribution with four bins. Bottom: Associated covariance matrix. Similar to Figure 8.13.

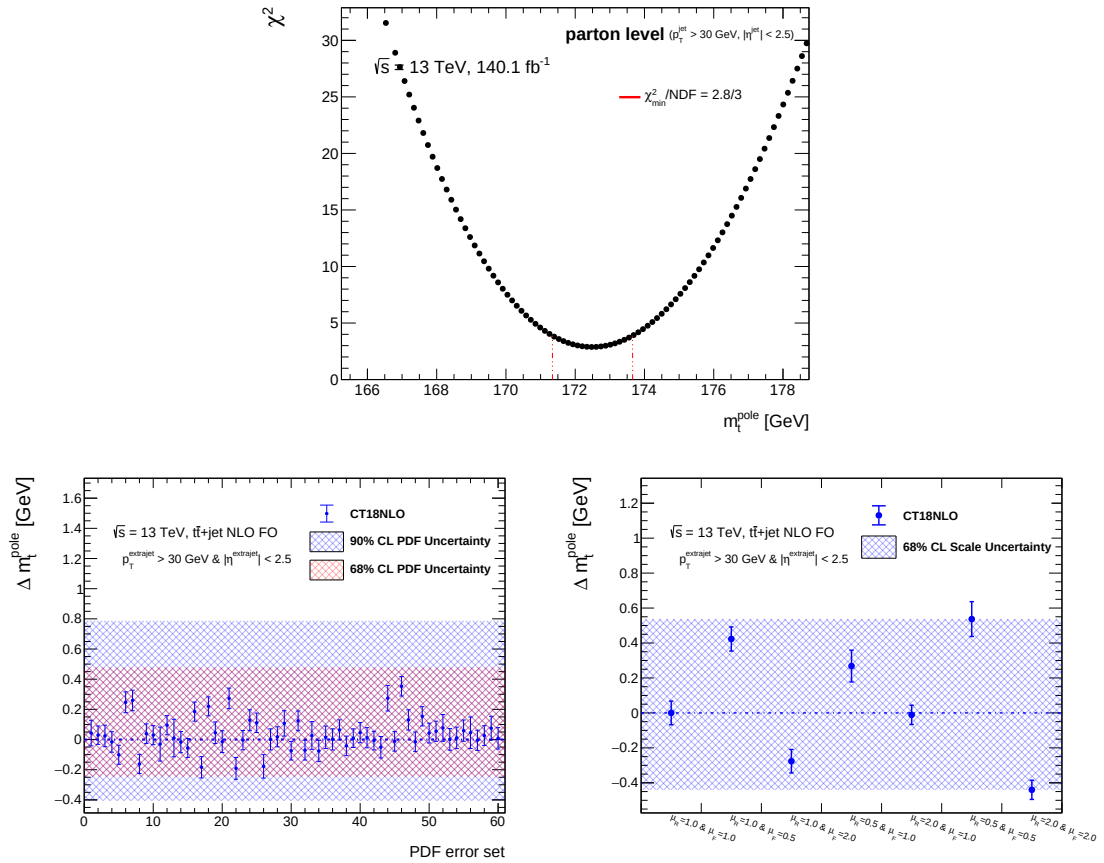


Figure G.7: Top:  $\chi^2$  distribution of the fit to the Asimov dataset using the  $\mathcal{R}$  distribution with four bins. Bottom: PDF and scale uncertainties for the extraction of  $m_t^{\text{pole}}$  derived using the CT18NLO PDF set.

## $\mathcal{R}$ distribution with seven bins

The full Asimov analysis is performed using the  $\mathcal{R}$  observable binned following the bin edges:  $\rho_s = \{0, 0.25, 0.325, 0.425, 0.525, 0.675, 1\}$ . This binning is similar to the one employed by the ATLAS collaboration in the measurement of the top quark mass using the  $\mathcal{R}$  observable in the semileptonic final state of the  $t\bar{t}$  +jet system at 8 TeV [7].

The resulting distribution and its associated total covariance matrix from the profiled maximum likelihood fit when using this binning are depicted in Figure G.8. Additionally, Figure G.7 presents the  $\chi^2$  distribution resulting from the fit and, as well as the plots illustrating the PDF and the scale uncertainties for the CT18NLL0 PDF set. The resulting top quark pole mass extracted from the Asimov dataset for this binning configuration is:

$$m_t^{\text{pole}} = 173.16 \pm 0.75 \text{ (fit)}_{-0.30}^{+0.38} \text{ (PDF} + \alpha_s)_{-0.42}^{+0.46} \text{ (scale) GeV} \quad , \quad (\text{G.7})$$

The result obtained using the seven-bin configuration is compatible with the result obtained using the nominal five-bin configuration used in the analysis. However, as this bin only has a single bin in the  $\rho_s > 0.7$  region, the inclusion of two more bins in the distribution in the regions that we are less interested in, the region with  $\rho_s < 0.7$ , increases the number of parameters of interest in the maximum likelihood fit, making the extraction of the latter more important bins in the region  $\rho_s > 0.7$  less precise, leading to the reduction in the precision of the mass determination. Additionally, the second to last bin in the distribution starts at 0.675 instead of 0.7 as in the nominal configuration, which also makes this bin less sensitive to the top quark pole mass.



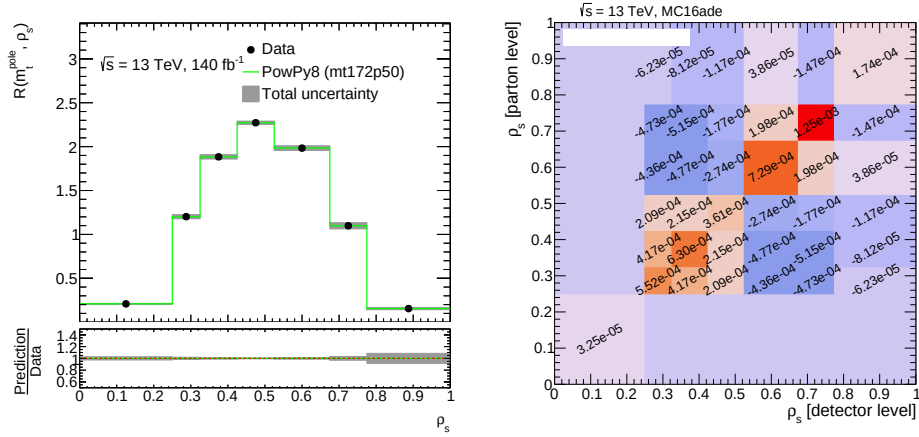


Figure G.8: Top: Normalized parton level unfolded distribution of the Asimov dataset when using the  $\mathcal{R}$  distribution with seven bins. Bottom: Associated covariance matrix. Similar to Figure 8.13.

