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Study of the di-tau Drell-Yan process with the ATLAS experiment: a probe for new physics in the Standard Model flavour sector

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*A Vito, Gabriella
e Vittorio*

“The Standard Model is the sea of particle physics, what does it conceal in particle physics that is new and more fundamental? The discovery of the tau was new land in the sea of two generations. Perhaps the tau will lead us out of the sea of the Standard Model.”

MARTIN L. PERL - Nobel Laureate in 1995 for the discovery of the tau lepton.

Abstract

The ATLAS experiment at the Large Hadron Collider (LHC) has recorded 140 fb^{-1} of proton-proton (pp) collisions at $\sqrt{s} = 13 \text{ TeV}$ in the years 2015-2018. This dataset is fully exploited in this thesis to perform a search for leptoquark particles in di-tau Drell-Yan final states. The main aspects of the analysis are outlined, with particular attention to the estimate of the background of hadronic jets misidentified as hadronic taus. Part of the thesis is also devoted to the ATLAS L0Muon barrel trigger upgrade project, which is ongoing in view of the upcoming High-Luminosity LHC program, with focus on the Sector Logic readout firmware design and implementation.

Acknowledgments

This thesis is the outcome of the work of three years in the ATLAS experiment, which I joined as a PhD student in Sapienza University of Rome. The work I have done has been performed in close collaboration with several people, which I would like to thank very much.

Many thanks to my thesis advisors, Dr. Matteo Bauce and Prof. Stefano Giagu for making this project possible and for your supervision during the three years. I am deeply grateful to have had the possibility to work on a quite interesting topic, which is in my opinion also very well set in view of the upcoming physics programs of the LHC and beyond. Thank you also to Dr. Aleandro Nisati, which served as PhD board referee for this project, and contributed to its development with many useful suggestions.

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Introduction

The Standard Model (SM) of particle physics is currently the most accurate description of the elementary constituents of matter and the fundamental forces: the weak, the strong, and the electromagnetic interactions. Nevertheless the SM cannot be considered a complete theory and beyond Standard Model scenarios are investigated at the large Hadron Collider (LHC). The ATLAS experiment is one of the particles detectors installed at the LHC and recorded in the years 2015-2018 a dataset of pp collisions at a center-of-mass energy of $\sqrt{s} = 13$ TeV, which is exploited in this thesis.

According to the Standard Model, leptons are divided into three families, having equal quantum numbers and differing solely in their mass: electrons, muons and taus. Interest has been raised in recent years for precision measurements involving tau leptons, as the B -physics anomalies [24], measured by the LHCb experiment at the LHC, hint for new physics more strongly coupled to the third generation of leptons and quarks, hence violating the SM lepton flavour universality in the third generation [42]. Such new physics models predict the existence of leptoquark particles, consisting in exotic mediators carrying both leptonic and color quantum numbers, and therefore able to couple to both leptons and quarks in the same interaction vertex. The Drell-Yan process with tau leptons, $pp \rightarrow \tau\tau$, plays a crucial role in this context, as exotic leptoquark models predict diagrams generating excesses of events and interference with the SM Drell-Yan diagram, and can therefore be detected as anomalies in the precision study of the Drell-Yan process.

This thesis presents as main topic a search for leptoquark particles in di-tau Drell-Yan final states, with the ATLAS detector. The analysis is focused on events with a di-tau invariant mass in a range from the Z pole to $O(1)$ TeV and exploits both the semi-leptonic channel, in which one tau decays hadronically and the other decays into an electron or a muon, and the fully-hadronic channel, in which both taus decay hadronically. All aspects of the analysis are covered: the objects definition, trigger pre-selection, events selection, experimental and modelling systematics and the statistical interpretation. The analysis led to the exclusion of vector leptoquark models, in a parameters phase space region very near to the one preferred to explain the B -physics anomalies and further strengthened the exclusions already obtained by the CMS experiment [62].

One of the most critical aspects in the analyses exploiting hadronic taus final states is the presence of a consistent background of hadronic jets misidentified as fake hadronic taus, which has to be carefully estimated. The assessment of this background is performed in the ATLAS Collaboration via a specific technique - the Fake Factors method - based on the measurement of fake-rates directly from

data. This thesis also presents a detailed explanation of this methodology, together with validation studies covering single- and di-tau final states and an analysis of the sources of uncertainty affecting the extrapolated backgrounds of fake taus.

A part of this thesis has also been devoted to hardware work for the Phase-II upgrade of the muon trigger system of the ATLAS experiment, in view of the upcoming High-Luminosity LHC program. The High-Luminosity LHC (HL-LHC) is the CERN long term program aiming at fully exploiting the LHC physics potential by operating the accelerating machine to the highest luminosity achievable. An instantaneous luminosity of $\mathcal{L} = 7.5 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ is foreseen, corresponding to approximately 200 pp interactions per bunch-crossing and to up to 4000 fb^{-1} integrated luminosity delivered to the experiments at the end of the program.

The ATLAS Collaboration has endorsed a Phase-II trigger architecture based on a single Level-0 hardware trigger using calorimeter and muon spectrometer information with an output readout rate of 1 MHz and a maximum latency of 10 μs , followed by an Event Filter software system, delivering an output rate of 10 kHz to the permanent storage [168]. The L0 muon barrel trigger exploits signals coming from the Resistive Plate Chambers (RPC) gaseous detectors, which are processed in each sector of the ATLAS barrel region by the Sector Logic (SL), an electronic device in charge of assessing the trigger decision.

The Sector Logic of the Phase-II trigger will run a new revised trigger algorithm capable of exploiting the installation of new RPC chambers and recover the acceptance inefficiencies characterizing the current implementation. My role in this part of the project has been to fully re-design and implement the readout functionality of the barrel SL, which is necessary to keep in memory the muon data, while the trigger decision is processed, and propagating the data in case of positive trigger decision.

The Phase-II upgrade of the muon trigger system will contribute also to the development of the physics program of the ATLAS experiment, including measurement and searches involving tau-lepton final states. Since the tau lepton can decay into muons and neutrinos, the upgrade of the muon system will improve the measurement of the leptonically decaying taus. In particular, the upgrade of the trigger electronics, will enable the ATLAS experiment to cope with the very high rate of physics events in the high-luminosity environment of Phase-II, while keeping at the same time the trigger thresholds low, enlarging the phase-space fiducial regions in which physics measurements can be done.

For this reason the hardware upgrades of the ATLAS experiment, as well as the improvements in the experimental techniques for the measurement of tauonic final states will constitute the baseline for future strategies in looking for new physics via the precision study of the Standard Model.

Personal contributions

The work presented in this thesis has been completed within the ATLAS Collaboration in close contact with colleagues. I hereby give a summary of the main contributions coming from my own activity, which are also specified at the beginning of each chapter in *italic*. Figures and tables produced by others are referred as such

and a citation is included in each caption. All other figures not presenting a citation have been produced by me in collaboration with others or by my own.

Search for leptoquarks in di-tau Drell-Yan final states. This is the main physics result delivered in this thesis, and is reported in Chapter 4. I have been one of the main analysers in this physics analysis, joining the team from the very beginning (even in the preliminary phase before the official ATLAS kick-off meeting), to the very end. I have been involved in almost all aspects of the analysis, more in detail:

- I collaborated on defining the physics goals and setting the analysis strategy, taking into account of the status of the art on tau physics in the ATLAS Collaboration previous to this work;
- I worked in the development of the software framework to process the dataset and calibrate all the physics analysis objects;
- I collaborated in the identification of the main analysis backgrounds, to be modelled via Monte Carlo simulation. I have developed the data-driven estimate of the background of hadronic jets misidentified as hadronic taus. This part of the analysis has been developed almost entirely by me;
- I studied the modelling uncertainties to be attributed to this measurement, with particular attention to the top and ttbar modelling systematics;
- I collaborated in processing the inputs for the statistical interpretation of the results, and the comparison of the analysis results to the predictions made by theorists.

The Fake Factors method for the estimate of fake hadronic taus. The Fake Factors method is the standard technique in the ATLAS Collaboration to measure with a data-driven approach the background of hadronic jets misidentified as hadronic taus. The results on this topic, reported in Chapter 3, are classified among the Tau Combined Performance works, whose aim is to improve the general techniques to measure tau leptons in ATLAS, providing benefits to all ATLAS analyses with taus.

My role in this context has been that of using the di-tau search for leptoquarks, which is the main topic of this thesis, to deliver a validation of the Fake Factors method with di-tau final states. I used a same-sign validation region (equal to the opposite sign signal region of the leptoquark physics analysis but requiring that the two taus have the same charge), to demonstrate that the Fake Factors Method can be implemented even in di-tau final states, taking into account of all the combinatorial possibilities in which fake taus can contribute to a di-tau final state. I also scrutinized all the possible sources of uncertainties which can arise in the method implementation, and proposed a new methodology to estimate some uncertainties, alternative to the one used as standard in ATLAS, which I presented to the collaboration in Tau Combined Performance meetings.

Readout firmware for the Phase-II L0 Muon barrel trigger. This part of the work is classified among the hardware developments in preparation for the High-Luminosity LHC program, and is reported in Chapter 5. I joined the team which is working to the re-design of the L0Muon barrel trigger and participated in the design and test of the Sector Logic board, which will be used to run the muon trigger algorithm in Phase-II.

I designed from scratch the Sector Logic readout functionality, in charge of acquiring and keep data in memory, while the accept/reject decision is taken from the trigger algorithm. I developed the firmware in VHDL language, simulated it via the Vivado simulation toolkit, and implemented it in a Xilinx FPGA. I also contributed to the integration of this firmware with the other components (trigger firmware and I/O firmware) to deliver the complete SL firmware to ATLAS, and participated in the preliminary testing campaigns of the board prototype at the CERN Laser Room experimental facility. The complete firmware has passed the ATLAS Preliminary Design Review in 2022, after examination by a board of experts.

Muon desk operations in the ATLAS control room. This is an operations activity, which is briefly described in Appendix B. I have been qualified during the PhD years as muon desk shifter and attended shifts in the ATLAS Control Room. I participated to the Run 3 data acquisition taking shifts at the muon desk in the years 2023 and 2024.

Hepscape! The high energy physics escape room. This is an outreach project to which I participated along the three years of the PhD and is briefly described in Appendix C. The project consists in running an escape room focused on particle physics topics to young people and children. I have been one of the beginners of this project, which started in 2021 with an outreach funding grant from Sapienza University assigned to me and other two PhD students in Rome, and I joined the runs of the activity in several festivals and fairs in the years 2021-2023. The project has spread over several institutes in Italy, and has recently been endorsed by the INFN third mission committee with a stable annual financing. More than 4500 people have visited “Hepscape!” as of today.

Publications including the thesis work

The original work presented in this thesis will be included in ATLAS publications.

A first paper will include the results of the leptoquark search presented in Chapter 4, together with an unfolded cross section measurement of the di-tau Drell-Yan process. This paper is in the process of being written, after several iterations with the relative Editorial Board. A second paper will be issued, including the results on the Fake Factors method. Also this publication is currently at the level of the Editorial Board formed and paper editors have been appointed to start the writing. The hardware work is included in ATLAS internal technical documentation, and specifically in Ref. [170]. The outreach activities have been documented in conference proceedings, specifically in Refs. [190, 191].

Chapter 1

Theoretical foundations and motivations

In this chapter, after outlining the Standard Model formalism, I present the flavour anomalies and how they can be used to build beyond Standard Model theories to search for new physics. This material is the outcome of personal study of the status of the art, as well as direct interaction and discussion with theorists involved in proposing the precision study of the Standard Model flavour sector as an alternative strategy to access new physics, other than trying to address the Higgs hierarchy problem.

The Standard Model of Particle Physics (SM) is currently the most accurate description of fundamental interactions between elementary particles and has been tested to an unprecedented accuracy in decades of precision measurements. Nevertheless experimental evidences (dark matter and dark energy, the neutrino masses, the matter/antimatter asymmetry) show that the SM is not the ultimate theory of Nature, motivating the search for new physics. Interest has been raised recently in investigating the Standard Model flavour sector, looking for new physics, which could manifest as processes violating lepton flavour universality or exotic mediators coupling both to leptons and quarks, called leptoquarks.

This chapter presents a general overview of the theoretical framework in which the physics part of this thesis is embedded. A summary of the SM and its features is given in Section 1.1, with a particular focus on the SM flavour sector, provided in Section 1.2. A description with the flavour anomalies, measured by experimental collaborations in B mesons decays, is presented in Section 1.3, while leptoquarks are described in Section 1.4 and are proposed as a possible explanation for these anomalies. Finally, Section 1.5 describes the Drell-Yan process with tau leptons in the final state and its usage for searching leptoquarks particles, which is the main topic of this thesis.

1.1 The Standard Model of Particle Physics

The Standard Model of Particle Physics (SM) describes three out of the four fundamental forces of nature, the strong, the electromagnetic and the weak force.

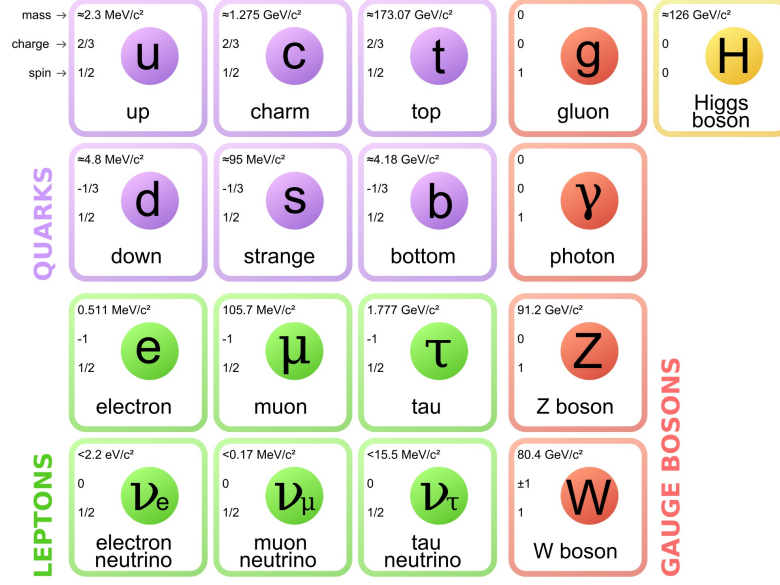


Figure 1.1. Summary of Standard Model elementary particles and their properties.

The gravitational force appears to have its effects on a significantly different energy scale and is not described by this theory. The fundamental components of the Universe are called elementary particles and can be divided in *matter* particles and *mediators*, with the latter generating the interactions between the former. An overview is presented in Figure 1.1.

The matter component is made of spin $1/2$ particles, called *fermions*. Fermions are organised in three *generations* of increasing proper mass, each of which is made by an electrically charged lepton (e^- , μ^- , τ^-) and its neutrino (ν_e , ν_μ , ν_τ) together with an up type (u , c , t) and a down type (d , s , b) quark. Up- and down- type quarks have a fractional electric charge of $2/3$ and $-1/3$ respectively, while neutrinos have zero charge. Quarks also carry a *colour charge* which is a property of the theory of strong interactions.

The interactions between matter particles are mediated by spin 1 vector bosons. In particular, the $W^\pm$ and the Z bosons are associated to the weak interaction, the photon (γ) to the electromagnetic interaction, while the eight gluons (g) are associated to the strong force. The Higgs boson is instead a spin 0 particle which belongs to the matter component of the SM, but is also responsible for generating the mass of the particles.

1.1.1 Symmetries and gauge theories

From a formal viewpoint, the Standard Model is a quantum field theory [1] [2] in which particles are described by local excitations of fields $\psi(x)$, evaluated in the space-time point x . Dynamics can be described by a lagrangian density $\mathcal{L}(\psi, \partial_\mu \psi)$, which is a function of the field and its space-time derivatives. The lagrangian structure can be identified in the theoretical framework of Gauge Theories, developed by Yang and Mills and further used by Glashow, Salam and Weinberg to build the

SM, starting from the definition of the gauge group of local transformations which leaves the lagrangian invariant. The gauge group itself can be identified looking for the experimental observation of conservation of physical quantities¹ or via physical intuition. The fundamental feature of gauge theories is that they predict the existence of *gauge bosons*, in a number equal to the number of generators of the gauge group, which correspond to mediator particles.

The SM is a gauge theory with lagrangian density

$$\mathcal{L}_{SM} = \mathcal{L}_{QCD} + \mathcal{L}_{EW}$$

which is locally invariant under gauge transformations belonging to the symmetry group

$$SU(3)_C \otimes SU(2)_W \otimes U(1)_Y.$$

The $SU(3)_C$ group refers to colour, the conserved charge of Quantum Chromodynamics (QCD), which describes the interactions between quarks and gluons. The $SU(2)_W \otimes U(1)_Y$ group refers to the electroweak interactions, which conserve weak isospin I and weak hypercharge Y .