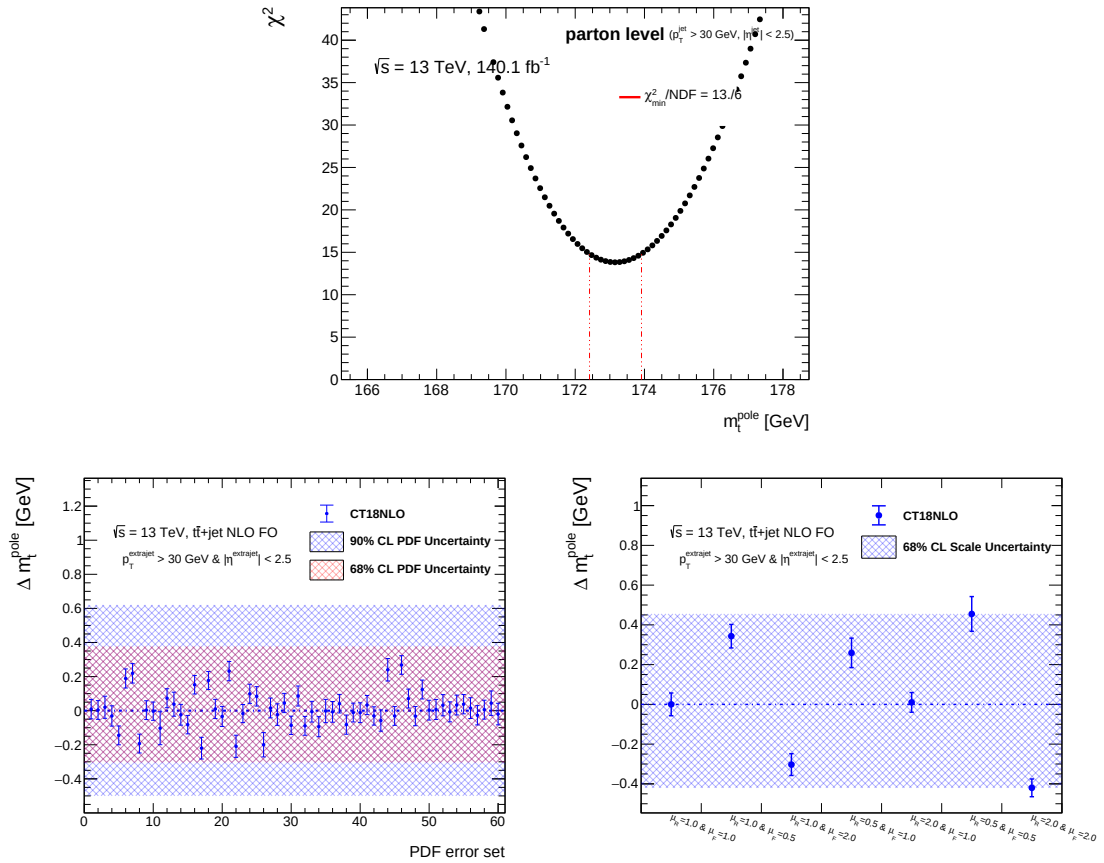


Figure G.9: Top:  $\chi^2$  distribution of the fit to the Asimov dataset using the  $\mathcal{R}$  distribution with seven bins. Bottom: PDF and scale uncertainties for the extraction of  $m_t^{\text{pole}}$  derived using the CT18NLO PDF set.



# Resum

## El Model Estàndard de física de partícules

El Model Estàndard de física de partícules (SM) és la teoria que millor descriu el coneixement actual sobre les partícules elementals i les seues interaccions. És una teoria construïda dins del marc teòric de la teoria quàntica de camps, pel que combina relativitat especial i mecànica quàntica. En les teories quàntiques de camps, les partícules es descriuen com a excitacions dels camps quàntics, i les seues interaccions mitjançant l'intercanvi de partícules anomenades *bosons*. El SM inclou les interaccions electromagnètiques, fortes, i febles. Aquestes forces estan descrites mitjançant el grup de simetries  $SU(3)_C \times SU(2)_L \times U(1)_Y$ , on la component  $SU(3)_C$  descriu les interaccions fortes, mentre que la component  $SU(2)_L \times U(1)_Y$  descriu la interacció unificada electro-feble. La Figura 10.10 mostra de manera esquemàtica les partícules fonamentals que conformen el Model Estàndard.

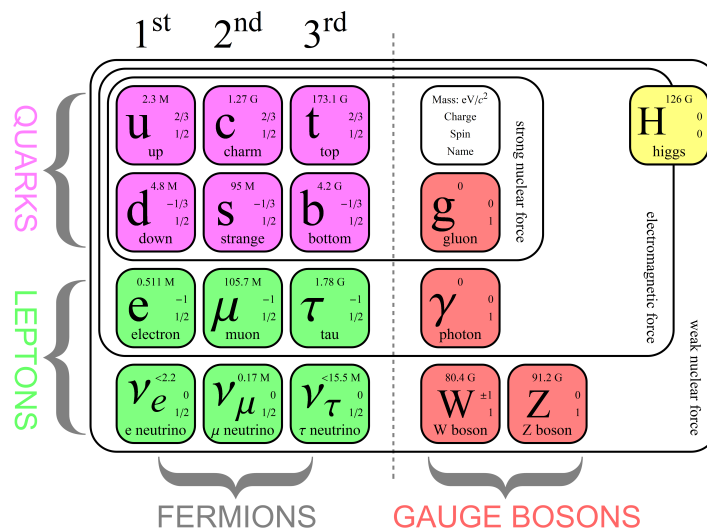


Figura 10.10: Les partícules fonamentals del Model Estàndard [2].

D'acord amb el seu espí, aquestes partícules es classifiquen en dos grups:

- **Fermions:** Els fermions són les partícules que constitueixen la matèria, ja que al tindre spin- $\frac{1}{2}$ , han d'obeir el principi d'exclusió de Pauli, el que els permet formar estructures complexes com són els àtoms i els nuclis. Alhora, els fermions es classifiquen en dos grups, depenent de si senten o no la interacció forta:
  - **Leptons:** Els leptons són els fermions que interactuen via la interacció electromagnètica i feble però no la forta. El grup està compost per tres partícules elèctricament carregades, l'electró ( $e$ ), el muó ( $\mu$ ) i el tau ( $\tau$ ), amb càrrega elèctrica  $Q = -1$ , i per tres partícules elèctricament neutres associades a les anteriors, el neutrí electrònic ( $\nu_e$ ), el neutrí muònic ( $\nu_\mu$ ) i el neutrí tauònic ( $\nu_\tau$ ).
  - **Quarks:** Els quarks són els fermions que interactuen via la interacció electromagnètica, feble i forta. Aquest grup està format per tres quarks de tipus *up* amb càrrega elèctrica  $Q = +2/3$ : l'*up* ( $u$ ), el *charm* ( $c$ ) i el *top* ( $t$ ), i tres quarks de tipus *down* amb càrrega elèctrica  $Q = -1/3$ : el *down* ( $d$ ), l'*strange* ( $s$ ) i el *bottom* ( $b$ ).
- **Bosons:** els bosons són partícules de spin enter (spin-0, 1) responsables de mediar en les interaccions entre partícules. En aquest grup podem trobar el mediador de la interacció electromagnètica, el fotó ( $\gamma$ ), els bosons que medien la interacció feble,  $W^\pm$  i  $Z$ , i els gluons ( $g$ ), encarregats de mediar la interacció forta. A més a més, el grup que formen els bosons també inclou l'anomenat *bosó de Higgs* ( $H$ ), una partícula fonamenta d'espí-0 que interacciona amb tots els fermions del SM (excepte amb els neutrins), amb els bosons mediadors de la interacció feble ( $W^\pm$  i  $Z$ ), i amb sí mateix. La interacció del bosó de Higgs amb aquestes partícules dona origen a la seua massa mitjançant el mecanisme de la Ruptura Espontània de la Simetria (SSB). Aquest bosó va ser observat per primera vegada en 2012 en el Gran Col·lisionador d'Hadrons (LHC) per les col·laboracions ATLAS i CMS [XX].

És important recordar que, per cada partícula fermiònica en el SM, existeix una partícula d'antimatèria associada que té la mateixa massa, però amb nombres quàntics oposats (càrrega elèctrica, isospí feble, càrrega de color, etc).

El Model Estàndard és una teoria que ha sigut testejada en multitud d'experiments i que ha reportat resultats consistents amb la majoria de mesures. No obstant això, i malgrat el seu èxit, sabem que el SM no pot ser la teoria final que descriu la natura, ja que hi ha diversos fenòmens que aquesta teoria no pot explicar com són l'origen de la massa dels neutrins, l'origen de la matèria en l'univers, o les observacions cosmològiques que han donat origen a la hipòtesi de l'existència de matèria i energia fosca. A més a més, aquest model no inclou una descripció de la força gravitatòria perquè una teoria quàntica de la relativitat general no ha sigut formulada de forma exitosa.

## El quark top i la seua massa

### La física del quark top

El quark top és una partícula fonamental d'espí- $\frac{1}{2}$  i càrrega  $Q = +\frac{2}{3}$  predita pel Model Estàndard com el company d'isospí feble del quark bottom, tots dos pertanyents a la tercera generació de fermions. Es tracta, a més a més, de la partícula més massiva del SM, amb una massa d'aproximadament 170 GeV. A causa del gran valor de la seua massa, el temps de vida mitjà del quark top és de l'ordre de  $\tau_t = 1/\Gamma_t \sim 0.5 \times 10^{-24}$  s, significativament menor que l'escala de temps d'hadronització,  $\tau_{\text{QCD}} \sim 1/\Lambda_{\text{QCD}} \sim 10^{-23} - 10^{-24}$  s. Atés el curt temps de vida mitjà del quark top, aquest decau abans de dur a terme el procés d'hadronització, per la qual cosa no hi ha estat hadrònics formats per quarks tops. En conseqüència d'això, el quark top només es pot observar experimentalment a través dels seus productes de decaïment.

Al LHC, els quarks top es produeixen predominantment en parells quark-antiquark (producció  $t\bar{t}$ ) mitjançant la interacció forta. La producció d'un parell  $t\bar{t}$  en col·lisionadors protó-protó pot iniciar-se, a primer ordre en teoria de pertorbacions (LO), pel procés de fusió de gluons ( $gg \rightarrow t\bar{t}$ ), o per l'aniquilació d'un parell quark-antiquark ( $q\bar{q} \rightarrow t\bar{t}$ ). A la Figura 10.11 es mostren dos diagrames de Feynman representatius d'aquest procés de producció.

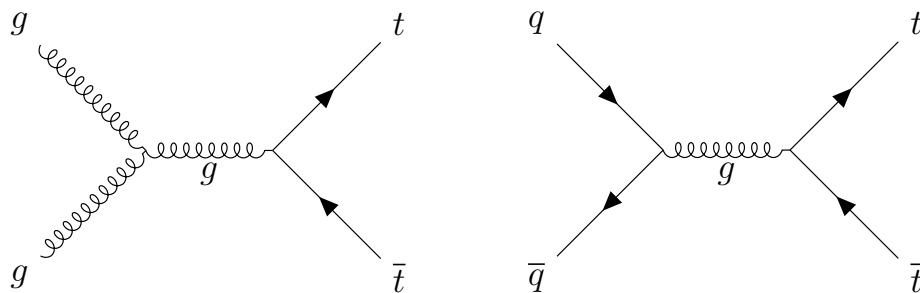


Figura 10.11: Diagrames de Feynman representatius de la producció d'un parell top-antitop mitjançant el procés de fusió de gluons (esquerra) i aniquilació d'un parell quark-antiquark (dreta).

Produït un quark top, aquest decau via la interacció feble a un bosó  $W$  i un quark bottom ( $b$ ) aproximadament un 100% de les vegades. Alhora, el bosó  $W$  també té un temps mitjà de vida molt curt, fent que només pugui ser estudiat a través dels seus productes de decaïment. A primer ordre en teoria de perturbacions, aquest bosó pot decaure en un parell quark-antiquark de diferent tipus ( $W \rightarrow q\bar{q}'$ ), o en un leptó carregat i el seu corresponent antineutrí ( $W^\pm \rightarrow l^\pm\nu$ ).

Depenent del mode en què decaïga cadascú dels bosons  $W$  provinents del decaïment del quark top i antitop d'un parell  $t\bar{t}$ , el decaïment d'aquest sistema es pot classificar en tres canals diferents:

- **Completament hadrònic:** Els dos bosons  $W$  provinents del decaïment del sistema  $t\bar{t}$  decauen hadrònicament a un parell quark-antiquark,  $t\bar{t} \rightarrow W^+bW^-\bar{b} \rightarrow b\bar{b}q\bar{q}'q''\bar{q}'''$ .
- **Dileptònic:** Els dos bosons  $W$  provinents del decaïment del sistema  $t\bar{t}$  decauen leptònicament a un leptó carregat i el seu corresponent neutrí,  $t\bar{t} \rightarrow W^+bW^-\bar{b} \rightarrow b\bar{b}l^+\nu_l l'^-\bar{\nu}_{l'}$ .
- **Semileptònic:** Un dels bosons  $W$  provinents del decaïment del sistema  $t\bar{t}$  decau hadrònicament a quarks, mentre que l'altre decau leptònicament a un leptó carregat i el seu corresponent neutrí,  $t\bar{t} \rightarrow W^+bW^-\bar{b} \rightarrow b\bar{b}q\bar{q}'\bar{b}l\nu_l$ .

L'estat final resultant de cadascun dels canals de decaïment produeix un senyal molt distintiu al detector. Els diferents anàlisis experimentals han d'escollir el o els canals que volen estudiar per adaptar-se i explotar els avantatges de cadascun, mentre minimitzen els seus inconvenients.

## Mètodes per mesurar la massa del quark top

El quark top és la partícula més massiva del SM el que fa que el seu acoblament Yukawa amb el bosó de Higgs també siga el més gran de tots ( $y_t \sim 1$ ). El valor del seu acoblament Yukawa fa que el quark top tinga un paper molt important en el procés de ruptura espontània de la simetria del SM, a més a més, també el converteix en una peça fonamental per a la cerca de física més enllà del Model Estàndard (BSM).

La massa del quark top és un dels paràmetres lliures del MS, per aquest motiu, només pot ser determinat de forma experimental. Els mètodes utilitzats per mesurar la massa d'aquesta partícula es poden classificar en dues categories:

- **Directes:** Mesuren la massa del quark top a partir de la reconstrucció de les propietats kinemàtiques dels seus productes de decaïment. Aquests mètodes han assolit un nivell de precisió de  $\sim 0.2\%$ , però el valor obtingut d'aquestes mesures no té una interpretació teòrica clara.
- **Indirectes:** Es basen en la mesura de distribucions d'observables sensibles a la massa del quark top i per als quals hi ha càlculs teòrics. El nivell de precisió assolit per aquest mètodes és menor que en el cas dels mètodes directes, però la interpretació teòrica del valor de la massa obtingut és més clara. Alguns exemples d'aquests observables són les seccions eficaces inclusives i diferencials del sistema  $t\bar{t}$ .

## L'experiment ATLAS al gran col·lisionador d'hadrons

El Gran Col·lisionador d'Hadrons (LHC) és el col·lisionador de partícules més gran mai construït, ubicat als laboratoris del CERN, prop de Ginebra. L'LHC està format per dos anells superconductors de 26.7 km emplaçats a  $\sim 100$  m de profunditat, en el túnel on abans es trobava el gran col·lisionador electró positró (LEP). Aquest col·lisionador està dissenyat per a col·lidir feixos de protons a una energia en centre de masses de  $\sqrt{s} = 14$  TeV, encara que també està capacitat per col·lidir nuclis pesants (Pb). Per assolir aquestes energies, els feixos de partícules són accelerats utilitzant cavitats de radiofreqüència, alhora que s'utilitzen imants dipolars per garantir que la seua trajectòria es mantinga dins de l'anell de l'LHC. A

més d'imants dipolars, a l'LHC també s'utilitzen imants quadrupolars i octupolars per a comprimir i focalitzar els grups de protons, respectivament.

Les col·lisions entre els feixos de protons de l'LHC es produeixen cada 25 ns en quatre punts d'interacció situats al voltant de l'anell. En aquests punts d'interacció s'emplacen els quatre experiments principals de l'LHC: ALICE, LHCb, CMS i ATLAS. Les dades utilitzades per a la realització d'aquesta tesi van ser preses pel detector ATLAS a una energia en centre de masses de  $\sqrt{s} = 13$  TeV, entre els anys 2015-2018, durant l'anomenada Run 2 de l'LHC.

L'experiment ATLAS (A Toroidal LHC ApparatuS) és un detector de partícules multipropòsit compost de diversos sistemes de subdetectors, cadascun d'ells especialitzat en la mesura del senyal depositat per diferents tipus de partícules. El detector està ubicat envoltant un dels punts d'interacció on col·lisionen els feixos de protons de l'LHC. Una vista esquemàtica del detector ATLAS es pot trobar a la Figura 10.12. Des de la localització més propera al punt de col·lisió cap a fora, el detector ATLAS està format pels següents sistemes de detectors:

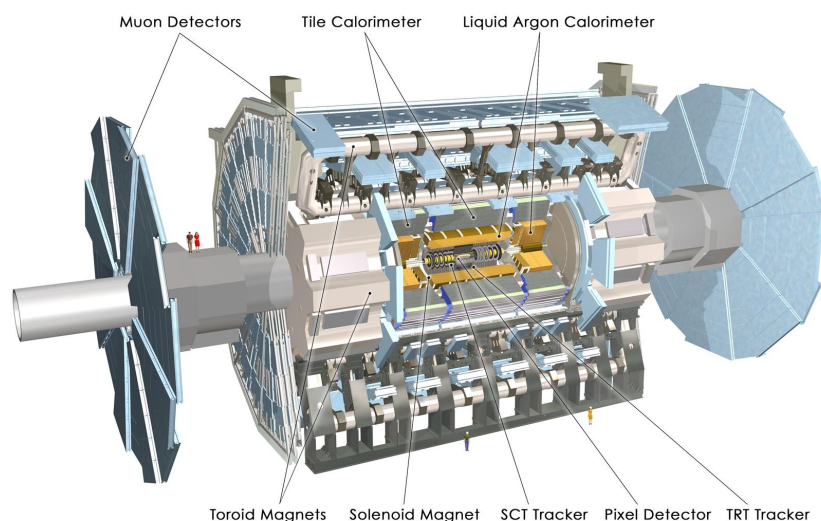


Figura 10.12: Representació esquemàtica del detector ATLAS i els seus components [110].