1.1.2 Quantum Electrodynamics

A first illustrative example of how symmetries play a role in the way the lagrangian density function is written is Quantum Electrodynamics (QED). QED is an abelian gauge theory describing an electrically charged particle with spin 1/2 and mass m , represented by the field ψ , and a massless vector boson, the photon, accounting for the electromagnetic field and represented by the field A_μ .

The lagrangian density reads

$$\mathcal{L}_{QED} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \bar{\psi}(i\gamma^\mu D_\mu - m)\psi \quad (1.1)$$

where γ^μ are the Dirac matrices², $\bar{\psi} = \psi^\dagger \gamma^0$ is the adjoint field, $F_{\mu\nu}$ is the electromagnetic tensor³ and the covariant derivative D_μ is defined by

$$D_\mu = \partial_\mu - ieA_\mu.$$

The lagrangian is invariant under the unitary joint transformations

$$\begin{aligned} \psi(x) &\rightarrow U(x)\psi(x) = e^{i\alpha(x)}\psi(x) \\ A_\mu &\rightarrow A_\mu(x) + \frac{1}{e}\partial_\mu\alpha(x) \end{aligned}$$

¹In fact, Noether's theorem states that "Each continuous symmetry of the lagrangian density yields to a conserved current and hence to a conserved charge". This implies that, starting from the observation of a conservation law, one can infer the symmetry of the lagrangian generating that conservation.

²It holds $\{\gamma^\mu\gamma^\nu\} = 2g^{\mu\nu}I$, where $g^{\mu\nu}$ is the metric tensor in flat space-time and I is the identity matrix.

³The electromagnetic tensor is defined by

$$F_{\mu\nu} = \partial_\nu A_\mu - \partial_\mu A_\nu.$$

where $\alpha(x)$ is an arbitrary function of space-time coordinates. The symmetry group of these transformations is $U(1)$ and the photon is the gauge boson corresponding to its generator.

The coupling constant between the fermion and the photon fields is e , the electric charge of the fermion, representing the intensity of the electromagnetic interaction between the two particles. As consequence of invariance of $\mathcal{L}_{QED}$ under $U(1)$ transformations, the Noether's current $J^\mu = \psi\gamma^\mu\psi$ and the electric charge are conserved.

1.1.3 Strong Interactions

The strong force involves quarks and gluons in interactions which conserve the colour charge; quarks and gluons appear in six different colours (red, green, blue and their corresponding anticolours).

Evidence of colour as a quantum number conserved in the strong interactions has been provided both by the decay of the Δ^{++} resonance and by the study of $R = \sigma_{\text{hadrons}}/\sigma_{\text{muons}}$ at increasing $\sqrt{s}$ in e^+e^- scattering. Coloured particles have never been observed singularly (*colour confinement*), i.e. only colour-neutral (*white*) states can be measured.

QCD is the non-abelian gauge theory which describes strong interactions. The gauge group of the theory is $SU(3)$: if we assume only one quark flavour is involved, a quark field changes under a transformation of this group as

$$q(x) \rightarrow U(x)q(x) = e^{-igs\alpha_a(x)T_a}q(x), \quad (1.2)$$

where $g_S = 4\pi\alpha_S$ is the coupling constant of strong interactions, α_a are arbitrary functions and T_a are the eight generators of $SU(3)$ ⁴.

The lagrangian density of QCD can be written as

$$\mathcal{L} = -\frac{1}{4} \sum_a F_{\mu\nu}^a F^{a,\mu\nu} + \bar{q} (i\gamma^\mu D_\mu - m) q, \quad (1.3)$$

where $F_{\mu\nu}^a$ are tensors defined as

$$F_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a - g_S f^{abc} G_\mu^b G_\nu^c, \quad (1.4)$$

and the covariant derivative is

$$D_\mu = \partial_\mu + igT_a G_\mu^a. \quad (1.5)$$

According to gauge theories, the eight generators of $SU(3)$ call for the introduction of eight fields, the gluons G^a , which are the mediators of the strong interaction and transform as

$$G_\mu^a \rightarrow G_\mu^a - \frac{1}{g_S} \partial_\mu \alpha_a - f_{abc} \alpha_b G_\mu^c. \quad (1.6)$$

⁴It holds

$$[T_a T_b] = if_{abc} T_c,$$

where f_{abc} are the structure constants of $SU(3)$. Notice that structure constants explicitly show non-abelianity of the theory: for an abelian theory $f_{abc} = 0$. Notice also that U and T_a are 3×3 matrices ($a, b, c = 1, 2, 3$) and summation over repeated indices is implied.

An important feature of QCD is *asymptotic freedom*: quarks interact weakly at high energies, hence allowing for perturbative calculations and the free-quark approximation, but strongly at low energies, preventing the unbinding of baryons and mesons.

1.1.4 Electroweak Interactions

The roots of the electroweak theory fall back to 1934, when Enrico Fermi provided a theoretical description of the β radioactive decay [3]

$$n \rightarrow p + e^- + \bar{\nu}_e$$

which happens at very low rates due to the involvement of weak interactions rather than electroweak or strong interactions. Fermi's description happens via the contact interaction

$$\mathcal{L} = -G_F \left(\bar{\psi}_p \gamma^\mu \psi_n \right) \left(\bar{\psi}_e \gamma^\mu \psi_\nu \right) + \text{h.c.},$$

where G_F is the Fermi constant. This picture is not renormalizable⁵; thus it offers a good effective description of weak interactions at low energies⁶. Experiments show that weak interactions involve both charged and neutral currents: the first account for transitions between the up- and down-type leptons or quarks, the latter conserve flavour.

The electroweak theory aims at unifying the theory of weak interactions and electromagnetic interactions. The symmetry group of the theory is

$$SU(2)_W \otimes U(1)_Y.$$

Fermions are classified according to their chirality eigenstate, i.e. in left-handed and right-handed fields $\psi_{L,R}$, where

$$\begin{aligned} \psi_L &= P_L \psi = \frac{1}{2} (1 - \gamma^5) \psi, \\ \psi_R &= P_R \psi = \frac{1}{2} (1 + \gamma^5) \psi, \end{aligned}$$

and $P_{L,R}$ is the left (right)-handed projection operator, while $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$. Left-handed fermions are paired in doublets with isospin $I = 1/2$, while right-handed ones are $I = 0$ singlets. Leptons are replicated in three families with the same quantum numbers,

$$L^i = \left\{ \begin{pmatrix} \nu_e \\ e \end{pmatrix}_L, \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix}_L, \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}_L \right\}, \quad e_R^i = \{(e)_R, (\mu)_R, (\tau)_R\},$$

⁵Renormalizability arises when the overall dimension of the operators in the lagrangian is $[E]^n$ with $n \leq 4$. Here $[\psi] = [E]^{3/2}$, so the overall dimension of $\mathcal{L}$ is $[E]^6$. The correct dimensionality is achieved introducing the gauge boson propagator, which gives a contribution $[E]^{-2}$.

⁶Precisely, the effective Fermi theory works for energies $E \ll m_{W,Z} \approx 80$ GeV. For higher energies the W and Z bosons propagators become non-negligible and the complete (renormalizable) electroweak theory is needed.

and analogously quarks,

$$Q_L^i = \left\{ \begin{pmatrix} u \\ d \end{pmatrix}_L, \begin{pmatrix} c \\ s \end{pmatrix}_L, \begin{pmatrix} t \\ b \end{pmatrix}_L \right\}, \quad u_R^i = \{(u)_R, (c)_R, (t)_R\}, \quad d_R^i = \{(d)_R, (s)_R, (b)_R\}.$$

while right-handed neutrinos are not involved in electroweak interactions. Weak hypercharge and electric charge are linked to weak isospin by the Gell-Mann–Nishijima formula

$$Q = I_3 + \frac{Y}{2},$$

where I_3 is the third component of the weak isospin.

Hypercharge symmetry involves both chiralities, i.e. the lagrangian density is invariant under the transformations of the $U(1)$ group,

$$\psi_{L,R} \rightarrow e^{i\alpha(x)Y} \psi_{L,R},$$

while weak isospin symmetry involves only left-handed doublets, with invariance under transformations of $SU(2)$,

$$\psi_L \rightarrow e^{i\beta_a(x)\frac{\tau^a}{2}} \psi_L,$$

where $\tau^a/2$ are the generators of $SU(2)$ ⁷ and summation over the index $a = 1, 2, 3$ is implied.

According to gauge theories the general form for a lagrangian invariant under the transformations group defined by the generators λ^a reads

$$\mathcal{L} = -\frac{1}{4} \sum_V F_V^{\mu\nu} F_{V,\mu\nu} + i \sum_f \bar{f} \gamma^\mu D_\mu f, \quad (1.7)$$

where summations run over all gauge vector bosons V and fermion fields f . The covariant derivative D_μ is defined as

$$D_\mu = \partial_\mu - ig_V (\lambda^a V_a)_\mu,$$

where the g_V is the generic coupling constant of a fermion to the V field and V^a is the field tensor representing the gauge boson. Considering the electroweak gauge group and a single fermion field ψ Eq. (1.7) explicitly becomes

$$\mathcal{L}_{EW} = -\frac{1}{4} W_{\mu\nu}^a W_a^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} + i \bar{\psi} \gamma^\mu D_\mu \psi \quad (1.8)$$

with

$$\begin{aligned} W_{\mu\nu}^a &= \partial_\nu W_\mu^a - \partial_\mu W_\nu^a - g\epsilon^{abc} W_\mu^b W_\nu^c, \\ B_{\mu\nu} &= \partial_\nu B_\mu - \partial_\mu B_\nu, \end{aligned}$$

and

$$D_\mu = \partial_\mu - ig W_\mu^a I_a - i \frac{g'}{2} B_\mu Y,$$

⁷We adopt the convention in which τ^a ($a = 1, 2, 3$) are the Pauli matrices.

where g and g' are the $SU(2)$ and $U(1)$ coupling constants respectively. Four gauge fields have been introduced corresponding to the generators of the gauge group: the triplet of fields W_μ^i ($i = 1, 2, 3$) corresponds to the three generators of $SU(2)$, while the B_μ field corresponds to the generator of $U(1)$. Physical fields representing the real observed bosons - the photon, the Z boson and the $W^\pm$ bosons - can be obtained with the linear combinations

$$A^\mu = \sin \theta_W W_3^\mu + \cos \theta_W B^\mu, \quad (1.9a)$$

$$Z^\mu = \cos \theta_W W_3^\mu - \sin \theta_W B^\mu, \quad (1.9b)$$

$$W_\pm^\mu = \frac{W_1^\mu \pm iW_2^\mu}{\sqrt{2}}, \quad (1.9c)$$

where θ_W is the Weinberg angle that is linked to the coupling constants g and g' via the relations

$$\sin \theta_W = \frac{g'}{\sqrt{g^2 + g'^2}},$$

$$\cos \theta_W = \frac{g}{\sqrt{g^2 + g'^2}}.$$

Moreover, the electric charge e can be written as $e = g \sin \theta_W$.

The interaction lagrangian of fermions with gauge bosons can be explicitly obtained substituting Eq. (1.9a) (1.9b) (1.9c) into the third term of Eq. (1.8) and neglecting all fermions kinetic terms

$$\begin{aligned} \mathcal{L}_f^{\text{int}} = & \frac{g}{\sqrt{2}} \left(J^{\mu-} W_\mu^+ + J^{\mu+} W_\mu^- \right) \\ & + \frac{g}{\cos \theta_W} \left[J_3^\mu - \sin^2 \theta_W J_{\text{em}}^\mu \right] Z_\mu + g \sin \theta_W J_{\text{em}}^\mu A_\mu \end{aligned} \quad (1.10)$$

where

$$J_-^\mu = \bar{\psi}_L \gamma^\mu \tau^- \psi_L, \quad J_+^\mu = \bar{\psi}_L \gamma^\mu \tau^+ \psi_L, \quad (1.11a)$$

$$J_3^\mu = \bar{\psi}_L \gamma^\mu \frac{\tau^3}{2} \psi_L, \quad (1.11b)$$

$$J_{\text{em}}^\mu = \bar{\psi}_L \gamma^\mu Q \psi_L + \bar{\psi}_R \gamma^\mu Q \psi_R, \quad (1.11c)$$

$\tau^\pm = \frac{1}{2} (\tau^1 \pm i\tau^2)$ and Q is the charge operator. Notice that charged $W^\pm$ vector bosons are coupled to the left-handed fermions only, while the neutral Z boson and the photon are coupled to both to left- and right-handed fermions, through the electromagnetic current J_{em}^μ .

1.1.5 The Higgs boson and spontaneous symmetry breaking

The Higgs boson is the particle responsible for mass acquisition of all the SM matter content via the *Higgs-Brout-Englert* mechanism [4] [5]. The Higgs field is a scalar

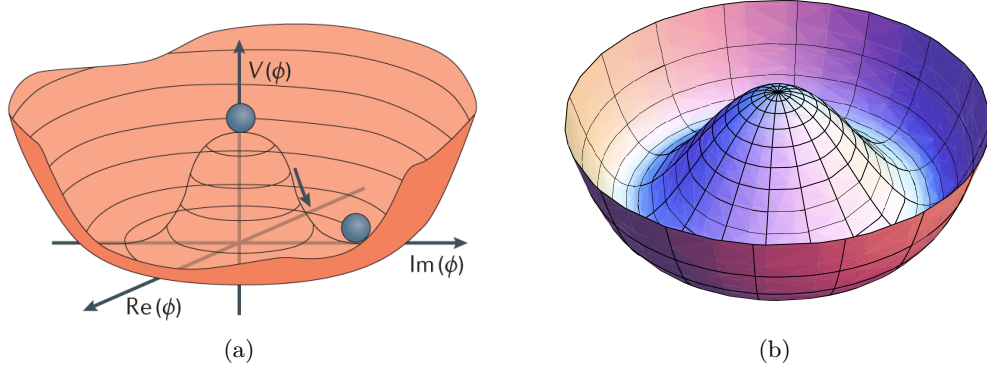


Figure 1.2. Graphical representation of the Higgs potential $V(\phi)$, often called *mexican hat* due to its shape.

isospin doublet, eigenstate of weak isospin with $I = 1/2$, $I_3 = -1/2$ and hypercharge $Y = 1$ ⁸,

$$\phi(x) = \begin{pmatrix} \phi^+(x) \\ \phi^0(x) \end{pmatrix} = \begin{pmatrix} \frac{\pi_1(x) + i\pi_2(x)}{\sqrt{2}} \\ \frac{\sigma(x) + i\pi_3(x)}{\sqrt{2}} \end{pmatrix} \quad (1.12)$$

where ϕ^+ and ϕ^0 are complex fields, while $\vec{\pi} = (\pi_1, \pi_2, \pi_3)$ and σ represent their real components. An additional term is introduced in the lagrangian density, which reads as

$$\mathcal{L}_H = (D_\mu \phi)^\dagger (D^\mu \phi) - V(\phi), \quad (1.13)$$

where the potential term is expressed as

$$V(\phi) = -\mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2 = -\mu^2 \phi^2 + \lambda \phi^4, \quad (1.14)$$

with $\lambda > 0$ and $-\mu^2 < 0$. The potential V defined in Eq. (1.14) has a finite lower bound and defines a ground state $|0\rangle$ (the *vacuum state*) which is infinitely degenerate in $(\sigma, \vec{\pi})$ space.

The degeneracy can be removed via the spontaneous symmetry breaking (SSB) procedure, which consists in adding a *driving term* in the lagrangian

$$\mathcal{L}' = \mathcal{L} + h\sigma,$$

which forces the potential to get a unique minimum in

$$\phi = \phi_0 = \begin{pmatrix} 0 \\ \frac{v}{\sqrt{2}} \end{pmatrix} \equiv \begin{pmatrix} 0 \\ \eta \end{pmatrix},$$

and then taking the limit of arbitrary small driving term ($h \rightarrow 0$). The expectation value of the field ϕ in the vacuum state is non-zero

$$\langle 0 | \phi | 0 \rangle = \frac{v}{\sqrt{2}} \equiv \eta \neq 0.$$

⁸Using the Gell-Mann Nishijima formula the electric charge is $Q = 0$ for the lower field component and $Q = 1$ for the upper one.

and $v = \sqrt{\mu^2/\lambda}$ holds in the limit $h \rightarrow 0$. The limit of arbitrary small driving term ($h \rightarrow 0$) restores the original symmetry of the lagrangian, however a preferential direction has been chosen in $(\sigma, \bar{\pi})$ space for the ground state and the minimum energy configuration is no longer symmetric. We therefore say that the symmetry is spontaneously broken by the ground state⁹.