- **El detector intern:** El detector intern (ID) és el sistema més proper al punt d'interacció dels feixos de protons. Aquest sistema està dissenyat per a mesurar la trajectòria de les partícules carregades que el travessen. Aquest detector es troba dins d'un imant superconductor capaç de crear un camp

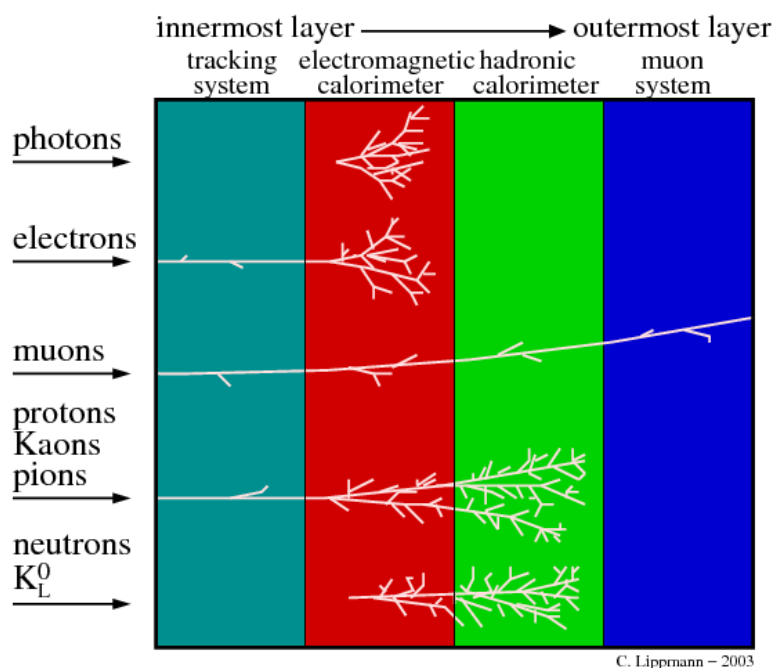


magnètic de 2 T. La presència d'aquest camp magnètic doblega la trajectòria de les partícules, permetint així poder mesurar la càrrega i el moment lineal d'aquestes partícules.

- **El sistema de calorímetres:** El sistema de calorímetres es troba just després de l'imant superconductor que envolta el detector intern. És un sistema dissenyat per aturar i mesurar l'energia de la majoria de les partícules originades al punt d'interacció dels protons. Aquest sistema es compon de dos tipus de calorímetres: calorímetres electromagnètics, optimitzats per mesurar les partícules que interaccionen electromagnèticament, i els calorímetres hadrònics, optimitzats per detectar les partícules que interaccionen mitjançant la interacció forta.
- **Les càmeres de muons:** Les càmeres de muons (MS) formen el sistema de detectors que està més allunyats del punt d'interacció dels protons i es troben envoltant la resta de l'experiment. Aquest sistema està dissenyat per detectar i determinar la trajectòria dels muons, les úniques partícules amb càrrega elèctrica que no s'aturen en travessar els calorímetres. Per mesurar el signe càrrega i el moment lineal dels muons, algunes de les càmeres de muons estan posicionades a l'interior d'imants toroidals, els quals produeixen un camp elèctric total de  $\sim 4$  T.

## Reconstrucció dels objectes al detector ATLAS

Per poder usar-los als anàlisis, els senyals elèctrics registrats pels diferents components del detector ATLAS i produïts per les partícules provinents del punt d'interacció han de ser processats per poder identificar i reconstruir els objectes físics que els van originar. Un exemple il·lustratiu dels senyals produïts al detector per diferents tipus de partícules es pot trobar a la Figura 10.13.



C. Lippmann – 2003

Figura 10.13: Il·lustració dels senyals generada per diferents tipus de partícules en travessar les capes d'un detector multipropòsit [230].

Seguint l'esquema, a aquesta figura es pot observar que les trajectòries de les partícules elèctricament carregades, com són els electrons, muons, i protons, es reconstrueixen al sistema de detecció de traces (ID en ATLAS). Al calorímetre electromagnètic els electrons són absorbits i la seua energia és mesurada. Els fotons també són absorbits en el calorímetre electromagnètic, però com són partícules elèctricament neutres, la seua trajectòria no és visible al sistema de detecció de traces. Per la seua part, al calorímetre hadrònic, els pions i tots els altres tipus d'hadrons són absorbits i la seua energia és mesurada. Els hadrons elèctricament neutres, com ara el pió neutre, també són absorbits en el calorímetre hadrònic, però la seua traça no és visible al detector intern. Els muons són capaços de travessar tot el detector sense ser absorbits, per la qual cosa són capaços d'assolir les càmeres de muons, el sistema de detectors utilitzat per mesurar el

seu moment. Finalment, els neutrins no interaccionen amb cap dels components del detector ATLAS, escapant sense ser detectats. No obstant això, la presència d'un neutrí en l'esdeveniment enregistrat pel detector pot ser deduïda mitjançant la detecció d'un desequilibri en el moment transversal del sistema (MET).

## Determinació de la massa del quark top utilitzant esdeveniments $t\bar{t} + \text{jet}$ en el canal de decaïment semileptònic amb el detector ATLAS a 13 TeV

### Definició de l'observable $\mathcal{R}$ en esdeveniments $t\bar{t} + \text{jet}$

En aquesta tesi, la massa del quark top s'extrau en l'esquema de renormalització *pole* utilitzant un mètode indirecte basat en esdeveniments en els quals un parell  $t\bar{t}$  és produït en associació amb un jet energètic,  $t\bar{t} + \text{jet}$ . En aquesta mena de topologies es pot reconstruir el següent observable:

$$\mathcal{R}(m_t^{\text{pole}}, \rho_s) = \frac{1}{\sigma_{t\bar{t}+\text{jet}}} \frac{d\sigma_{t\bar{t}+\text{jet}}}{d\rho_s}(m_t^{\text{pole}}, \rho_s), \quad \rho_s = \frac{2m_0}{\sqrt{s_{t\bar{t}+\text{jet}}}} \quad (10.8)$$

on  $m_0$  és una constant d'escala arbitrària, normalment fixada a  $m_0 = 170$  GeV, i  $s_{t\bar{t}+\text{jet}}$  és la massa invariant del sistema  $t\bar{t} + \text{jet}$ .

La Figura 10.14 presenta la distribució de l'observable  $\mathcal{R}(m_t^{\text{pole}}, \rho_s)$  per a diferents valors de la massa del quark top. Aquest observable mostra una gran sensibilitat a variacions en la massa del quark top, especialment en la regió  $\rho_s > 0.7$ . Les propietats cinemàtiques del jet addicional en aquestes distribucions estan delimitades a  $p_T^{\text{extrajet}} > 30$  GeV i  $|\eta^{\text{extrajet}}| < 2.5$ . Aquests requisits s'apliquen amb el propòsit d'incrementar la probabilitat que aquest jet a nivell partònic es convertisca en un jet identificable dins de la acceptància del detector ATLAS.

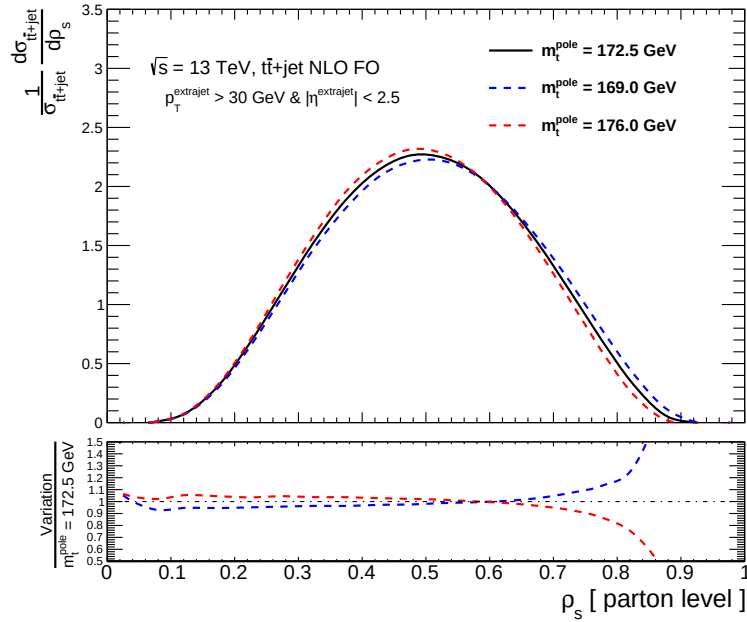


Figura 10.14: Prediccions de la secció eficaç diferencial normalitzada del sistema  $t\bar{t}$  +jet en funció de  $\rho_s$  a nivell partònic.

## Selecció dels esdeveniments i reconstrucció del sistema $t\bar{t}$ i $t\bar{t}$ +jet utilitzant tècniques d'aprenentatge automàtic

La variable  $\rho_s$  i l'observable  $\mathcal{R}$  són definits en esdeveniments  $t\bar{t}$  +jet. Per tant, per a reconstruir aquestes magnituds, l'anàlisi presentat en aquesta tesi busca identificar els esdeveniments en el detector que mostren senyals compatibles amb haver-se originat a partir d'un esdeveniment  $t\bar{t}$  +jet que decau semileptònicament, tal com s'il·lustra al diagrama de la Figura 10.15.

El senyal experimental previst en el detector per a l'estat final que es mostra a la Figura 10.15 consisteix en un leptó carregat (electró o muó), un mínim de cinc jets, dos dels quals originats a partir de l'hadronització d'un quark  $b$ , i una quantitat significativa d'energia transversa faltant per indicar la presència d'un neutrí no detectat.

A més, l'anàlisi també selecciona esdeveniments amb una topologia similar, però que contenen exactament quatre jets. Aquests esdeveniments són només compatibles amb ser originats per un procés  $t\bar{t}$  i no  $t\bar{t}$  +jet, i són utilitzats per a establir regions de control en les quals es reconstrueix l'observable  $M_{lb}$ . L'ús de regions de control amb aquest observable permet determinar simulatàniament

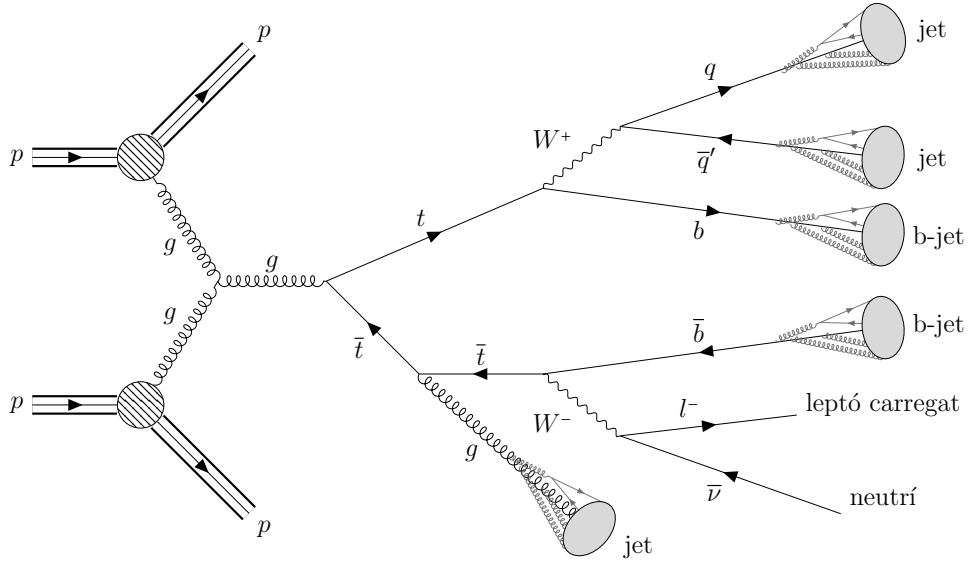


Figura 10.15: Diagrama il·lustratiu de la producció d'un parell de quarks top en associació amb un jet addicional en una col·lisió protó-protó i el seu posterior decaïment en el canal semileptònic.

el valor del paràmetre de la massa del quark top en el generador Monte Carlo, eliminant així possibles biaixos que aquest paràmetre pugui introduir a la mesura.

La reconstrucció del sistema  $t\bar{t}$  + jet i l'observable  $M_{lb}$  es realitza mitjançant un model d'aprenentatge automàtic construït amb el marc de treball conegut com a SPA-NET [186], dissenyat per escollir l'emparellament de cada un dels objectes físics reconstruïts al detector amb les partícules que els han originat a nivell partònic, i per reconstruir les propietats cinemàtiques del neutrí. Per entrenar el model s'han utilitzat els esdeveniments simulats  $t\bar{t}$  que han superat la selecció d'esdeveniments explicada anteriorment. Després de la reconstrucció, s'apliquen una sèrie de requisits addicionals per tal de millorar la proporció d'esdeveniments correctament reconstruïts a la mostra.

Els esdeveniments seleccionats i reconstruïts amb aquest model d'aprenentatge automàtic es divideixen en dues regions de senyal i dues regions de control, depenent del nombre de jets a l'esdeveniment i el nombre de jets etiquetats (*tagged*) com a  $b$ -jets a l'esdeveniment. A les regions de senyal, es considera la variable  $\rho_s$ , mentre que a les regions de control, es considera la variable  $M_{lb}$ . Aquesta divisió es realitza per millorar la sensibilitat de l'anàlisi a  $m_t^{\text{pole}}$  i  $m_t^{\text{MC}}$ . Un resum de les seleccions emprades a cada regió es pot trobar a la Taula 10.3. Les distribucions resultants per a cadascuna de les regions utilitzades a l'anàlisi es mostra a la Figura 10.16.

Taula 10.3: Resum de les regions utilitzades per a categoritzar els esdeveniments seleccionats a l'anàlisi.

| Regió       | leptons              | $n_{\text{jets}}$ | $n_{b\text{-tagged}}$ | Variable | Motivació                      |
|-------------|----------------------|-------------------|-----------------------|----------|--------------------------------|
| SRLjets5j2b | $e^\pm$ or $\mu^\pm$ | $\geq 5$          | 2                     | $\rho_s$ | Sensible a $m_t^{\text{pole}}$ |
| SRLjets5j1b | $e^\pm$ or $\mu^\pm$ | $\geq 5$          | 1                     | $\rho_s$ | Sensible a $m_t^{\text{pole}}$ |
| CRLjets4j2b | $e^\pm$ or $\mu^\pm$ | 4                 | 2                     | $M_{lb}$ | Sensible a $m_t^{\text{MC}}$   |
| CRLjets4j1b | $e^\pm$ or $\mu^\pm$ | 4                 | 1                     | $M_{lb}$ | Sensible a $m_t^{\text{MC}}$   |