The mass of $W^\pm$ and Z bosons

To identify the mass of the gauge bosons we have to translate the Higgs doublet in Eq. (1.12) into its exponential representation

$$\phi = e^{i \frac{\bar{\pi}(x) \cdot \bar{\tau}}{2v}} \begin{pmatrix} 0 \\ \frac{v+\sigma}{\sqrt{2}} \end{pmatrix},$$

and apply an $SU(2)_W$ rotation which brings to the unitary gauge¹⁰

$$\phi' = e^{i \bar{\alpha}(x) \cdot \frac{\bar{\tau}}{2}} \phi = \begin{pmatrix} 0 \\ \frac{v+\sigma}{\sqrt{2}} \end{pmatrix}, \quad (1.15)$$

where $\bar{\alpha}(x) = -\frac{\bar{\pi}(x)}{v}$ has been chosen. If we consider the kinetic part of the lagrangian density of Eq. (1.13), replacing ϕ with Eq. (1.15), one has¹¹

$$(D_\mu \phi)^\dagger (D^\mu \phi) = \frac{v^2}{8} \left[g^2 \left((W_\mu^1)^2 + (W_\mu^2)^2 \right) + (g' B_\mu - g W_\mu^3)^2 \right].$$

Using Eq. (1.9a) (1.9b) (1.9c) the boson masses can be identified: $m_W = gv/2$, Z , $m_Z = \sqrt{g^2 + g'^2}v/2$ and $m_\gamma = 0$. Finally, it holds

$$m_W/m_Z = \cos \theta_W. \quad (1.16)$$

The mass of the fermions

The mass of the fermions is generated by their Yukawa coupling with the Higgs field. The interaction lagrangian between the Higgs and the fermions reads

$$\mathcal{L}_{f\phi} = \sum_i g_i \left(\bar{L}^i \phi e_R^i + \bar{e}_R^i \phi^\dagger L^i \right), \quad (1.17)$$

where $L^i = (\nu_e^i, e^i)_L^T$ and index $i = 1, 2, 3$ runs over the three flavour families. Substituting the Higgs field in the form of Eq. (1.15) (i.e. after SSB, in the unitary gauge) the interaction lagrangian becomes

$$\mathcal{L}_{f\phi} = \sum_i g_i \frac{v+\sigma}{\sqrt{2}} \left(\bar{e}_L^i e_R^i + \bar{e}_R^i e_L^i \right) = \sum_i g_i \frac{v+\sigma}{\sqrt{2}} \bar{e}^i e^i.$$

⁹The adjective “spontaneously” means that the system *naturally* tends to manifest itself in an asymmetric solution, despite being intrinsically symmetric. The original symmetry of the lagrangian, in fact, is indeed restored in the limit $h \rightarrow 0$ as can be also understood thinking that the choice to privilege the σ direction in the dynamical solution is arbitrary. More precisely, we should talk of spontaneously *hidden* symmetry.

¹⁰The unitary gauge is the particular gauge in which Goldstone bosons, the massless particles predicted by Goldstone theorem, are cancelled. Goldstone bosons are non-physical particles which represent the longitudinal degree of freedom of the massive gauge bosons.

¹¹We put $\sigma = 0$ to avoid writing interactions terms between σ field and gauge bosons.

and we can recognize terms for the fermion masses, proportional to their coupling to the Higgs:

$$m_e = g_e \frac{v}{\sqrt{2}}, \quad m_\mu = g_\mu \frac{v}{\sqrt{2}}, \quad m_\tau = g_\tau \frac{v}{\sqrt{2}}.$$

1.2 The flavour sector of the Standard Model

Flavour deals with the fact that Standard Model leptons and quarks are replicated in three families (also called *generations*) described exactly by the same quantum numbers and differing solely in their mass, with the third family being much heavier than the first two. The dynamical behaviour of leptons with respect to the electroweak interaction is also the same: this implies that decay branching fractions and cross sections of processes involving leptons from different families are either exactly equal or differ by an amount corresponding only to the different kinematic phase-space factor. This experimental fact, called *lepton universality*, has been extensively tested over the years, first studying the muon decay into electrons in the '50s, then the tau lepton decays into muons and electrons in the '80s, finally measuring Z mediated processes with e^+e^- , $\mu^+\mu^-$, $\tau^+\tau^-$ in the '90s and is confirmed as of today.

Having the same quantum numbers, lepton fields of different flavour families transform in the same way under the electroweak gauge group $SU(2)_W \otimes U(1)_Y$. Hence, under the approximate assumption of null masses $m_e = m_\mu = m_\tau \approx 0$ the lagrangian is invariant under a rotation in flavour space for each fermion field. This yields a global *flavour symmetry* under the group

$$U(3)^5 = U(3)_L \otimes U(3)_{e_R} \otimes U(3)_{Q_L} \otimes U(3)_{u_R} \otimes U(3)_{d_R}, \quad (1.18)$$

which is an accidental symmetry of the SM, meaning it is not imposed a priori but rather emerges as a consequence of the assumptions on which the theory is constructed. Removing the assumption of null masses, the flavour symmetry group of Eq. (1.18) is broken by the Yukawa coupling of the quarks with the Higgs field, and reduces to

$$U(1)^5 = U(1)_B \otimes U(1)_{L_e} \otimes U(1)_{L_\mu} \otimes U(1)_{L_\tau} \otimes U(1)_Y,$$

corresponding to the conservation of baryon number (B), individual lepton family numbers L_e , L_μ , L_τ and the weak hypercharge Y .

Flavour dynamics, consisting in processes which involve lepton transformation from one family to another, appears solely in the quark sector. Flavour changing charged currents are mediated by $W^\pm$ bosons and transform up-quarks of one family into down-quarks of another family or vice versa, while flavour changing neutral currents (FCNC) are prohibited at tree level in the SM and can happen only at loop level with suppression ruled by the Glashow-Iliopoulos-Maiani (GIM) mechanism [6].

1.2.1 The origins of flavour physics

Our current understanding of flavour is the result of decades of experimental searches and theoretical intuition. The very first idea of quark mixing goes back to the experimental observation that the Fermi constant G_F extracted from the β decay of strange nucleons was smaller than the one measured in standard β decay [3].

In 1962 Nicola Cabibbo reconciled this observation with the universality of weak interactions by describing the weak charged current as an admixture of $\Delta S = 0$ and $\Delta S = 1$ currents [7].

$$J_+^\mu = \cos \theta_c J_+^\mu (\Delta S = 0) + \sin \theta_c J_+^\mu (\Delta S = 1) \quad (1.19)$$

where $J_+^\mu = \bar{Q}_L \gamma^\mu \tau^+ Q_L$ is the charged current, as reported in Eq. (1.11a), and θ_c is called the Cabibbo angle. In those times only u , d , s quarks were known, hence the only possibility to build two $SU(2)_W$ doublets was

$$Q_L^{\Delta S=0} = \begin{pmatrix} u \\ d \end{pmatrix}_L, \quad Q_L^{\Delta S=1} = \begin{pmatrix} u \\ s \end{pmatrix}_L.$$

Substituting those doublets into Eq. (1.19) and using charged current definition one obtains

$$J_+^\mu = \bar{u} \gamma^\mu \frac{1 - \gamma^5}{2} (\cos \theta_c d + \sin \theta_c s)$$

which means that the charged current can be equivalently written considering only one quark doublet

$$Q'_L = \begin{pmatrix} u \\ d' \end{pmatrix}_L \quad \text{with} \quad d' = \cos \theta_c d + \sin \theta_c s. \quad (1.20)$$

This picture was not yet satisfying as, if one substitutes the doublet in Eq. (1.20) in the neutral currents expressions (see Eq. (1.11b) (1.11c)), terms mixing fields of different flavour are obtained and this is in contrast with experimental evidence that FCNC are absent at tree level in the Standard Model. To solve this issue a fourth quark was introduced, the *charm*, which was also necessary to implement the GIM mechanism, explaining the suppression of FCNC in the SM at loop level. In this broadened picture, two quark doublets are present

$$Q_L^1 = \begin{pmatrix} u \\ d' \end{pmatrix}_L, \quad Q_L^2 = \begin{pmatrix} c \\ s' \end{pmatrix}_L \quad \text{with} \quad \begin{pmatrix} d' \\ s' \end{pmatrix} = \begin{pmatrix} \cos \theta_c & \sin \theta_c \\ -\sin \theta_c & \cos \theta_c \end{pmatrix} \begin{pmatrix} d \\ s \end{pmatrix}$$

and one of the fundamental concepts in flavour dynamics is set: flavour changing charged currents connect up-quark with down-quark fields, each of which is a unitary combination of all down-quark fields via a *rotation in flavour space*.

1.2.2 Quarks mixing and the CKM matrix

Flavour mixing in the quark sector has been finally formalized by Kobayashi and Maskawa, which extended the concept of unitary combination of quark fields to all the three families of the SM, constructing the Cabibbo-Kobayashi-Maskawa (CKM) matrix [8].

To derive the CKM definition, let's consider the Yukawa coupling lagrangian between the quarks and the Higgs field, which reads

$$\begin{aligned} \mathcal{L}_{q\phi} = \sum_{ik} y_d^{ik} \bar{Q}_L^i \phi d_R^k + (y_d^{ik})^* \bar{d}_R^k \phi^\dagger Q_L^i \\ + y_u^{ik} \bar{Q}_L^i \phi_C u_R^k + (y_u^{ik})^* \bar{u}_R^k \phi_C^\dagger Q_L^i, \end{aligned}$$

where $\phi_C = i\sigma_2\phi^*$ is the conjugate Higgs field and y_d^{ik}, y_u^{ik} are two generic complex matrices (with indices $i, j = 1, 2, 3$ running over the flavour families). Substituting the Higgs exponential representation in the broken phase (i.e. Eq. (1.15)), one obtains

$$\mathcal{L}_{q\phi} = \frac{v}{\sqrt{2}} \sum_{ik} y_d^{ik} \bar{d}_L^i d_R^k + \left(y_d^{ik}\right)^* \bar{d}_R^k d_L^i + y_u^{ik} \bar{u}_L^i u_R^k + \left(y_u^{ik}\right)^* \bar{u}_R^k u_L^i ,$$

and the quark mass matrices can be recognized (dropping the indices)

$$\mathcal{M}_u = y_u \frac{v}{\sqrt{2}} , \quad \mathcal{M}_d = y_d \frac{v}{\sqrt{2}} .$$

The mass matrices are in general non-diagonal, but they can be separately diagonalised by means of two unitary matrices¹²

$$\mathcal{M}_{uD} = U_L^\dagger \mathcal{M}_u U_R \quad \mathcal{M}_{dD} = K_L^\dagger \mathcal{M}_d K_R \quad (1.21)$$

Let's now consider the lagrangian representing charged current interactions between the quarks and the gauge bosons, which reads

$$\mathcal{L}_q^{\text{int,cc}} = \frac{g}{\sqrt{2}} \sum_i \bar{u}_L^i \gamma^\mu d_L^i W_\mu^- + \bar{d}_L^i \gamma^\mu u_L^i W_\mu^+ \quad (1.22)$$

The quarks fields will rotate under transformations ruled by Eq. (1.21) as

$$u_L^j = (U_L)^{jk} u_L'^k \quad \bar{u}_L^j = \bar{u}_L'^i (U_L^\dagger)^{ij} \quad (1.23a)$$

$$d_L^j = (K_L)^{jk} d_L'^k \quad \bar{d}_L^j = \bar{d}_L'^i (K_L^\dagger)^{ij} . \quad (1.23b)$$

Substituting Eq. (2.10) into Eq. (1.22) one obtains

$$\mathcal{L}_q^{\text{int,cc}} = \frac{g}{\sqrt{2}} \sum_{ik} \bar{u}_L^i V_{\text{CKM}}^{ik} \gamma^\mu d_L^k W_\mu^- + \bar{d}_L^i \left(V_{\text{CKM}}^\dagger\right)^{ik} \gamma^\mu u_L^k W_\mu^+ \quad (1.24)$$

where the CKM matrix is identified as $V_{\text{CKM}} = U_L^\dagger K_L$ and is a non-trivial combination of the unitary operators rotating up- and down-quarks in the diagonalised mass basis.

It is worth notice that the quarks interaction lagrangian with neutral currents, instead, contains fields combinations coupling up-type quarks only or down-type quarks only: $\bar{u}_L^i \gamma^\mu u_L^i$ or $\bar{d}_L^i \gamma^\mu d_L^i$. This implies that substituting Eq. (2.10) yields only trivial unitary operators combinations $U_L^\dagger U_L = K_L^\dagger K_L = \text{I}$, which cancel the summations over different flavour families. This technically implements in this formalism the absence of flavour changing neutral currents at tree level in the SM. Notice also that this discussion can analogously be replied in the lepton sector, with the crucial difference that there is no mass term for neutrinos, since in the SM there is no right-handed neutrino field. As a consequence leptons fields can be directly chosen to be mass eigenstates and there is no CKM matrix in the lepton sector¹³.

¹²This is ruled by an algebra theorem which ensures that “For every non-singular matrix M there exist two unitary operators such that $M_D = U_L^\dagger M U_R$, where M_D is diagonal”.

¹³Recent observations have shown that instead neutrinos *do* have mass. The minimal extension of the SM able to describe this consists in adding three sterile neutrinos, yielding a non-trivial mixing in the lepton sector, which is ruled by the Pontecorvo–Maki–Nakagawa–Sakata (PMNS) matrix.

1.2.3 The CKM matrix parametrisations and unitarity

The CKM matrix is a 3×3 unitary matrix, whose elements connect up- and down-type quarks fields

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

The total number of degrees of freedom of its representation is $N^2 - (2N - 1)$, where $N(N - 1)/2$ are real parameters, and the remaining are complex phases. Using $N = 3$ one obtains that the CKM can be written in terms of three real parameters and one phase. The most intuitive parametrisation of the CKM is the standard one, in which the matrix is expressed as product of three rotation matrices around the d , s , b quarks axes in flavour space:

$$V_{\text{CKM}} = \begin{pmatrix} c_{12}c_{13} & s_{12}c_{13} & s_{13}e^{-i\delta} \\ -s_{12}c_{23} - c_{12}s_{23}s_{13}e^{i\delta} & c_{13}c_{23} - s_{12}s_{23}s_{13}e^{i\delta} & s_{23}c_{13} \\ s_{12}s_{23} - c_{12}c_{23}s_{13}e^{i\delta} & -c_{12}s_{23} - s_{12}c_{23}s_{13}e^{i\delta} & c_{23}c_{13} \end{pmatrix}, \quad (1.25)$$

where $s_{ij} = \sin \theta_{ij}$, $c_{ij} = \cos \theta_{ij}$ are the real parameters and δ is the complex phase. Experimentally we know that $s_{13} \ll s_{23} \ll s_{12} \ll 1$, which implies that V_{CKM} is very similar to the identity matrix. This hierarchy is made more evident in the Wolfenstein parametrisation

$$V_{\text{CKM}} = \begin{pmatrix} 1 - \frac{\lambda^2}{2} & \lambda & A\lambda^3(\rho - i\eta) \\ -\lambda & 1 - \frac{\lambda^2}{2} & A\lambda^2 \\ A\lambda^3(1 - \rho - i\eta) & -A\lambda^2 & 1 \end{pmatrix} + \mathcal{O}(\lambda^4), \quad (1.26)$$

which is obtained from Eq. (1.25) using

$$\begin{aligned} \sin \theta_{12} &= \lambda & \sin \theta_{13} &= A\lambda^3 \\ \sin \theta_{23} &= A\lambda^2 & e^{i\delta} &= \rho + i\eta. \end{aligned}$$

Following CKM unitarity, constraints on its components can be derived

$$\sum_k V_{ki} V_{kj}^* = \delta_{ij}, \quad (1.28)$$

for $i, j = 1, 2, 3$, whose validity can be measured with experiments and consists in a powerful test of the SM construction. Among them the particular choice $i = 1, j = 3$ yields

$$V_{ud}V_{ub}^* + V_{cd}V_{cb}^* + V_{td}V_{tb}^* = 0,$$

which is usually referred to as *unitarity triangle* as can be represented in such a shape into the complex plane, with the principal vertex being in $(\bar{\rho}, \bar{\eta}) = (\rho, \eta) (1 - \lambda^2/2)$.

It can be shown that $\mathbb{CP}$ symmetry is conserved by the interaction lagrangian of quarks only if the CKM matrix is real. This implies that the value of η in the Wolfenstein parametrisation is a measure of $\mathbb{CP}$ violation in weak interactions.

1.3 The flavour anomalies as a hint for New Physics

The Standard Model describes fundamental interactions and particles with extremely high accuracy and its predictions have been extensively tested in a wide range of scales. Despite its phenomenological success, still clear experimental evidences are left which show it cannot be the ultimate theory of Nature and some new physics should exist beyond the SM theory: the lack of a description of gravitational effects, the evidence for dark matter and dark energy, the neutrino masses and the excess of matter over antimatter. Interest has been raised recently in the flavour sector of the Standard Model, as anomalous measurements in that sector (the *flavour anomalies*) constitute a promising handle to build new physics models, alternative to the traditional way of accessing new physics through addressing the Higgs hierarchy problem.

1.3.1 The flavour puzzle

Along with the already mentioned experimental evidences, some theoretical issues also mark the SM as an unsatisfactory theory, which are often used as starting points for new physics model building.

One of these theory questions is the *hierarchy problem* (or *naturalness problem*) [9], which consists in the fact the SM predicts at tree level a mass for the Higgs boson with an extremely high value with respect to the experimental value $m_H = 125$ GeV, measured at the Large Hadron Collider. For this reason, huge high-order corrections are needed in order to match with the experimental measurement, and this looks quite unnatural and unsatisfying from a theoretical point of view. A large amount of effort has been made in the last decade to develop beyond-SM theories making leverage on a solution of the hierarchy problem to predict some new physics experimental effect. One example is Super-Symmetry (SUSY), an exotic theory predicting the existence of a super-symmetric partner for each SM particle, which was built as an attempt to solve the hierarchy problem and also provides axions as possible candidates for dark matter particles. Several other models have been constructed, following the same paradigm of finding a solution to the hierarchy problem: extra-dimensional theories, conformal theories, clockwork models, none of these, unfortunately, has been confirmed by experimental searches.

However, a second conceptual difficulty hidden in current formulation of the Standard Model is the so called *flavour puzzle*, consisting in the fact the SM is not able to explain why leptons and quarks are structured in three identical families with identical quantum numbers, the only difference being their non-degeneracy in mass. In contrast to the gauge sector of the SM, the flavour sector contains a large number of free parameters which, after being fixed to reproduce the measured quarks and leptons properties, show a highly non-trivial structure whose origin is not known. The ultimate hope is that flavour might come from a New Physics sector providing a more economic and symmetric description, able to predict the observed masses and mixings in terms of a reduced number of parameters. This explains why flavour anomalies measured in B mesons decays have gained theorist's attention: as some of these measurements suggest a violation of lepton flavour universality, flavour anomalies can be used to drive the building of new physics models which might also

help us to gain a deeper understanding of flavour in general. This sets effectively a new paradigm for model building, which is alternative and complementary to the one based on the naturalness problem, and looks promising for continuing the quest for new physics in the years to come.

1.3.2 The experimental measurement of B -physics anomalies

The flavour anomalies represent a set of observables measured in semi-leptonic B mesons decays, which deviate from the SM prediction. Such measurements usually consist in branching-fractions, or ratios of branching-fractions, evaluated across different leptonic decay channels to test lepton universality. Despite the processes and the decay channels studied by the experimental collaborations are several, the underlying partonic transitions involved in the anomalies are mainly two:

- the charged current $b \rightarrow c\tau\bar{\nu}$ transition,
- the neutral current $b \rightarrow s\ell^+\ell^-$ transition, with $\ell = \mu, e$.

The current overall picture of flavour anomalies hints to the presence of new physics, which should be lightly and universally coupled to leptons and quarks of first and second family and more coupled to leptons of the third family, thus violating SM lepton universality in the third generation. For this reason the charged current transition is currently the most promising for the detection of anomalous effects, as new physics is supposed to show-up more easily in a final state with third family tau leptons. However, the neutral current transition can also play a fair role in new physics detection, as one-loop suppression of this flavour changing neutral current in the SM allows any slight exotic effect to compete with the little SM background of this rare process.

Overview of experimental facilities for B -physics

Current B mesons experimental measurements are primarily conducted via B -factories at e^+e^- colliders or at the LHC using pp collisions. B -factories operate at a center-of-mass energy close to the $\Upsilon(4S)$ resonance, which decays exclusively into a pair of B mesons. Examples of these colliders were PEP-II and KEK, hosting BaBar [10] and Belle [11] experiments, which both concluded their program, and SuperKEKB, which is currently hosting Belle II [12]. On the other hand, the LHC is producing b hadrons in high-energy pp collisions, with a center-of-mass energy of 13 TeV. The dominant production channel is gluon fusion, resulting in a pair of $b\bar{b}$ quarks, which quickly hadronise. The B -physics program of the LHC is mainly driven by LHCb [13] experiment, although ATLAS and CMS [14] also have dedicated measurements.

The two different production mechanisms reflect different experimental designs. In B -factories mesons are generated by almost back-to-back decays of the $\Upsilon(4S)$, hence detectors like Belle II have a full solid angle coverage. Conversely, at the LHC b -hadrons are usually produced close to the beam pipe and fly both in the same forward or backward direction, so they can be detected by a single-arm spectrometer with forward angular coverage like LHCb.

The background in which the observed particles decay is also very different: Belle II clearly operates in a cleaner environment, as the energy and momentum of B mesons is completely determined by the known collision energy and the absence of other decay products, while LHCb is challenged to deal with the composite nature of protons, whose collision generates plenty of spurious particles to be rejected. On the other hand, the LHC is the world's most intense source of b quarks and provides the large statistics that is necessary to study the rare processes involving B mesons. Moreover, the large collision energy grants access to the entire spectrum of b -hadrons: B_c , B_s , Λ_b , Ω_b and their excited states are produced, all of which are presently beyond the reach of Belle II.

One more aspect to keep in mind is the difference in performance between the two experiments in detecting muon and electrons. For Belle II the reconstruction of electrons and muons is very similar; at LHCb instead the high-energy electrons emit a significant amount of Bremsstrahlung, generating a difference in the reconstruction between the two channels. Also LHCb trigger efficiency is lower for electrons than for muons, due to the high occupancy of the calorimeters in comparison to the muons stations in the jet-enriched environment of the LHC. This explains why LHCb measurements testing e/μ lepton universality typically make use of *double ratio* techniques, designed to cancel from the final result all experimental biases which could generate differences between the electronic and muonic channels.

Finally we stress that also ATLAS and CMS have a B -physics program. CMS, in particular, has recorded during Run 2 of the LHC a specific dataset of unbiased B decays with the explicit purpose of contributing to the study of flavour anomalies [15].

The R_D/R_D^* anomaly in charged current transitions

The first set of observables displaying an anomaly has been measured in B mesons decays into D mesons and hint at new physics violating lepton universality in τ/ℓ ratios, where $\ell = e, \mu$. We define the following ratios of decay branching fractions

$$R_D = \frac{\mathcal{B}(\bar{B} \rightarrow D\tau^-\bar{\nu}_\tau)}{\mathcal{B}(\bar{B} \rightarrow D\ell^-\bar{\nu}_\ell)}, \quad R_{D^*} = \frac{\mathcal{B}(\bar{B} \rightarrow D^*\tau^-\bar{\nu}_\tau)}{\mathcal{B}(\bar{B} \rightarrow D^*\ell^-\bar{\nu}_\ell)}, \quad (1.29)$$

where $D^{(*)}$ corresponds to $D^{(*)0}$ or $D^{(*)+}$. The Heavy Flavor Averaging group (HFLAV) has evaluated the following SM prediction combining several theoretical computations [16]

$$R_D = 0.298 \pm 0.004, \quad R_{D^*} = 0.254 \pm 0.005,$$

which has to be compared with the experimental measurements that we now introduce. Notice that the SM expected value is not one, but this is only due to the difference in kinematic phase space, which follows from the difference in final state leptons mass: $m_\tau \ll m_\mu \approx m_e$.

The first measurement showing deviations from the SM was reported in 2012 by the BaBar collaboration [17]. Using the hadronic B -tagging, where one B -meson is fully reconstructed by detecting all of its decay products and then finding final states of the other B mesons in the event with one missing particle, BaBar measured

$$\text{Babar '12 : } R_D = 0.440 \pm 0.058 \pm 0.042, \quad R_{D^*} = 0.332 \pm 0.024 \pm 0.018.$$

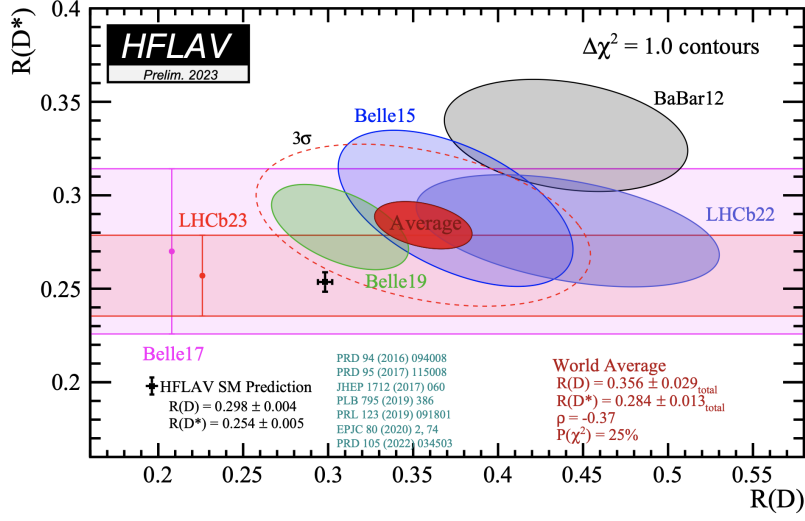


Figure 1.3. R_D and R_{D^*} measurements from different experiments, in comparison to world average and SM prediction [24].

where we adopt the convention that first uncertainty is statistical and the second systematic. Three years after, Belle also presented results using hadronic B -tags and the $\tau^- \rightarrow \ell^- \nu_\ell \bar{\nu}_\ell$ decay [18]

$$\text{Belle '15 : } R_D = 0.375 \pm 0.064 \pm 0.026, \quad R_{D^*} = 0.293 \pm 0.038 \pm 0.015.$$

Soon after, Belle repeated the measurement of R_{D^*} using the hadronic τ decays ($\tau^- \rightarrow \pi^- \bar{\nu}_\tau$, $\tau^- \rightarrow \rho^- \bar{\nu}_\tau$), finding [19]

$$\text{Belle '17 : } R_{D^*} = 0.270 \pm 0.035 \pm 0.027.$$

At this point, the collective measurements deviated from the SM predictions by approximately 3.9σ and experiments continued to pursue these observables. The Belle collaboration produced a new measurement using semileptonic $\bar{B} \rightarrow D^{(*)} \ell^- \bar{\nu}_\ell$ candidates for their tagged sample [20]

$$\text{Belle '19 : } R_D = 0.307 \pm 0.037 \pm 0.016, \quad R_{D^*} = 0.283 \pm 0.018 \pm 0.014.$$

In the meanwhile the LHCb collaboration joined the effort providing some first results in 2015 [21], followed by more precise combined measurements of $R_D - R_{D^*}$ with $\tau^- \rightarrow \ell^- \nu_\ell \bar{\nu}_\ell$ decays [22]

$$\text{LHCb '22 : } R_D = 0.441 \pm 0.060 \pm 0.066, \quad R_{D^*} = 0.281 \pm 0.018 \pm 0.024.$$

and the measurement of R_{D^*} with the hadronic tau decay [23]

$$\text{LHCb '23 : } R_{D^*} = 0.247 \pm 0.015 \pm 0.019.$$

The overall summary of these measurements is given in Figure 1.3, which also reports the current world average

$$R_D = 0.356 \pm 0.029_{\text{tot}}, \quad R_{D^*} = 0.284 \pm 0.013_{\text{tot}},$$

showing a 3.2σ deviation from the SM prediction [24]. Both ratios R_D and R_{D^*} show an increased value with respect to the predicted value, therefore, considering their definitions in Eq. (1.29), this anomaly hints for a new physics which is preferring decays into taus more than into electrons or muons.

The R_{Λ_c} measurement in charged current transitions

The LHCb collaborations has also released in 2022 a measurement which probes the $b \rightarrow c\tau\bar{\nu}$ transition in the Λ_b hyperon decay [25]. After measuring the ratio $\mathcal{K} = \mathcal{B}(\Lambda_b^0 \rightarrow \Lambda_c^+ \tau^- \bar{\nu}_\tau) / \mathcal{B}(\Lambda_b^0 \rightarrow \Lambda_c^+ \pi^- \pi^+ \pi^-)$, the decay branching fraction of $\Lambda_b^0 \rightarrow \Lambda_c^+ \tau^- \bar{\nu}_\tau$ is extracted and then compared to its equivalent in the muonic channel in the ratio

$$R_{\Lambda_c} = \frac{\mathcal{B}(\Lambda_b^0 \rightarrow \Lambda_c^+ \tau^- \bar{\nu}_\tau)}{\mathcal{B}(\Lambda_b^0 \rightarrow \Lambda_c^+ \mu^- \bar{\nu}_\mu)} = 0.242 \pm 0.026 \pm 0.040 \pm 0.059 ,$$

where the last uncertainty is due to the external branching fraction measurement from the channel $\Lambda_b^0 \rightarrow \Lambda_c^+ \mu^- \bar{\nu}_\mu$. The measurement results fairly in agreement with the SM prediction $R_{\Lambda_c}^{\text{SM}} = 0.324 \pm 0.004$ [26], but a slight 1σ tension is present.

The R_K/R_{K^*} measurements in neutral current transitions

Another set of measurements that plays a relevant role in the search for flavour anomalies can be constructed exploiting B mesons decays into K mesons, which probe the neutral current transition $b \rightarrow s\ell^+\ell^-$. Flavour changing neutral currents are absent in the SM at tree level, hence these processes are very rare and require a huge amount of data to be studied. Two ratios of branching fractions are defined

$$R_K = \frac{\mathcal{B}(B \rightarrow K\mu^+\mu^-)}{\mathcal{B}(B \rightarrow Ke^+e^-)} , \quad R_{K^*} = \frac{\mathcal{B}(B \rightarrow K^*\mu^+\mu^-)}{\mathcal{B}(B \rightarrow K^*e^+e^-)} , \quad (1.30)$$

with $K^{(*)}$ corresponding to $K^{(*)0}$ or $K^{(*)+}$. These ratios test lepton universality between electrons and muons and their expected value from theory is ≈ 1 , since there is no significant difference in the decay phase space factor between the two channels.

The first evaluations of these constants were performed by the LHCb collaboration, which detected anomalies reaching 3.1σ in R_K [27] and 2.4σ in R_{K^*} [28], as shown in Figure 1.4. The measurement procedure had to deal with the different performance of the LHCb detector in measuring electrons and muons, which is mainly due to Bremsstrahlung emissions of electrons in pp collisions and lower trigger efficiency in the electron channel, as detailed in Section 1.3.2. For this reason, both R_K and R_{K^*} constants were experimentally measured as double ratios, using a normalisation to the $B \rightarrow J/\psi(\ell^+\ell^-)K$ decay, which is known to high accuracy as having exactly the same branching ratio on both electronic and muonic channel

$$R_K = \frac{\mathcal{B}(B \rightarrow K\mu^+\mu^-)}{\mathcal{B}(B \rightarrow J/\psi(\rightarrow \mu^+\mu^-)K)} / \frac{\mathcal{B}(B \rightarrow Ke^+e^-)}{\mathcal{B}(B \rightarrow J/\psi(\rightarrow e^+e^-)K)} .$$

The constants were measured in the interval $0.1 < q^2 < 6.0$ GeV, with q^2 being the invariant mass squared of the di-lepton system, to avoid contamination from

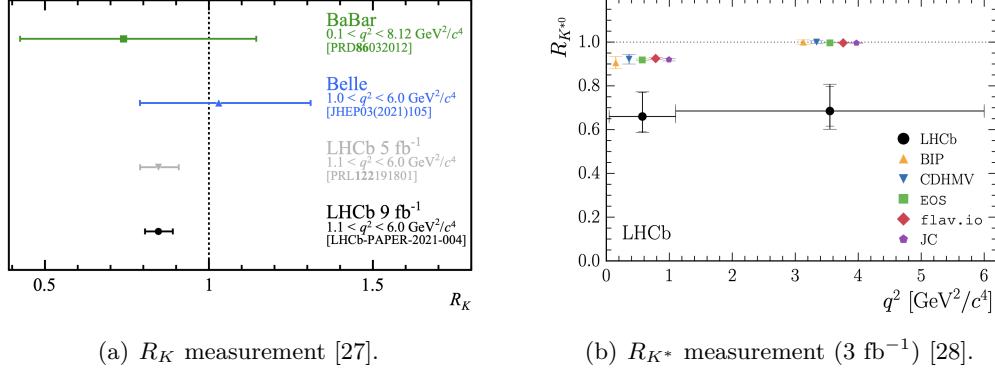


Figure 1.4. R_K and R_{K^*} measurements, obtained by the LHCb collaboration. Both measurements have been superseded further measurements obtained in 2022.

the $B \rightarrow J/\psi (\ell^+ \ell^-) K$ decays, which happen around the charmonium production energy $q^2 = 9.59 \text{ GeV}^2$. This first set of measurements raised lot of interest in the flavour physics community as pointed to a non-negligible evidence for some new phenomena violating lepton flavour universality in e/μ . However, a more detailed analysis and deeper understanding of the experimental procedure showed that these anomalies were mostly produced by an asymmetric behavior of the LHCb detector with respect to first and second family leptons.