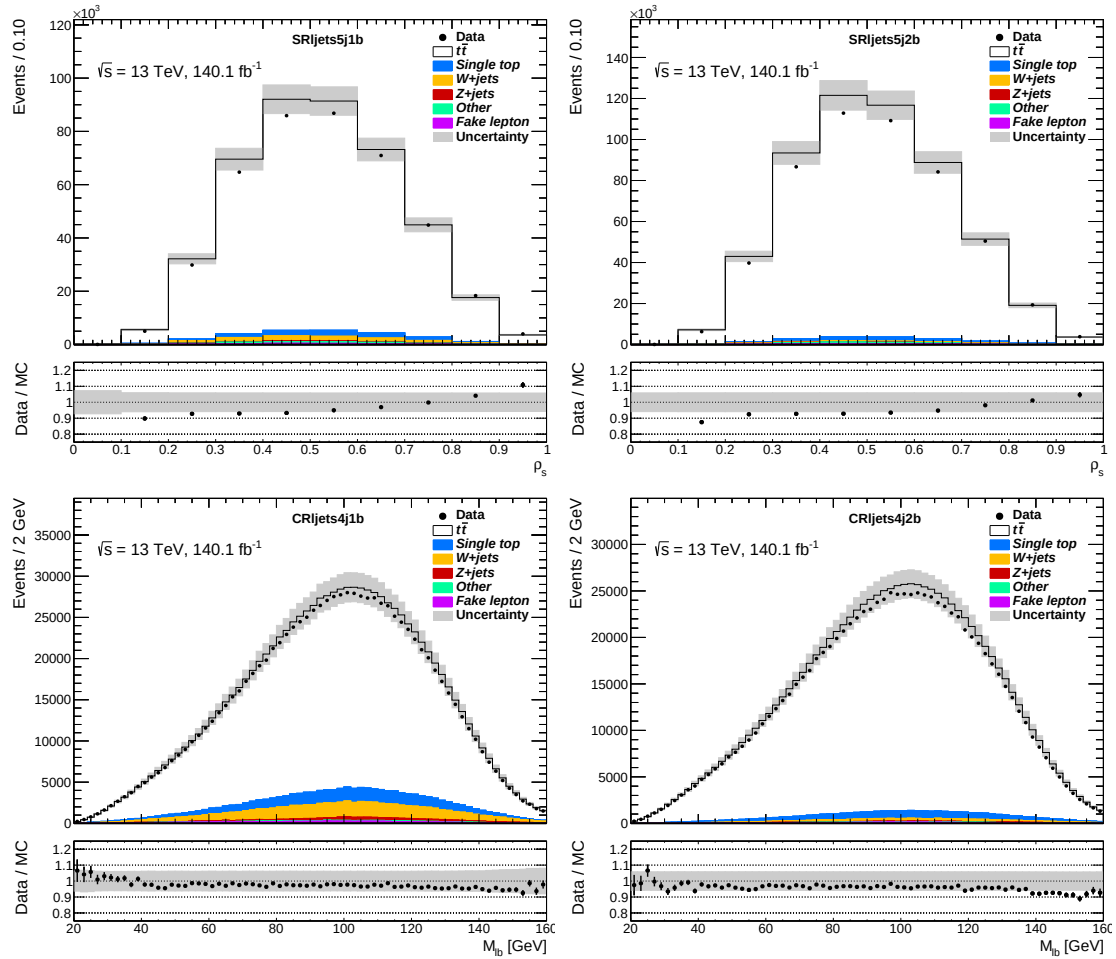


Figura 10.16: Comparació entre les distribucions de dades i les prediccions de l'observable  $\rho_s$  i  $M_{lb}$  reconstruïts utilitzant el model d'aprenentatge automàtic construït amb SPA-NET i després de la selecció final d'esdeveniments.

## Determinació de la massa MC del quark top i la secció eficaç diferencial $t\bar{t}+\text{jet}$ a nivell partònic

Per determinar la massa MC del quark top ( $m_t^{\text{MC}}$ ) i la distribució de l'observable  $\mathcal{R}$  a nivell partònic, aquest anàlisi fa servir un model estadístic basat en les tècniques d'estimació de màxima versemblança perfilada (*profile maximum likelihood* en anglès). En aquest model, el nombre total d'esdeveniments esperats a cada un dels intervals  $i$  de les distribucions de les regions de senyal i de control ( $\nu_i^{\text{SR}}$  i  $\nu_i^{\text{CR}}$ ) es poden expressar de la següent manera:

$$\nu_i^{\text{SR}}(\vec{\mu}_{t\bar{t}+\text{jet}}, m_t^{\text{MC}}, \vec{w}, \vec{\theta}) = \sum_{k=1}^{n_{\text{bin}}^{\rho_s}} S_i^k(\mu_{t\bar{t}+\text{jet}}^k, m_t^{\text{MC}}, \vec{\theta}) + \sum_j B_i^j(w_j, \vec{\theta}), \quad (10.9)$$

$$\nu_i^{\text{CR}}(\mu_{t\bar{t}}^{\text{CR}}, m_t^{\text{MC}}, \vec{w}, \vec{\theta}) = s_i(\mu_{t\bar{t}}^{\text{CR}}, m_t^{\text{MC}}, \vec{\theta}) + \sum_j b_i^j(w_j, \vec{\theta}), \quad (10.10)$$

on  $\mu_{t\bar{t}+\text{jet}}^k$  representa el paràmetre de normalització associat al interval  $k$  de la distribució de  $\rho_s$  a nivell partònic,  $m_t^{\text{MC}}$  el paràmetre de la massa MC del quark top, i  $\vec{w}$  i  $\vec{\theta}$  els paràmetres d'incertesa (*nuisance parameters* en anglès) associats a la normalització dels processos de fons, i a totes les altres incerteses sistemàtiques, respectivament.  $S_i^k$  indica el nombre d'esdeveniments de senyal esperats generats pel interval  $k$  de la distribució de  $\rho_s$  a nivell partònic,  $s_i$  el nombre total d'esdeveniments de senyal esperats a la regió de control, i  $B_i^j$  i  $b_i^j$  el nombre d'esdeveniments de fons esperats a la regió de senyal i a la regió de control, respectivament.

Realitzant l'ajust de les distribucions de dades a aquest model estadístic, es poden determinar els paràmetres  $\mu_{t\bar{t}+\text{jet}}^k$  i  $m_t^{\text{MC}}$  de forma simultània, tenint en compte totes les incerteses que els afecten. A més, a partir dels paràmetres  $\mu_{t\bar{t}+\text{jet}}^k$ , es pot obtenir la distribució  $\mathcal{R}$  corregida a nivell partònic mitjançant un canvi de variables.

En el moment d'escriure aquesta tesi, l'anàlisi utilitzant les dades reals del detector ATLAS està emmascarat. Per aquest motiu, els resultats presentats a aquesta tesi corresponent a la validació de l'anàlisi emprant una mostra de pseudo-dades coneguda com a *Asimov*, generada a partir de simulacions MC. Fent servir aquesta mostra de pseudo-dades, les quatre distribucions utilitzades per a l'ajust es mostren a la Figura 10.17.

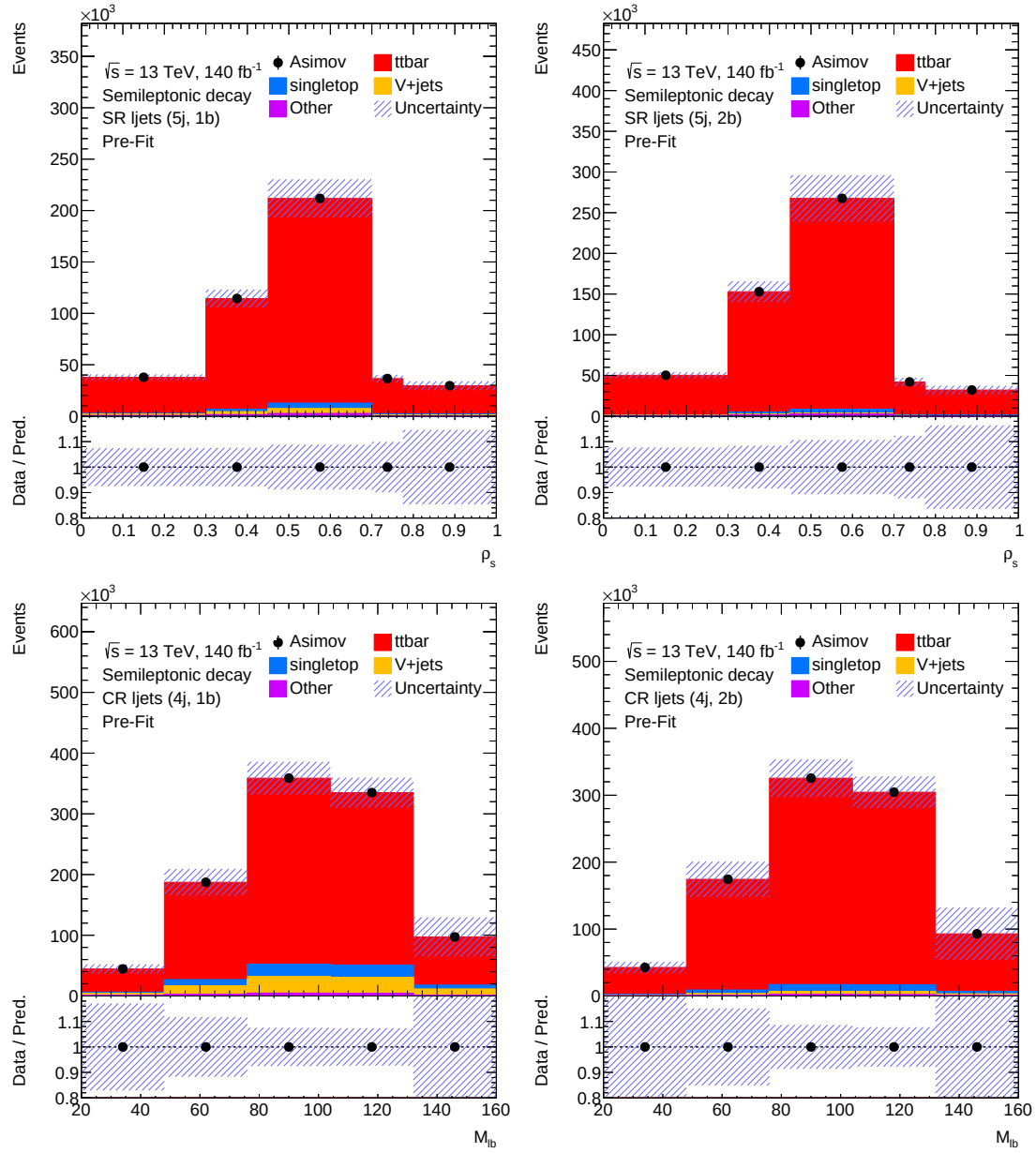


Figura 10.17: Comparació entre les distribucions d'Asimov i les prediccions de MC abans de l'ajust de màxima versemblança per a les dues regions de senyal i les dues regions de control utilitzades a l'anàlisi.