In 2022 the LHCb collaboration has done a re-analysis of the same 9 fb^{-1} dataset with tighter identification criteria for the electrons and adding in the analysis procedure improved techniques for rejection of backgrounds of misidentified hadrons, obtaining the following results [29]

$$\begin{aligned} \text{low } q^2 \quad & \begin{cases} R_K &= 0.994^{+0.090}_{-0.082}(\text{stat})^{+0.029}_{-0.027}(\text{syst}) , \\ R_{K^*} &= 0.927^{+0.093}_{-0.087}(\text{stat})^{+0.036}_{-0.035}(\text{syst}) , \end{cases} \\ \text{central } q^2 \quad & \begin{cases} R_K &= 0.949^{+0.042}_{-0.041}(\text{stat})^{+0.022}_{-0.022}(\text{syst}) , \\ R_{K^*} &= 1.027^{+0.072}_{-0.068}(\text{stat})^{+0.027}_{-0.026}(\text{syst}) . \end{cases} \end{aligned}$$

were low- q^2 refers to the interval $0.1 < q^2 < 1.1 \text{ GeV}^2$ and central- q^2 to $1.1 < q^2 < 6.0 \text{ GeV}^2$. All the four measurements agree with the SM prediction and supersede previous results, ruling out new physics scenarios with lepton universality violation between electrons and muons. These measurements, however, do not play a decisive role in excluding scenarios in which new physics is mainly coupled to the third family of leptons and quarks and is lightly and universally coupled to first and second generations. In this hypothesis, new physics phenomena lepton-universal in electrons and muons would give equal contributions in numerator and denominator of Eq. (1.30) and would be compatible with the measured values of the R_K - R_{K^*} constants around unity.

Differential distributions and asymmetry in neutral current transitions

The ratios $R_K^{(*)}$, $R_D^{(*)}$, R_{Λ_c} discussed in previous sections are scalar quantities which can be measured and compared with the theoretical predictions, directly showing

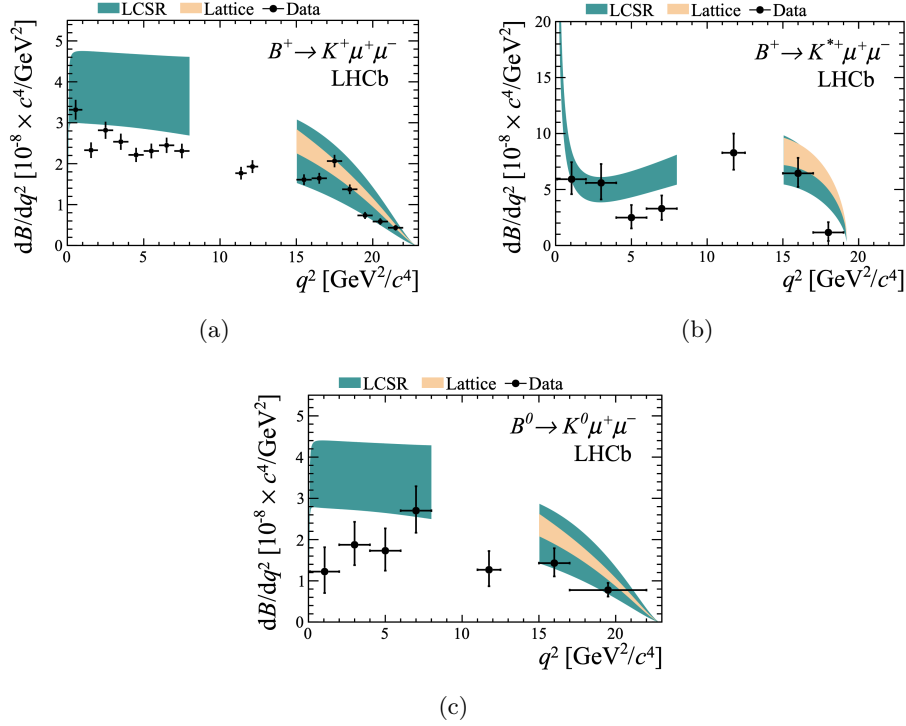


Figure 1.5. Differential branching fraction for (a) $B^+ \rightarrow K^+ \mu^+ \mu^-$, (b) $B^+ \rightarrow K^{*+} \mu^+ \mu^-$ decays, (c) $B^0 \rightarrow K^0 \mu^+ \mu^-$. The shaded regions show the theoretical predictions. [30].

the presence or not of a flavour anomaly. However, other new physics features can also be recognised as deviations in distributions of sensible quantities characterising flavour decays. If present, such deviations, are usually not sufficient to claim the detection of an anomaly, but they are often able to show up some common pattern, which constitutes valuable inception for theorists in building new models.

The LHCb collaboration has extensively measured the differential branching rate of $B^+ \rightarrow K^+ \mu^+ \mu^-$, $B^+ \rightarrow K^{*+} \mu^+ \mu^-$ and $B^0 \rightarrow K^0 \mu^+ \mu^-$ [30] [31], with results shown in Figure 1.5. As can be seen these differential rates show a pattern of deviations, being systematically lower than the SM prediction in the region below the charmonium threshold. Furthermore, the same trend has been observed by LHCb in the differential rates $B_s \rightarrow \phi \mu^+ \mu^-$ and $\Lambda_b \rightarrow \Lambda \mu^+ \mu^-$ [32] [33].

In addition to the differential branching ratios, LHCb measured the angular distributions for the above modes. In this case, a scan in di-lepton invariant mass squared (q^2) has been done for the optimised angular variable $P_{5'}$ [34] [35], as shown in Figure 1.6(a). The local discrepancies are 2.5σ in the bin $q^2 = [4, 6] \text{ GeV}^2$ and 2.9σ in the bin $q^2 = [6, 8] \text{ GeV}^2$. Belle collaboration has also performed this measurement (see Figure 1.6(b)), reporting a 2.3σ discrepancy in the bin $q^2 = [4, 6] \text{ GeV}^2$. ATLAS and CMS also joined this effort (Figures 1.6(c), 1.6(d)), the former reporting a measurement larger than SM prediction in bin $q^2 = [4, 6] \text{ GeV}^2$, the latter reporting no deviation from predicted shape.

It is worth to underline that the angular observables and the differential distributions are difficult quantities to evaluate, since long-distance QCD effects can

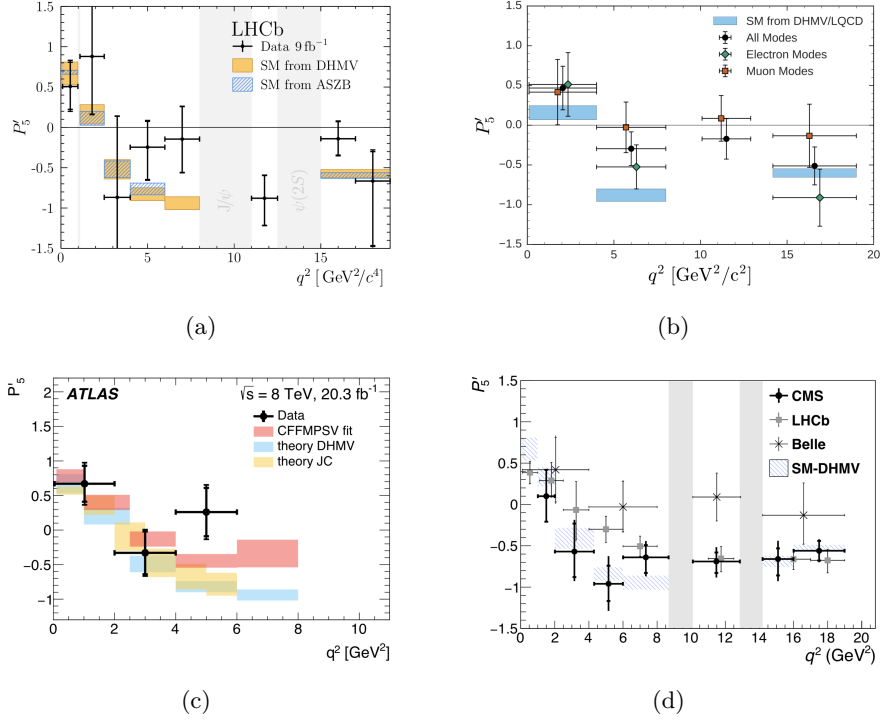


Figure 1.6. The CP-averaged observable $P_{5'}$ in bins of squared di-lepton invariant mass q^2 measured by: (a) LHCb [35], (b) Belle [36], (c) ATLAS [37], (d) CMS [38].

severely affect the precision of the prediction. The current methods used to derive the SM predictions rely on either the light-cone sum rules (LCSR) or lattice QCD, but are subject to large uncertainty. For this reason, the anomalies detected in these distributions are not singularly sufficient to draw any conclusion; however if considered jointly in an effective field theory fit, they can be interpreted as hinting at some new physics contribution universally coupled to electrons and muons, as will be further detailed in Section 1.3.3.

1.3.3 EFT interpretation of the B -physics anomalies

The flavour anomalies and measurements previously presented can be reinterpreted in an Effective Field Theory (EFT) approach. The EFT framework is useful to translate the anomalous experimental measurements into constraints on new physics operators, which constitute a joint model independent interpretation of several measurements. This is useful to gain more evidence for new physics effects and also to provide theorist some insight on new physics structure while building new models.

The joint EFT interpretation of charged currents and neutral currents anomalies detailed in Section 1.3.2, points to evidence for a new physics with subleading and universal coupling to light leptons families (electrons and muons) and major coupling to taus and third family quarks, thus violating lepton flavour universality in the third generation. If confirmed, such evidence can be further interpreted in the context of leptoquark models, pointing to the existence of a new gauge mediator which should

manifest as coupling to both quarks and leptons, with preferential coupling to third family.

Effective field theories for modelling new physics

Physics often deals with multi-scale problems, i.e. problems characterized by a multitude of energy scales, each of which is connected with a specific set of degrees of freedom characterising the phenomenon under investigation. Dealing with many scales at the same time is both complex and unnecessary, since typically not all degrees of freedom are equally relevant for the problem at hand.

The most prominent example in particle physics is given by the Fermi theory of electroweak neutron decay. Fermi described this decay as a single vertex four-fermion interaction between the involved fields, happening in one point of space-time and ruled by the Fermi constant G_F , obtaining predictions for decay rates very well in agreement with experiments. We know today that charged currents in electroweak interactions are mediated by $W^\pm$ gauge bosons exchange and that two vertices are involved, located at distinct points of space-time; however the “internal” degree of freedom made by the gauge boson mediator propagating among the two vertices was not probed in low energy¹⁴ neutron decay and could effectively be neglected.

Following the same approach, we can develop an effective field theory to parameterise new physics, exploiting the difference between two energy scales: the scale Λ_{NP} at which new phenomena are expected to be localised and the scale E at which we probe particle interactions to detect anomalies. We believe that new physics is indeed located at considerably higher energies than the electroweak scale and that only low-energy tail effects are probed at the scale at which the LHC is operated (i.e. $\lambda = E/\Lambda_{\text{NP}} \ll 1$). This means that it’s possible, as a first approximation, to neglect all “internal” degrees of freedom of new physics (e.g. eventual exotic gauge bosons mediating new physics interactions) and describe it via field operators verifying the only requirement of being invariant under the SM gauge group.

In the Standard Model Effective Field Theory (SMEFT) framework, the lagrangian density is extended with an operators series expansion in powers of $1/\Lambda_{\text{NP}}$, such that the overall dimension of each term is $d = 4$

$$\begin{aligned}\mathcal{L}_{\text{SMEFT}} &= \mathcal{L}^{(d=4)} + \mathcal{L}^{(d=5)} + \mathcal{L}^{(d=6)} + \dots \\ &= \mathcal{L}_{\text{SM}} + \frac{1}{\Lambda_{\text{NP}}} \sum_{i=1}^{N_5} \mathcal{C}_i^{(5)} \mathcal{O}_i^{(5)} + \frac{1}{\Lambda_{\text{NP}}^2} \sum_{i=1}^{N_6} \mathcal{C}_i^{(6)} \mathcal{O}_i^{(6)} + \dots\end{aligned}\tag{1.31}$$

where the $\mathcal{C}_i$ are real numbers called *Wilson coefficients* and parameterise new physics operators $\mathcal{O}_i$ contributions. Order by order, the SMEFT lagrangian includes all operators of a given dimension compatible with SM gauge symmetry: at dimension four the SM lagrangian is recovered, at dimension five only one operator is present - the Weinberg operator - which violates lepton number and generates the Majorana mass term for neutrinos, at dimension six many more contributions are generated. Dimension six operators are the ones interesting for flavour anomalies parametrisation, higher dimensions being more suppressed and negligible as a first approximation. A complete list of dimension six operators was presented in Ref. [39], and was

¹⁴In this context “low energy” means $E \ll m_W \approx 80$ GeV.

reduced to a basis in Ref. [40], which is usually referred to as the *Warsaw basis* of SMEFT. Ignoring flavour structure and assuming baryon number conservation, this basis contains only 59 independent operators, out of the 2499 possible ones.

EFTs are extremely powerful tools for phenomenological analysis and are widely used by theorists for model building, with a typical procedure that can be summarised as follows. First of all, a subset of operators is selected from the Warsaw basis, following some symmetry requirement or physical intuition. Then, amplitudes of physical processes are written as combinations of operators matrix elements

$$\mathcal{A}_{\text{eff}} = \sum_{n=0}^m \sum_i \mathcal{C}_i^{(n)} \langle f | \mathcal{O}_i^{(n)} | i \rangle + \mathcal{O}(\lambda^m) , \quad (1.32)$$

and fit to experimental data to extract constraints on the relevant Wilson coefficients. Fit results are used to understand features of new physics (which could for example manifest as *patterns* in Wilson coefficients values) and to drive the development of a specific new physics model, with its lagrangian and model-dependent parameters. As can be seen, this is a *bottom-up* approach: from data to the model. Eventually, constraints on Wilson coefficients can be translated into constraints of the model's parameters, giving it more fine-tuning. Finally, the new physics model is used make predictions (this corresponds to a *top-down* step) which are then tested by experimental collaborations in exotic searches.

EFT interpretation of charged currents anomalies

Charged current flavour anomalies presented in Section 1.3.2 can be jointly interpreted in an EFT framework to extract information on the physics content suggested by such measurements. The relevant field operators for the analysis of charged currents are

$$\begin{aligned} \mathcal{O}_{LL}^{ij\alpha\beta} &= \left(\bar{Q}_L^i \gamma_\mu L^\alpha \right) \left(\bar{L}^\beta \gamma^\mu Q_L^j \right) \\ \mathcal{O}_{LR}^{ij\alpha\beta} &= \left(\bar{Q}_L^i \gamma_\mu L^\alpha \right) \left(\bar{e}_R^\beta \gamma^\mu d_R^j \right) \\ \mathcal{O}_{RR}^{ij\alpha\beta} &= \left(\bar{d}_R^i \gamma_\mu e_R^\alpha \right) \left(\bar{e}_R^\beta \gamma^\mu d_R^j \right) \end{aligned} \quad (1.33)$$

which connect quarks and leptons fields in four-fermion vertices and can be rewritten as combinations of dimension-six operators of the Warsaw basis [41]. With the EFT analysis the following phenomenological relations can be derived [42]

$$\frac{R_D}{R_D^{\text{SM}}} = |1 + \mathcal{C}_{LL}^c|^2 - 3.00 \text{ Re} [(1 + \mathcal{C}_{LL}^c) \mathcal{C}_{LR}^{c*}] + 4.12 |\mathcal{C}_{LR}^c|^2 , \quad (1.34a)$$

$$\frac{R_{D^*}}{R_{D^*}^{\text{SM}}} = |1 + \mathcal{C}_{LL}^c|^2 - 0.24 \text{ Re} [(1 + \mathcal{C}_{LL}^c) \mathcal{C}_{LR}^{c*}] + 0.16 |\mathcal{C}_{LR}^c|^2 , \quad (1.34b)$$

$$\frac{R_{\Lambda_c}}{R_{\Lambda_c}^{\text{SM}}} = |1 + \mathcal{C}_{LL}^c|^2 - 1.01 \text{ Re} [\mathcal{C}_{LR}^c + \mathcal{C}_{LL}^c \mathcal{C}_{LR}^{c*}] + 1.34 |\mathcal{C}_{LR}^c|^2 . \quad (1.34c)$$

where $\mathcal{C}_{LL}^c$ and $\mathcal{C}_{LR}^c$ globally represent interactions of new physics operators with left and right handed fields and are non-trivial combinations of the Wilson coefficients $\mathcal{C}_{LL/LR/RR}^{ij\alpha\beta}$ relative to operators in Eq. (1.33).

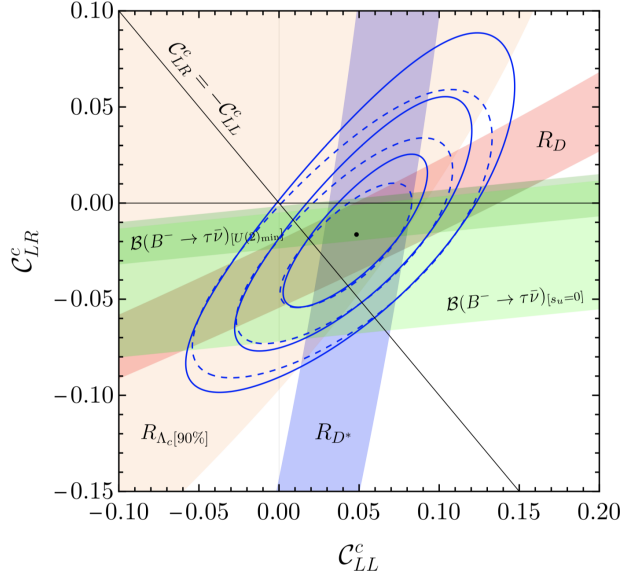


Figure 1.7. Determination of C_{LL}^c and C_{LR}^c from a χ^2 EFT fit of charged current flavour anomalies. The Wilson coefficients are assumed real and renormalized at the reference scale $\Lambda_{\text{NP}} = 1$ TeV. The black dot is the best fit point of $(0.05, -0.02)$ while blue ellipses represent 1, 2 and 3σ contours. The dashed lines are obtained including also $\mathcal{B}(B_u^- \rightarrow \tau \bar{\nu})$ information in the fit [42].

A χ^2 -fit can be performed, looking for the values of C_{LL}^c and C_{LR}^c which best accommodate R_D - R_{D^*} and R_{Λ_c} experimental measurements according to Eq. (1.34). Results are shown in Figure 1.7, assuming Wilson coefficients are real and renormalized at a conventional new physics scale $\Lambda_{\text{NP}} = 1$ TeV. The best fit point is found at $C_{LL}^c = 0.05$, $C_{LR}^c = -0.02$ and is located at 3σ distance from the $C_{LL}^c = C_{LR}^c = 0$ point, for which the SM is recovered. We can therefore argue that charged current anomalies jointly suggest the evidence for new physics via their EFT interpretation. Wilson coefficients are constrained in a region compatible with both the hypothesis of pure left-handed interaction ($C_{LR}^c = 0$) as well as the case with equal magnitude right-handed and left-handed currents, $|C_{LL}^c| = |C_{LR}^c|$. It is worth notice that the case $C_{LL}^c = -C_{LR}^c$ is particularly relevant as it is recognized as a natural benchmark for a flavour non-universal gauge model, where both left- and right-handed third-family quarks and leptons are unified in fundamental representations of $SU(4)$ [43].

The same analysis can be repeated including the branching ratio $\mathcal{B}(B_u^- \rightarrow \tau \bar{\nu})$ as additional information. The PDG average is used as experimental measurement $\mathcal{B}(B_u^- \rightarrow \tau \bar{\nu})^{\text{exp}} = 1.09(24) \times 10^{-4}$ [44], UTfit value as theory prediction $\mathcal{B}(B_u^- \rightarrow \tau \bar{\nu})^{\text{SM}} = 0.812(54) \times 10^{-4}$ [45] and the following phenomenological relation [42]

$$\frac{\mathcal{B}(B_u^- \rightarrow \tau \bar{\nu})}{\mathcal{B}(B_u^- \rightarrow \tau \bar{\nu})^{\text{SM}}} = |1 + C_{LL}^u - 2 \chi_u C_{LR}^u|^2, \quad (1.35)$$

where C_{LL}^u and C_{LR}^u are Wilson coefficients combinations (similar to C_{LL}^c and C_{LR}^c) and $\chi_u = m_{B^+}^2 / [m_\tau (m_b + m_u)] \approx 3.75$. As shown by the dashed blue curves in Figure 1.7, the addition of $\mathcal{B}(B_u^- \rightarrow \tau \bar{\nu})$ leaves the preferred phase-space region

almost unchanged, slightly disfavouring the hypothesis of sizable right-handed currents.

EFT interpretation of neutral currents anomalies

The neutral current transitions can also be interpreted via EFT, similarly to charged current transitions. As described in Section 1.3.2 neutral currents anomalies show up as deviations in several distributions, hence a joint EFT interpretation synthesizing information in few phenomenological coefficients is of particular interest to extract hints on eventual new physics.

Following Ref. [41] we can select the relevant operators for EFT analysis of $b \rightarrow s\ell\ell$ transitions:

$$\mathcal{O}_9^{bs\ell\ell} = (\bar{s}_L \gamma_\mu b_L)(\bar{\ell} \gamma^\mu \ell) , \quad \mathcal{O}_{10}^{bs\ell\ell} = (\bar{s}_L \gamma_\mu b_L)(\bar{\ell} \gamma^\mu \gamma_5 \ell) , \quad (1.36)$$

where ℓ is the lepton field and we have neglected the possible operators with the flavour changing right-handed quark currents. Since new physics can eventually violate lepton flavour universality, we can parameterise the relative Wilson coefficients as

$$\mathcal{C}_i^{bs\mu\mu} = \mathcal{C}_i^{\text{univ}} + \Delta\mathcal{C}_i^{bs\mu\mu} , \quad (1.37a)$$

$$\mathcal{C}_i^{bsee} = \mathcal{C}_i^{\text{univ}} , \quad (1.37b)$$

in which $\mathcal{C}_i^{\text{univ}}$ represents new physics contributions with equal behaviour across e and μ families, while $\Delta\mathcal{C}_i^{bs\mu\mu}$ represent lepton flavour violation across first and second generations. Following again Ref. [41], the following relation holds for lepton flavour universality breaking terms

$$\Delta\mathcal{C}_9^{bs\mu\mu} = -\Delta\mathcal{C}_{10}^{bs\mu\mu} .$$

A χ^2 fit can be performed using all neutral currents measurements to constrain $\mathcal{C}_9$ and $\mathcal{C}_{10}$ Wilson coefficients, with results graphically shown in Figure 1.8 [46]. The best fit points are:

$$\begin{aligned} \mathcal{C}_9^{\text{univ}} &= -0.64 \pm 0.22 , \\ \Delta\mathcal{C}_9^{bs\mu\mu} &= -\mathcal{C}_{10}^{bs\mu\mu} = -0.11 \pm 0.06 . \end{aligned}$$

and also $\mathcal{C}_{10}^{\text{univ}} \approx 0$. We note from the results that the lepton flavour violating component $\Delta\mathcal{C}_9^{bs\mu\mu}$ is compatible with zero, whereas the universal new physics coefficient $\mathcal{C}_9^{\text{univ}}$ shows a significant deviation from the null SM value. We therefore conclude that the EFT analysis of neutral currents anomalies hints to the presence of new physics lepton flavour universal across first and second generations.

1.4 Leptoquark models and phenomenology

Leptoquarks (LQ) are hypothetical particles able to interact both with leptons and quarks, hence carrying both baryon (B) and lepton (L) quantum numbers. They

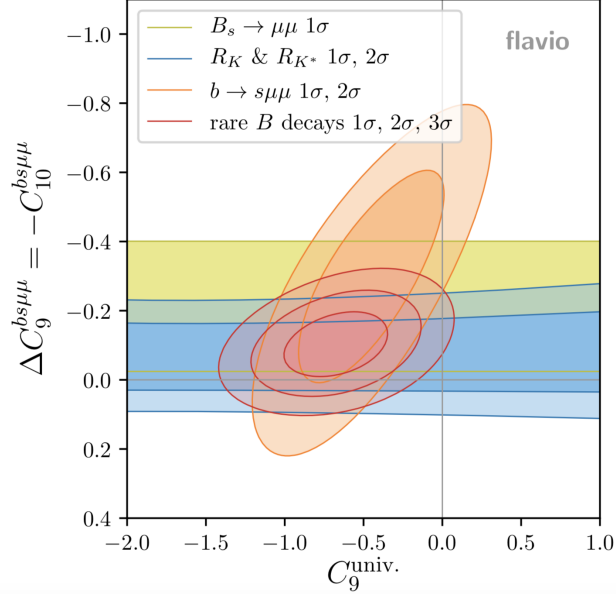


Figure 1.8. Determination of $C_9^{\text{univ.}}$ and $\Delta C_9^{bs\mu\mu} = -C_{10}^{bs\mu\mu}$ from a χ^2 EFT fit of charged current flavour anomalies [46].

can be either scalar (spin 0) or vector (spin 1) and are charged under weak isospin and weak hypercharge.

Renewed interest has raised in leptoquarks as they are among the most promising candidates to predict the charged and neutral current anomalies in B mesons decays, reported in Section 1.3.2, and are hinted by the anomalies EFT interpretation, which results in non-null Wilson coefficients for new physics operators involving both leptons and quarks fields (see for example Eq. (1.33) and Eq. (1.36) in Section 1.3.3). Nevertheless, leptoquarks models had also been studied in past decades, as they were recognised as a possible extension of the SM in various sectors. The first leptoquark model, in fact, dates back to Pati-Salam studies [47], who developed a theory addressing the $SU(4)$ symmetry as a possible extension of the SM gauge group, but many other beyond-SM frameworks have also involved such particles, as for example grand-unification theories based on $SU(5)$ and $SO(10)$, supersymmetric theories, composite quarks and leptons models.

Current interest is directed to lepton-flavour non-universal extensions of the Pati-Salam $SU(4)$ model, able to predict lepton flavour violation hinted in the B -anomalies flavour sector. Such models also predict deviations in observables that can be probed at hadron colliders, providing an independent and complementary source of experimental testing.

1.4.1 Models for vector and scalar leptoquarks

Current leptoquark models are divided in vector and scalar candidates, depending on the spin of the particle. In the following we describe the most prominent examples present in current state of the art. Among the various, the U_1 vector leptoquark model is the most renowned, as it best fits flavour anomalies and can be easily

extended to a UV-complete renormalizable theory.

The U_1 vector leptoquark model

The U_1 vector leptoquark model addresses a massive spin 1 particle, which is a singlet under $SU(2)_W$ and has weak hypercharge $y = 2/3$. This construction is a simplified model and is not UV-complete (i.e. not renormalizable), nevertheless it is able to generate predictions for all UV-insensitive flavour anomalies.

The model lagrangian reads

$$\begin{aligned} \mathcal{L}_U = & -\frac{1}{2}U_{\mu\nu}^\dagger U^{\mu\nu} + M_U^2 U_\mu^\dagger U^\mu - ig_s(1 - k_c) U_\mu^\dagger T^a U_\nu G^{\mu\nu,a} \\ & -\frac{2}{3}ig_Y(1 - k_Y) U_\mu^\dagger U_\nu B^{\mu\nu} + \frac{g_U}{\sqrt{2}} \left(U^\mu J_\mu^U + \text{h.c.} \right), \end{aligned} \quad (1.39)$$

where M_U is the mass associated to the leptoquark field U_μ and we use $U_{\mu\nu} = D_\mu U_\nu - D_\nu U_\mu$ and $D_\mu = \partial_\mu - ig_s G_\mu^a T^a - i\frac{2}{3}g_Y B_\mu$. Here G_μ^a ($a = 1, \dots, 8$) and B_μ denote the $SU(3)_c$ and $U(1)_Y$ gauge bosons, g_s and g_Y are the corresponding gauge couplings, and T^a are the generators of $SU(3)_c$. Moreover, k_c and k_Y are arbitrary constants which can be chosen to select the *minimal coupling scenario* ($k_c = k_Y$), in which the LQ is identified as originating from the gauge symmetry (under the particular choice $k_c = k_Y = 0$), and the *Yang-Mills scenario* ($k_c \neq k_Y$), in which the leptoquark can also arise from a strongly coupled sector. The interaction current of the U_1 leptoquark with SM fermions is

$$J_\mu^U = \beta_L^{i\alpha} \left(\bar{Q}_L^i \gamma_\mu L^\alpha \right) + \beta_R^{i\alpha} \left(\bar{d}_R^i \gamma_\mu e_R^\alpha \right), \quad (1.40)$$

where β_L and β_R are two 3×3 matrices which encode the flavour structure of the interactions, as it arises from the analysis of the flavour anomalies of B mesons decays. Based on the EFT studies discussed in Section 1.3.3 we assume the following structure

$$\beta_L = \begin{pmatrix} 0 & 0 & \beta_L^{d\tau} \\ 0 & \beta_L^{s\mu} & \beta_L^{s\tau} \\ 0 & \beta_L^{b\mu} & 1 \end{pmatrix}, \quad \beta_R = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \beta_R^{b\tau} \end{pmatrix}, \quad (1.41)$$

where $|\beta_L^{d\tau,s\mu}| \ll |\beta_L^{s\tau,b\mu}| \ll 1$, $\beta_R^{b\tau} = \mathcal{O}(1)$, and the g_U normalisation is chosen such that $\beta_L^{b\tau} = 1$. All the null entries have to be interpreted as neglected, having a small impact on the observables tested by experiments.

It can be shown [41] that the following matching relations between the $\beta_{L/R}$ parameters of the U_1 model and the Wilson coefficients $\mathcal{C}_{LL/LR/RR}^{ij\alpha\beta}$ of the EFT operators in Eq. (1.33) hold

$$\mathcal{C}_{LL}^{ij\alpha\beta} = C_U \beta_L^{i\alpha} \left(\beta_L^{j\beta} \right)^*, \quad \mathcal{C}_{LR}^{ij\alpha\beta} = C_U \beta_L^{i\alpha} \left(\beta_R^{j\beta} \right)^*, \quad \mathcal{C}_{RR}^{ij\alpha\beta} = C_U \beta_R^{i\alpha} \left(\beta_R^{j\beta} \right)^*,$$

with $C_U \equiv g_U^2 v^2 / (4M_U^2)$ and $v = (\sqrt{2}G_F)^{-1/2} \approx 246$ GeV. These relations can be used to translate constraints on the Wilson coefficients evaluated in EFT studies into constraints on the parameters of the U_1 model (see some examples in Figure 1.9) which can give more adaptation of the model to data, or more insight to the theorist for further model building.

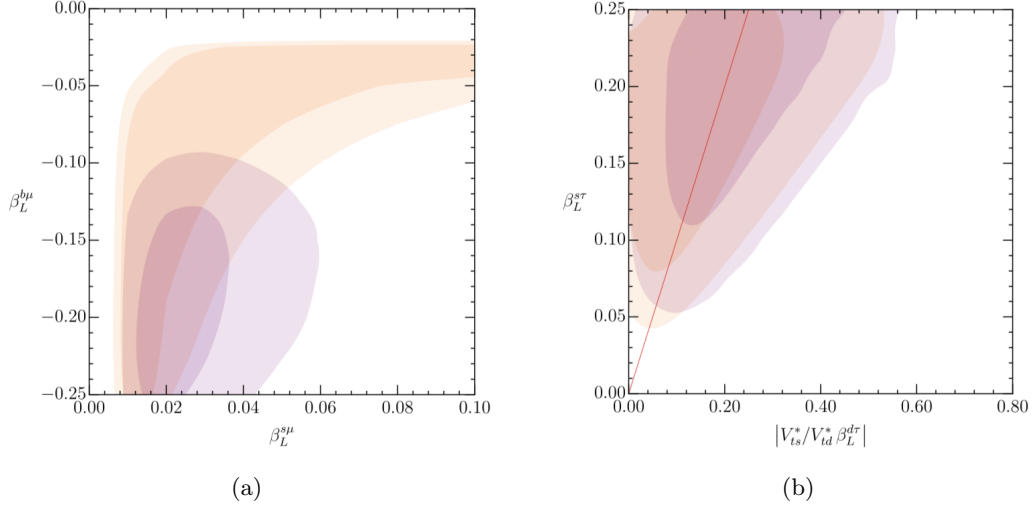


Figure 1.9. Constraints on U_1 leptoquark model parameters obtained fitting flavour anomalies. The two colours correspond to $\beta_R^{b\tau} = 0$ (orange) and $\beta_R^{b\tau} = -1$ (purple). Darker and lighter regions correspond to 1σ and 2σ contours [41].