Després de l'ajust de màxima versemblança perfilada, el valor determinat pel paràmetre de la massa del quark top en el MC per a mostra d'Asimov és el següent:

$$m_t^{\text{MC}} = 172.50 \pm 0.41 \text{ GeV}. \quad (10.11)$$

Com era d'esperar, el valor determinat coincideix amb el valor utilitzat en la generació dels esdeveniments a la mostra d'Asimov. L'error associat a aquesta determinació correspon al nivell de precisió esperat en la mesura d'aquest paràmetre a les dades reals. Aquest nivell de precisió és altament competitiu, ja que és comparable a la precisió assolida en diversos anàlisis realitzats per les col·laboracions ATLAS i CMS en el canal de desintegració semileptònic [222, 223].

El resultat de l'ajust per a la distribució  $\mathcal{R}$  corregida a nivell partònic i la seua corresponent matriu de covariàncies es mostren a la Figura 10.18. La matriu de covariàncies conté la informació sobre la incertesa en la mesura del valor de cada un dels intervals de la distribució  $\mathcal{R}$  i les correlacions entre ells.

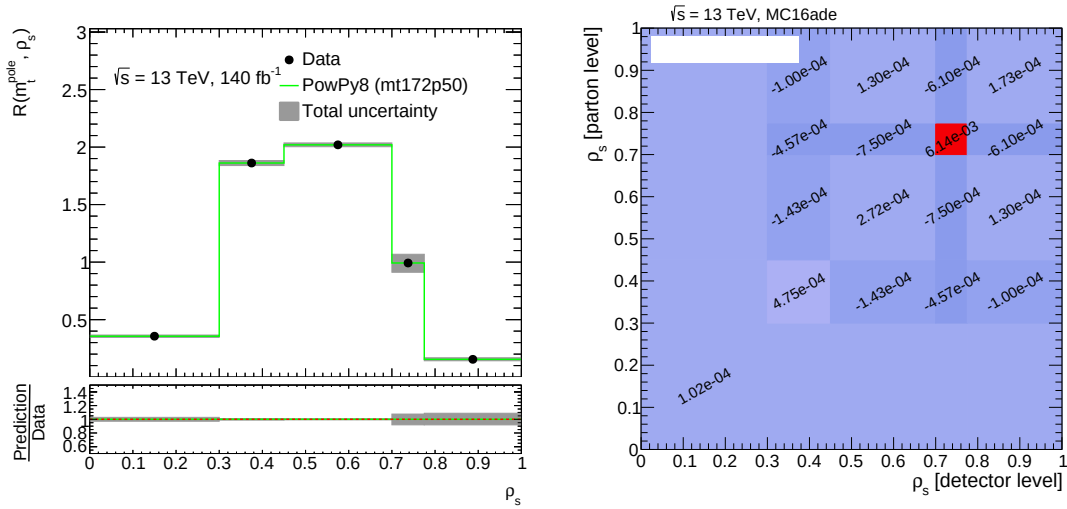


Figura 10.18: Distribució d' $\mathcal{R}$  corregida a nivell partònic per a la mostra d'Asimov i la seua corresponent matriu de covariàncies.

## Mesura de la massa polo del quark top

El valor de la massa polo del quark top ( $m_t^{\text{pole}}$ ) i la seua incertesa associada al fit són determinats a partir de la distribució  $\mathcal{R}$  d'Asimov corregida a nivell partònic. Aquesta extracció és realitza mitjançant un ajust  $\chi^2$  a les prediccions teòriques  $t\bar{t} + \text{jet@NLO}$  a ordre fixe (FO) calculades utilitzant el procés **Powheg-Box-v2**  $t\bar{t}J$  [95]. En l'ajust  $\chi^2$ , el valor determinat de  $m_t^{\text{pole}}$  és el valor que minimitza la següent expressió:

$$\chi^2 = \sum_{i,j} \left[ \mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}} - \mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}}) \right] [V^{-1}]_{ij} \left[ \mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}} - \mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}}) \right]_j, \quad (10.12)$$

on  $\mathcal{R}_{\text{data}}^{t\bar{t}+\text{jet}}$  representa la distribució de dades corregida a nivell partònic,  $\mathcal{R}_{\text{theo@NLO}}^{t\bar{t}+\text{jet}}(m_t^{\text{pole}})$  és la parametrizació de les prediccions teòriques calculades a  $t\bar{t} + \text{jet@NLO}$  FO, i  $V_{ij}^{-1}$  la matriu de covariancies associada a la distribució de dades corregida. Com  $\mathcal{R}$  és una distribució normalitzada, el primer interval de la distribució ( $0 < \rho < 0.3$ ) s'exclou del sumatori de l'Equació 10.12. La distribució dels valors de  $\chi^2$  obtinguts després de l'ajust es mostra a la Figura 10.19.

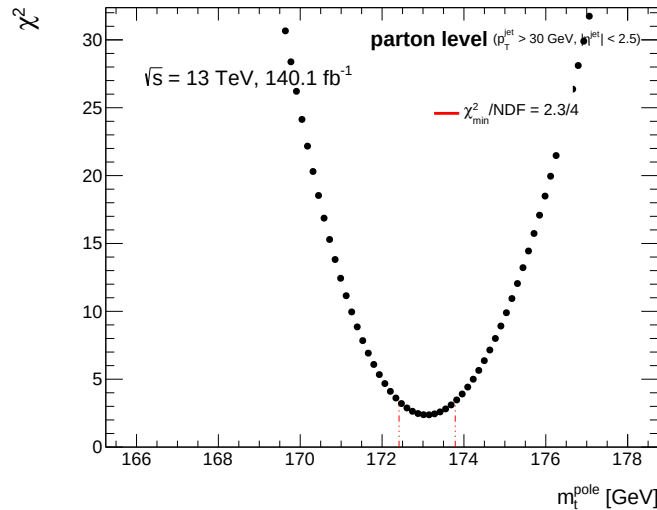


Figura 10.19: Distribució  $\chi^2$  obtinguda mitjançant la comparació entre la distribució d'Asimov  $\mathcal{R}$  corregida a nivell partònic i els càlculs teòrics  $t\bar{t} + \text{jet@NLO}$  FO utilitzant l'Equació 10.12.

La incertesa associada al valor obtingut de l'ajust s'extrau de la variació de massa resultant d'incrementar la distribució  $\chi^2$  una unitat respecte al seu mínim,  $\Delta\chi^2 = 1$ . Aquesta incertesa inclou totes les incerteses estadístiques i sistemàtiques considerades a la determinació de la distribució  $\mathcal{R}$  a nivell partònic.

A més d'aquesta incertesa, és necessari tindre en compte la incertesa teòrica associada als càlculs de les prediccions teòriques  $t\bar{t} + \text{jet@NLO}$  FO. Aquestes incerteses depenen de diversos factors, com són la funció de densitat de partons (PDF) utilitzada en els càlculs, el valor de la constant d'interacció forta ( $\alpha_S$ ) utilitzat en els càlculs, i les variacions en les escales de factorització i renormalització en els càlculs. Considerant totes aquestes incerteses, el resultat obtingut per a massa polo del quark top determinat en la mostra d'Asimov, utilitzant quatre PDFs diferents, són els següents:

**CT18NLO** [218]:

$$m_t^{\text{pole}} = 173.09 \pm 0.69 (\text{fit})_{-0.21}^{+0.34} (\text{PDF} + \alpha_S)_{-0.31}^{+0.43} (\text{scale}) \text{ GeV} \quad , \quad (10.13)$$

**NNPDF3.0** [215]:

$$m_t^{\text{pole}} = 172.93 \pm 0.69 (\text{fit}) \pm 0.45 (\text{PDF} + \alpha_S)_{-0.50}^{+0.37} (\text{scale}) \text{ GeV} \quad , \quad (10.14)$$

**PDF4LHC21** [216]:

$$m_t^{\text{pole}} = 173.07 \pm 0.70 (\text{fit})_{-0.29}^{+0.31} (\text{PDF} + \alpha_S)_{-0.47}^{+0.37} (\text{scale}) \text{ GeV} \quad , \quad (10.15)$$

**ABMP16NLO** [217]:

$$m_t^{\text{pole}} = 172.84 \pm 0.67 (\text{fit})_{-0.17}^{+0.22} (\text{PDF} + \alpha_S)_{-0.29}^{+0.32} (\text{scale}) \text{ GeV}. \quad (10.16)$$

El valor de la incertesa obtingut correspon al nivell de precisió esperat en la mesura d'aquest paràmetre quan es fan servir dades reals. En comparació amb les mesures anteriors de  $m_t^{\text{pole}}$  utilitzant l'observable  $\mathcal{R}$ , l'anàlisi descrita en aquesta tesi té el potencial d'aconseguir la mesura més precisa d'aquest paràmetre en esdeveniments  $t\bar{t} + \text{jet}$  quan s'aplique a les dades reals del detector.



# Acronyms

|               |                                                                             |
|---------------|-----------------------------------------------------------------------------|
| <b>ALICE</b>  | <b>A</b> <b>L</b> arge <b>I</b> on <b>C</b> ollider <b>E</b> xperiment      |
| <b>ATLAS</b>  | <b>A</b> <b>T</b> oroidal <b>L</b> H <b>C</b> <b>A</b> pparatu <b>S</b>     |
| <b>BSM</b>    | <b>B</b> eyond the <b>S</b> tandard <b>M</b> odel                           |
| <b>CERN</b>   | <b>C</b> onseil <b>E</b> uropeen pour la <b>R</b> eserche <b>N</b> ucleaire |
| <b>CMS</b>    | <b>C</b> ompact <b>M</b> uon <b>S</b> olenoid                               |
| <b>CKM</b>    | <b>C</b> abibbo- <b>K</b> obayashi- <b>M</b> askawa                         |
| <b>CL</b>     | <b>C</b> onfidence <b>L</b> evel                                            |
| <b>CR</b>     | <b>C</b> olor <b>R</b> econnection                                          |
| <b>ECAL</b>   | <b>E</b> lectromagnetic <b>C</b> ALorimeter                                 |
| <b>EFT</b>    | <b>E</b> ffective <b>F</b> ield <b>T</b> heory                              |
| <b>EW</b>     | <b>E</b> lectro <b>W</b> eak                                                |
| <b>FF</b>     | <b>F</b> orward- <b>F</b> olding                                            |
| <b>FSR</b>    | <b>F</b> inal- <b>S</b> tate <b>R</b> adiation                              |
| <b>HCAL</b>   | <b>H</b> adronic <b>C</b> ALorimeter                                        |
| <b>HL-LHC</b> | <b>H</b> igh- <b>L</b> uminosity <b>L</b> H <b>C</b>                        |
| <b>ID</b>     | <b>I</b> nnner <b>D</b> etector                                             |
| <b>IR</b>     | <b>I</b> nfra <b>R</b> ed                                                   |
| <b>ISR</b>    | <b>I</b> nital- <b>S</b> tate <b>R</b> adiation                             |
| <b>JER</b>    | <b>J</b> et <b>E</b> nergy <b>R</b> esolution                               |
| <b>JES</b>    | <b>J</b> et <b>E</b> nergy <b>S</b> cale                                    |
| <b>JMR</b>    | <b>J</b> et <b>M</b> ass <b>R</b> esolution                                 |

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|                |                                               |
|----------------|-----------------------------------------------|
| <b>JMS</b>     | <b>Jet Mass Scale</b>                         |
| <b>JVT</b>     | <b>Jet Vertex Tagger</b>                      |
| <b>LHC</b>     | <b>Large Hadron Collider</b>                  |
| <b>LHCb</b>    | <b>Large Hadron Collider beauty</b>           |
| <b>LL</b>      | <b>Leading Log</b>                            |
| <b>LO</b>      | <b>Leading Order</b>                          |
| <b>MC</b>      | <b>Monte Carlo</b>                            |
| <b>MPI</b>     | <b>Multi-Parton Interactions</b>              |
| <b>ME</b>      | <b>Matrix Element</b>                         |
| <b>MS</b>      | <b>Muon Spectrometer</b>                      |
| <b>NLO</b>     | <b>Next-to-Leading Order</b>                  |
| <b>NLL</b>     | <b>Next-to-Leading Log</b>                    |
| <b>NNLO</b>    | <b>Next-to-Next-to-Leading Order</b>          |
| <b>NP</b>      | <b>Nuisance Parameter</b>                     |
| <b>PDF</b>     | <b>Parton Density Function</b>                |
| <b>pdf</b>     | <b>probability density function</b>           |
| <b>PLF</b>     | <b>Profile Likelihood Fit</b>                 |
| <b>PLU</b>     | <b>Profile Likelihood Unfolding</b>           |
| <b>POI</b>     | <b>Parameter Of Interest</b>                  |
| <b>PS</b>      | <b>Parton Shower</b>                          |
| <b>QCD</b>     | <b>Quantum ChromoDynamics</b>                 |
| <b>QED</b>     | <b>Quantum ElectroDynamics</b>                |
| <b>QFT</b>     | <b>Quantum Field Theory</b>                   |
| <b>RGE</b>     | <b>Renormalization Group Equations</b>        |
| <b>SM</b>      | <b>Standard Model</b>                         |
| <b>SPA-Net</b> | <b>Symmetry Preserving Attention Networks</b> |
| <b>SSB</b>     | <b>Spontaneous Symmetry Breaking</b>          |
| <b>TA</b>      | <b>Track-Assisted</b>                         |

|                         |                                                                           |
|-------------------------|---------------------------------------------------------------------------|
| <b>UE</b>               | <b>U</b> nderlying <b>E</b> vent                                          |
| <b>UV</b>               | <b>U</b> ltra <b>V</b> iolet                                              |
| <b>WP</b>               | <b>W</b> orking <b>P</b> oint                                             |
| <br>                    |                                                                           |
| $pp$                    | proton-proton                                                             |
| $p\bar{p}$              | proton-antiproton                                                         |
| $\sqrt{s}$              | center-of-mass energy                                                     |
| $\overline{MS}$         | modified minimal subtraction renormalization mass scheme                  |
| MSR                     | MSR renormalization mass scheme                                           |
| $t\bar{t}$              | top-antitop pair                                                          |
| $t\bar{t} + \text{jet}$ | top antitop pair produced in association with an additional energetic jet |





# List of Publications

- [I] ATLAS Collaboration, “Measurement of the ATLAS Detector Jet Mass Response using Forward Folding with  $80 \text{ fb}^{-1}$  of  $\sqrt{s} = 13 \text{ TeV}$  pp data,” July 2020. [ATLAS-CONF-2020-022](#).  
*Responsible of the large- $R$  jet mass calibration from  $V$ +jets events.*
- [II] ATLAS Collaboration, “Measurement of the top quark pole mass in dileptonic  $t\bar{t}$  +jet events with the ATLAS detector at 13 TeV”, 2023. **Under internal approval**.  
→ Link for ATLAS members: [ATL-COM-PHYS-2020-177](#).  
*Contributions to the code development and cross-check studies.*
- [III] ATLAS Collaboration, “Measurement of the top quark MC mass parameter and the top quark pole mass in semileptonic  $t\bar{t}$  +jet events with the ATLAS detector at 13 TeV”, 2023. **Under internal approval**.  
→ Link for ATLAS members: [ATL-COM-PHYS-2023-863](#).  
*Responsible for training the ML model for the event reconstruction, the construction of the profile maximum likelihood fit to extract the top quark MC mass parameter, and the parton level fit to extract the top quark pole mass.*



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