The U_1 model can be used to predict flavour anomalies, whose agreement with experimental measurements serves as consistency test and validation. This is shown in Figure 1.10, where agreement with the experimental measurement of R_D - R_{D^*} constants is achieved, together with the agreement with the R_K - R_{K^*} measurement as reported in LHCb letter [27] (i.e. the R_K - R_{K^*} prediction here is not updated to the latest LHCb results, as reported in letter [29]).

UV-completion of the U_1 model

The U_1 leptoquark model is a simplified model and describes the massive particle without satisfying UV-completion, which makes it non renormalizable. The UV-completion of the simplified model is built starting from the $U(3)^5$ accidental flavour symmetry of the Standard Model, detailed in Eq. (1.18), which in the hypothesis of negligible electron and muon masses $m_e = m_\mu \approx 0$ (and non-negligible tau mass) reduces to

$$U(2)^5 = U(2)_L \otimes U(2)_{e_R} \otimes U(2)_{Q_L} \otimes U(2)_{u_R} \otimes U(2)_{d_R} ,$$

This global symmetry is further reduced via spontaneous symmetry breaking to the local gauge symmetry

$$\mathcal{G}_{4321} = SU(4) \times SU(3) \times SU(2) \times U(1) .$$

The most prominent UV-complete extension of the U_1 model is based on the symmetry group $\mathcal{G}_{4321}$ and is therefore called the “4321” model [41]. The symmetry $\mathcal{G}_{4321}$ consists in a modern revision of the original $SU(4)$ group proposed by Pati and Salam as a fundamental symmetry of Nature [47]. The Pati-Salam group offered a very elegant possibility for building a renormalizable theory, but described leptoquarks with a flavour-universal behaviour, while the “4321” group is able to

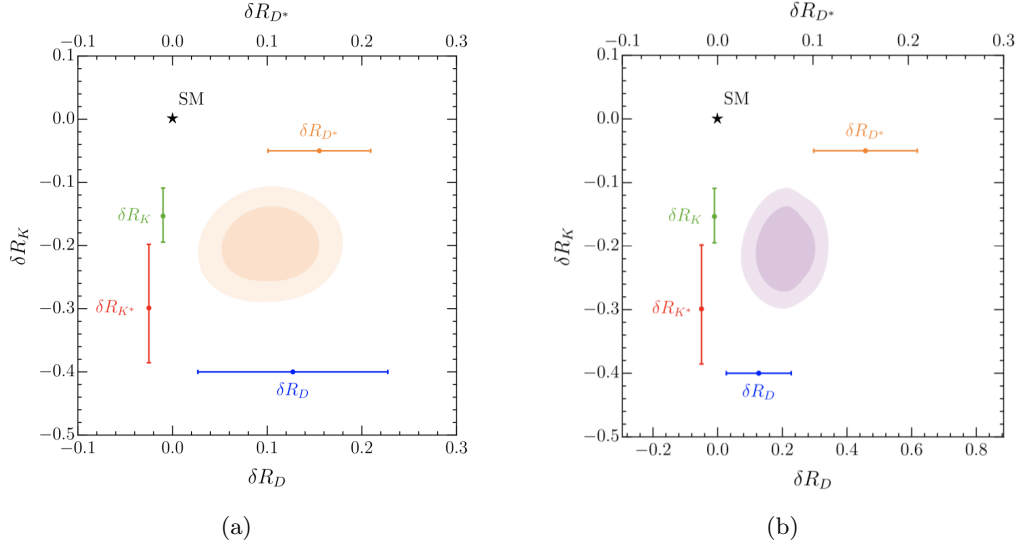


Figure 1.10. Preferred 1σ and 2σ regions for the $\delta R_{D^{(*)}}$ and $\delta R_{K^{(*)}}$ ratios, with $\delta R = (R - R_{\text{SM}})/R_{\text{SM}}$, predicted under the hypothesis $\beta_R^{b\tau} = 0$ (a) and $\beta_R^{b\tau} = -1$ (b). The coloured error bars represent experimental measurements of the ratios. These results are updated to LHCb results in Ref. [27] and not include results in [29]. Taken from [41].

accommodate violations of lepton universality and is hence more appropriate for the description of flavour anomalies.

In the “4321” model, several other particles are predicted, in addition to leptoquarks. In particular, eight colorons are introduced G' , together with a heavy resonance Z' , which couple mostly with the third generation of leptons and quarks and have small couplings with first and second generations, suppressed by factors g_s^2/g_U^2 and g_Y^2/g_U^2 respectively. Also vector-like leptons are predicted, consisting in doublets of exotic leptons, which decay into SM leptons. All these additional states have the common characteristic of generating multi-lepton final states and are searched in the LHC experiments constituting complementary test of the theory framework in which leptoquarks are embedded.

Scalar leptoquarks models

Scalar models have also been developed in literature, and are searched by LHC experiments, although the currently most prominent leptoquark model is the vector U_1 . Three scalar leptoquark candidates have been formulated, which are detailed in Ref. [48] and summarized in the following.

A first model describes the S_3 scalar leptoquark, which is a triplet under $SU(2)_W$ and has weak hypercharge $y = 1/3$. The Yukawa lagrangian of S_3 reads

$$\mathcal{L}_{S_3} = y_L^{ij} \bar{Q}^i i\tau_2 (\vec{\tau} \cdot \vec{S}_3) L^j + \text{h.c.} ,$$

where τ_k are the Pauli matrices ($k = 1, 2, 3$) and $y_{L(R)}^{ij}$ is the generic Yukawa coupling with quark (lepton) indices $i(j)$. This model was able to predict the $R_{K^*}R_{K^*}$

anomalies measured in Ref. [27], but cannot represent instead the anomalies R_D - R_{D^*} . Given that the anomalous R_K - R_{K^*} measurement has been mostly superseded by the last LHCb measurement in Ref. [29] showing no anomaly, interest in this model has currently decreased.

A second model describes the S_1 scalar leptoquark. This candidate is a singlet under $SU(2)_W$ and has weak hypercharge $y = 1/3$. The model lagrangian reads

$$\mathcal{L}_{S_1} = y_L^{ij} \bar{Q}^i i\tau_2 L^j S_1 + y_R^{ij} \bar{u}_R^i e_R^j S_1 + \text{h.c.} ,$$

where y_L and y_R are the LQ Yukawa matrices. This candidate is currently interesting, as it is able to address the flavour anomalies R_D - R_{D^*} .

The last candidate is the R_2 leptoquark. R_2 is a doublet under $SU(2)_W$, has weak hypercharge $y = 7/6$ and interacts via the lagrangian

$$\mathcal{L}_{R_2} = -y_L^{ij} \bar{u}_R^i R_2 i\tau_2 L^j + y_R^{ij} \bar{Q}^i R_2 e_R^j + \text{h.c.} , \quad (1.42)$$

where y_L and y_R are the LQ couplings to fermions. This candidate is also interesting as it is able to address flavour anomalies R_D - R_{D^*} and it is often cited in ATLAS papers, which typically show exclusion limits for the up- down- components of the doublet, referred as LQ^u and LQ^d .

1.4.2 Leptoquarks production and decay

Leptoquarks can interact in vertices involving both SM leptons and quark fields. There is no model-independent reason to require the generation number of the lepton to be the same as that of the quark, therefore in general LQ couplings are possible with all combinations of leptons and quarks fields.

Figure 1.11 reports the Feynman diagrams for the dominant production processes of leptoquarks at a hadron collider like the LHC. Leptoquarks can arise either via pair production or single production processes, yielding subsequent decays into leptons and quark pairs, or via the Drell-Yann process, in which the leptoquark is exchanged in the t -channel, connecting initial and final states. Assuming the simplified “minimal leptoquark” (MLQ) scenario, in which the leptoquark interacts with only one type of leptons and quarks¹⁵ with coupling constant λ , we can deduce the amplitude dependence on the couplings from diagrams inspection in Figure 1.11. Pair production diagrams from PP-1 to PP-4 yield amplitudes proportional to g_s^2 , having two interaction vertices coupling the leptoquark with gluons. The other diagrams show instead a dependence in λ : PP-5 and Drell-Yan (DY) diagrams yield amplitudes which scale as λ^2 , while single production SP-1 and SP-2 scales as $g_s \lambda$. These dependencies determine the dominance of one diagram or another in the total cross section: for small couplings ($\lambda \lesssim 1$) the pair production mode is dominant yielding an amplitude only dependent on the strong coupling, and hence leaving the leptoquark mass the only exotic parameter characterizing the process. For large leptoquark couplings instead ($\lambda \gtrsim 1$), single production e Drell-Yan become the leading processes, yielding amplitudes that are dependent on λ itself.

¹⁵This is equivalent to set to zero all β parameters of tensors in Eq (1.41) except one, e.g. $\beta_R^{b\tau} \neq 0$, $\beta_L^{i\alpha} = 0$ for $i, \alpha = 1, 2, 3$.

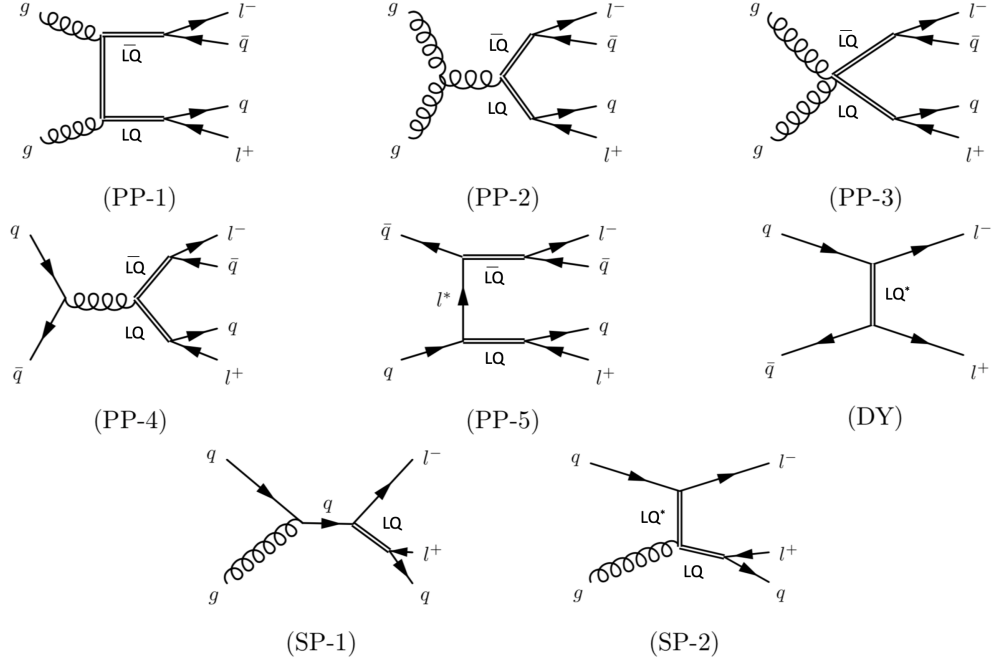


Figure 1.11. Leading order diagrams for leptoquark pair production (from PP-1 to PP-5), Drell-Yan t -channel exchange (DY) and single production (SP-1 and SP-2). The amplitudes from PP-1 to PP-4 are proportional to g_s^2 , PP-5 and DY scale as λ^2 , SP-1 and SP-2 as $g_2\lambda$ [49].

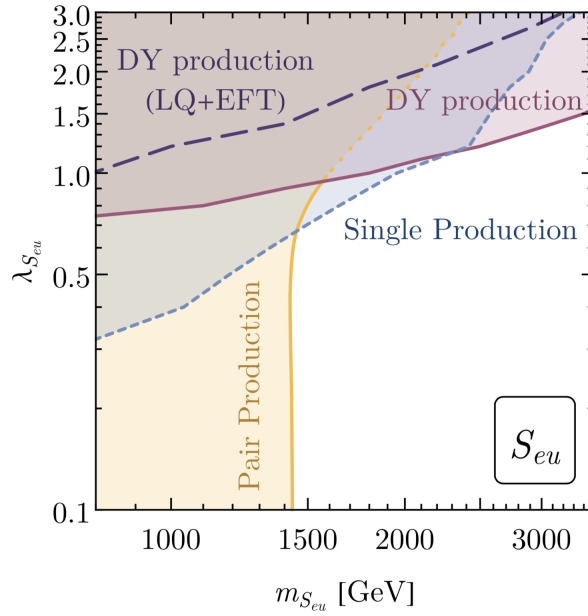


Figure 1.12. Expected bounds for leptoquark searches in the mass versus coupling constant space. The minimal leptoquark scenario is assumed with a scalar leptoquark coupling only to electrons and up-quarks [49].

The choice of production mode targeted by a collider experiment like ATLAS, determines the shape of the exclusion contour which is drawn in the leptoquark mass versus coupling constant phase space. Figure 1.12 shows an example of exclusion contours for a test scalar leptoquark, coupling only to electrons and up-quarks in the simplified MLQ scenario. The pair production mode provides the most significant bounds on leptoquark parameter space excluding low masses with a λ -independent contour (which acquires some dependence at large coupling via the diagram PP-5). Drell-Yan production is particularly effective in excluding the large mass and large coupling region and yields a λ -dependent contour. Single production generates instead a profile which is almost already covered by the other two production modes, adding only some small exclusion in the region where pair production and Drell-Yan bounds cross each other.

The decay width of the leptoquark can be evaluated and is ruled in first approximation by the particle mass M_U and the coupling λ only [49]. For a scalar particle, the decay width is given by

$$\Gamma_S = \frac{\lambda^2}{16\pi} M_U \left(1 - \frac{m_q^2}{M_U^2}\right)^2 \approx \frac{\lambda^2}{16\pi} M_U , \quad (1.43)$$

where m_q is the mass of the involved quark, which can be neglected in general (yielding considerable contributions only in the top-quark case). For a vector particle, instead, the decay width has the following expression

$$\Gamma_S = \frac{\lambda^2}{24\pi} M_U \left(1 - \frac{m_q^2}{M_U^2}\right)^2 \left(1 + \frac{m_q^2}{2M_U^2}\right) \approx \frac{\lambda^2}{24\pi} M_U , \quad (1.44)$$

where same definition and considerations apply for m_q .

1.4.3 Current status on leptoquarks searches

Several experimental searches for leptoquarks have been conducted to test the different models predicting these particles. We summarise in the following some recent results, focusing on collider searches conducted by the ATLAS Collaboration at the LHC, as these are the most related to the work presented in this thesis.

Searches are usually classified in categories based on the flavour of leptons and quarks produced in the leptoquark decay, which corresponds in probing different elements in the coupling tensors of the models (e.g. the β_L and β_R tensors of Eq. 1.41). More specifically, *same generation* searches probe leptoquarks decaying into leptons and quarks of the same family, while *cross-generational* searches look for leptoquarks decaying to fermions of different generations. Although leptoquarks can in general couple to all types of leptons and quarks, current ATLAS analyses cover final states involving mainly electrons, muons, b -jets, and to lesser extent taus and c -jets. This is because detector performance is optimal for b -tagging as well as for reconstruction of e , μ , sub-optimal for tau reconstruction and c -tagging and no jet-tagging is in general available for jets induced by other quarks flavours hadronization. Moreover, searches target mainly the pair production mode, yielding exclusions at low coupling constants, while single production and Drell-Yan have not been used so far.

A first ATLAS search looks for leptoquark pair production using $t\ell^+t\ell^-$ final states where $\ell = e, \mu$ [50]. This is a cross-generational search pointing to third family quarks and second family leptons. Since the top decays into a b -quark and a $W^\pm$ boson (subsequently decaying leptonically or hadronically) a multi-lepton and multi-jet final state is generated. The signal is selected looking for ≥ 2 light leptons, ≥ 2 jets, ≥ 1 b -jet and three signal regions are defined depending on the leptons multiplicity. Under the assumption of exclusive decays into te ($t\mu$), the corresponding lower limit on the scalar leptoquark mass is at 1.61(1.64) TeV, and on the vector leptoquark mass at 1.71(1.73) TeV in the minimal coupling scenario and at 2.0(2.0) TeV in the Yang-Mills scenario.

A second cross-generational search is reported in Ref. [51]. This analysis targets final states in which leptoquarks decay into third generation quarks (top or bottom) and second generation leptons (electron, muons and their neutrinos). The final state requires exactly one lepton, missing transverse momentum accounting for neutrinos and ≥ 4 hadronic jets coming from t - b -decays. Lower limits are set on the LQ mass separately for the μ (e) final state: 1.47(1.44) TeV for the up scalar LQ¹⁶, 1.37(1.39) TeV for the down scalar LQ, 1.71(1.62) TeV for the vector LQ in the minimal coupling scenario, 1.98(1.90) TeV for the vector LQ in the Yang-Mills scenario.

ATLAS has also used tau leptons to constrain leptoquarks models as reported in Ref. [52]. In this search a final state with two hadronically decaying tau leptons and two c -quarks is targeted, coming from the decay of a pair-produced leptoquarks. The analysis is challenged by the difficult reconstruction of hadronic taus and by the estimate of the multijet background of jets faking taus which is addressed via a data-driven technique based on jet $\rightarrow$ tau fake factor rates. Scalar leptoquarks models are considered and a lower limit on their mass is set at 1.3 TeV.

Same generation searches have been less exploited so far by ATLAS, Ref. [53] being currently the only example. In this search tau and b -jet couples are searched coming from the decay of pair-produced leptoquarks. This analysis is particularly interesting, as current theory scenarios hint to lepton flavour violation in the third family yielding leptoquarks more coupled to third generation fermions. At least one tau is required to decay hadronically and a data-driven technique based on fake rates is used to estimate the fake-tau background. Masses below 1.49 TeV are excluded for scalar LQs, while for vector leptoquarks the corresponding limit is 1.69(1.96) TeV in the minimal coupling (Yang Mills) scenario.

Summary plots of leptoquarks masses exclusions are shown in Figures 1.13 and 1.14. As can be seen, many results have been produced by the ATLAS collaboration, targeting mostly pair-produced scalar leptoquarks, with cross-generational couplings. Future searches by ATLAS are therefore expected to cover more vector leptoquarks models, with same-generation couplings and to exploit also the Drell-Yan production to cover the large-coupling phase-space region.

We report for completeness that also other searches have been conducted by ATLAS which do not directly target leptoquarks production, but nevertheless look for exotic particles predicted in theory scenarios addressing flavour anomalies. Examples

¹⁶Here we refer to a scalar LQ model in which the field is a doublet with an *up* and a *down* component. More details are given in Section 1.4.1 or in the ATLAS paper references.

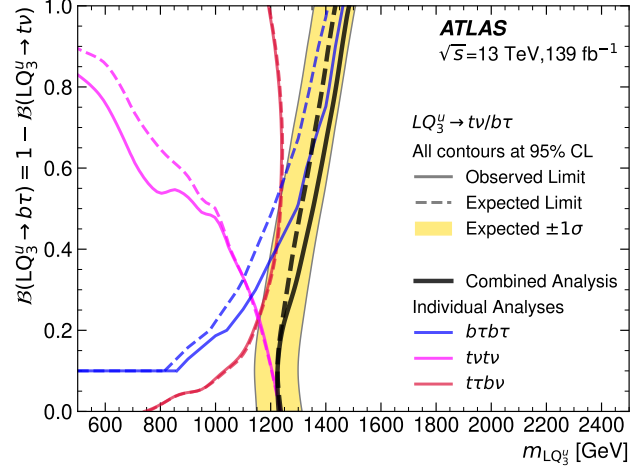


Figure 1.13. Summary plot for ATLAS searches of up-type third generation leptoquarks decaying into third generation quarks and leptons [54].

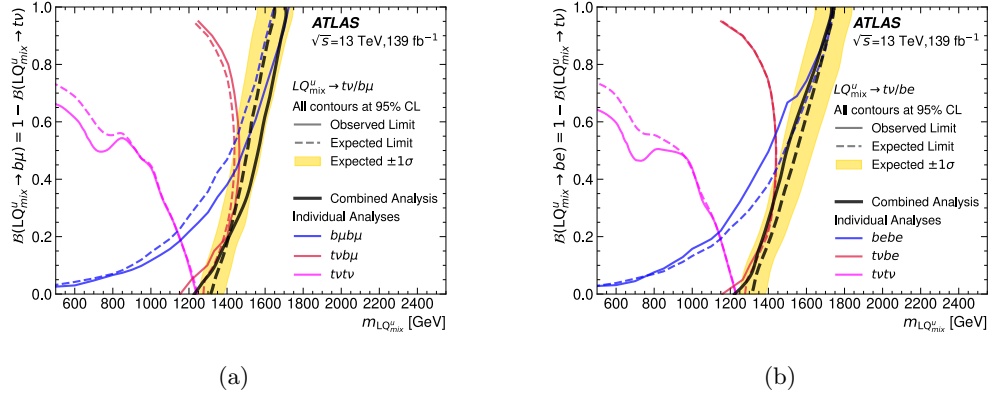


Figure 1.14. Summary plot for ATLAS searches of up-type scalar leptoquarks decaying into a third generation quark and (a) a muon (b) an electron [54].

of these results are the search for vector-like leptons [55] (composite doublets of leptons decaying into SM ordinary leptons) and the Z' heavy resonance decaying into third family leptons [56]. More details are given in the respective references.

1.5 The Drell Yan process with tau leptons

The Drell-Yan process, consisting in a pair production of massive leptons by quark-antiquark annihilation, is a fundamental process at hadron colliders and has been extensively measured to extract the properties of the electroweak and strong interactions. Interest has been raised recently in studying the Drell-Yan process with tau leptons in the final state, both in Standard Model measurements and in exotic searches for new physics. On the Standard Model side, such measurements are interesting for their own, as they complement already existing results in the electronic and muonic channels, and have not been done so far due to the difficulty of reconstructing tau leptons. On the exotics side, instead, the di-tau Drell-Yan can be used to test scenarios in which new physics is more coupled to the third family of leptons and quarks, which currently are the most prominent explanations for the flavour anomalies in B mesons decays.

We review in this Section the main features of pp collisions phenomenology and the Drell-Yan process, finally describing the relevance of the di-tau Drell-Yan in constraining leptoquarks models.

1.5.1 Phenomenology and theory description of pp interactions

The proton is a composite particle and therefore pp interactions in a hadron collider like the LHC are complex phenomena to describe. Protons are made by three valence quarks uud , which carry most of the hadron momentum, as well as sea quarks and gluons. These constituents are collectively called partons. At sufficiently high energy, pp collisions are inelastic and the fundamental interaction takes place between two individual partons (*hard scatter*).

A graphical description of a pp interaction is given in Figure 1.15. When the protons cross each other, two partons are selected for the partonic interaction, while the others are left almost unperturbed, generating only soft radiation which is conventionally called the *underlying event*. The two partons interact in the hard scatter, after having emitted some radiation before, which is called initial state radiation (ISR). A parton shower is generated from the hard scattering, producing a large amount of quarks and gluons carrying an increasingly smaller fraction of the initial energy. When the parton energy reaches values of the order of $\Lambda_{\text{QCD}} \approx 0.2 \div 0.3$ GeV, pole of the QCD running coupling, bounding potentials between coloured partons intervene and hadronisation occurs, generating mesons and baryons often grouped in collimated structures called jets. Further radiation can be emitted immediately after the hard scattering, called final state radiation (FSR) or even after, in the form of photons (photon radiation).

The momentum scale of the different physical processes involved in pp collisions are very different, ranging from $\mathcal{O}(1)$ TeV for the hard scatter interaction to $\mathcal{O}(1)$ GeV, which is the scale of hadronising partons. The hard interaction represents a scale at which QCD is perturbative and the matrix element can be effectively calculated,

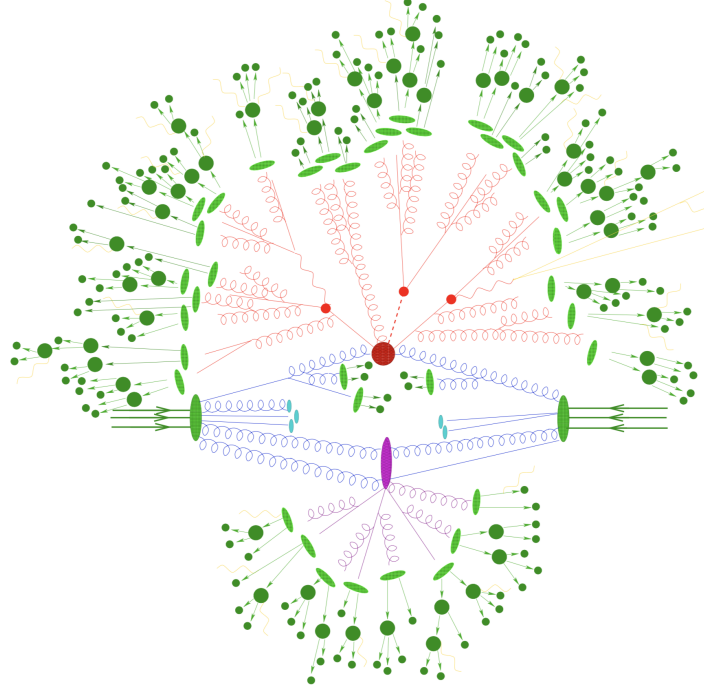


Figure 1.15. Graphical representation of a pp collision at hadron collider. In the picture are shown with different colours: the hard scatter, initial and final state radiation, the underlying event, hadronisation, the soft photon radiation. [57].

while the hadronisation scale is in the non-perturbative regime and processes can only be described via approximate phenomenological models.

Hard scattering cross sections calculation

The theoretical calculation of a pp interaction is a task which requires some care in accounting for the composite nature of the colliding particles and involves QCD methods.

It was first pointed out by Drell and Yan [58] that the parton model ideas developed for deep inelastic scattering could be extended to processes in hadron-hadron collisions. In particular, it was hypothesised that the hadronic cross section $\sigma(AB \rightarrow X)$ could be obtained starting from the partonic subprocess cross section $\sigma(q_a q_b \rightarrow X)$, calculated instead with ordinary QFT techniques. This is today formalised in the *factorisation theorem* of QCD, which states that the hadronic cross section can be evaluated averaging the partonic cross section over all possible momentum fractions x_a and x_b carried by the partons, and taking as weighting factors the parton distribution functions (PDFs), which represent the probability of a parton of having a certain momentum fraction. Formally we write

$$\sigma_{AB} = \int dx_a dx_b f_{a/A}(x_a, Q^2 = \mu_F^2) f_{b/B}(x_b, Q^2 = \mu_F^2) \hat{\sigma}_{ab \rightarrow X} . \quad (1.45)$$

where $\hat{\sigma}_{ab \rightarrow X}$ denotes the partonic cross section and $f_{a/A}$, $f_{b/B}$ are the PDFs, depending on the energy scale of the process Q^2 , which is normally taken equal to

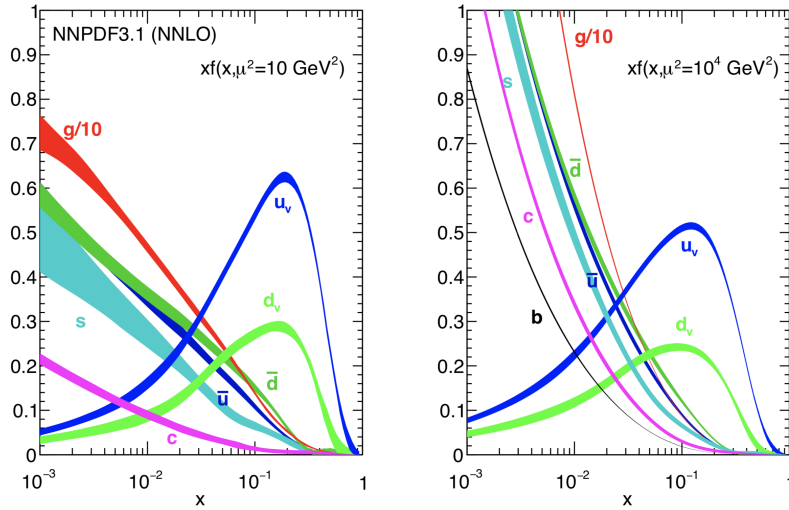


Figure 1.16. The NNPDF3.1 PDFs set, calculated at NNLO and evaluated at $Q^2 = 10 \text{ GeV}^2$ (left) and $Q^2 = 10^4 \text{ GeV}^2$ (right) [60].

the *factorisation scale* μ_F .

The PDFs cannot be calculated from first principles and have to be measured in experiments. This has been extensively done in the past decades in several deep inelastic scattering experimental campaigns, which took place for example at SLAC or at HERA collider and at Tevatron. Experimental measurements only yield the x dependence of the PDF at a fixed energy scale, while Q^2 dependence is ruled by the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equations [59], which are often used to evolve PDFs measured at a low energy scale till the LHC scale (see an example in Figure 1.16).

Divergences arise in the factorisation integral in Eq. (1.45), mainly due to large logarithms appearing from gluons emitted collinear with the incoming quarks. Some of these divergences have the same structure of the ones arising in the solution of the DGLAP equations, hence can be reabsorbed via a redefinition of the PDFs (which generates their dependence on Q^2), while other finite corrections are non-universal and have to be calculated separately for each process and integrated into the factorisation integral via a perturbative expansion

$$\sigma_{AB} = \int dx_a dx_b f_{a/A}(x_a, \mu_F^2) f_{b/B}(x_b, \mu_F^2) \times \left[\hat{\sigma}_0 + \alpha_S(\mu_R^2) \hat{\sigma}_1 + \dots \right]_{ab \rightarrow X}. \quad (1.46)$$

being μ_R is the *renormalisation scale* for the QCD running coupling α_S . The factorisation and renormalisation scales have to be assumed at some value, which is usually taken as the energy scale of the hadronic interaction. For a Drell-Yan process calculation, for example, the typical choice is to take them equal to the combined mass of the di-lepton final state, $\mu_F = \mu_R = M_{\ell\ell}$. This choice is however arbitrary and leads to some uncertainty, that can numerically be evaluated inserting several varied values for the two μ_F and μ_R parameters and measuring their impact on the final cross section calculation.

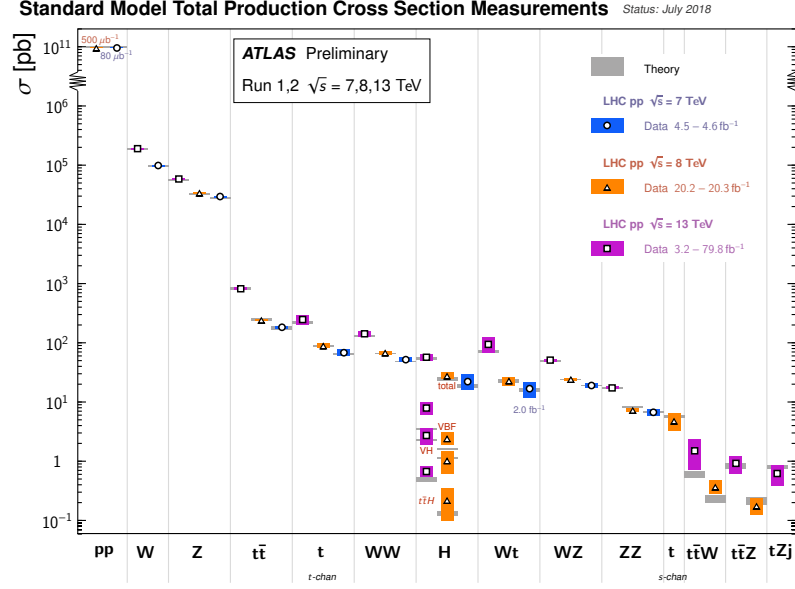


Figure 1.17. Summary of several SM total cross sections, measured by the ATLAS experiment [61].

Events simulation and Standard Model cross sections

The factorisation theorem scheme is implemented in current Monte Carlo event generators, which are used today for the modelling of physics processes at the LHC. Different algorithms are adopted, first to calculate the matrix elements (ME), then to perform the parton showering (PS) and model the effect of the underlying event. ME generators are able to describe with high accuracy the hard-scattering process, even if accompanied by few QCD emissions. Parton shower algorithms instead describe multiple emissions in the soft and collinear approximation, which is the regime dominating the cross section value. The final description of the events is achieved *matching* the predictions provided by the ME generator and the PS algorithm.

The comparison of theory predictions and experimental values for all SM cross sections measured by the ATLAS Collaboration is reported in Figure 1.17. The impressive agreement between theory and measurements can be noticed, which is reached across a wide variety of channels yielding cross sections which differ in more than ten orders of magnitude, manifesting the remarkable success of the Standard Model in describing elementary particles interactions.

1.5.2 Drell-Yan process kinematics and cross section

The leading order Feynman diagram of the Drell-Yan process $q\bar{q} \rightarrow Z/\gamma^* \rightarrow \ell^+\ell^-$ is represented in Figure 1.18: a quark and an anti-quark are selected from the two protons and annihilate, generating an off-shell Z boson or a massive photon, which subsequently decay into a couple of opposite sign leptons.

The kinematical features of the Drell-Yan process are easily calculable by direct application of special relativity. If we neglect initial state particles masses, the

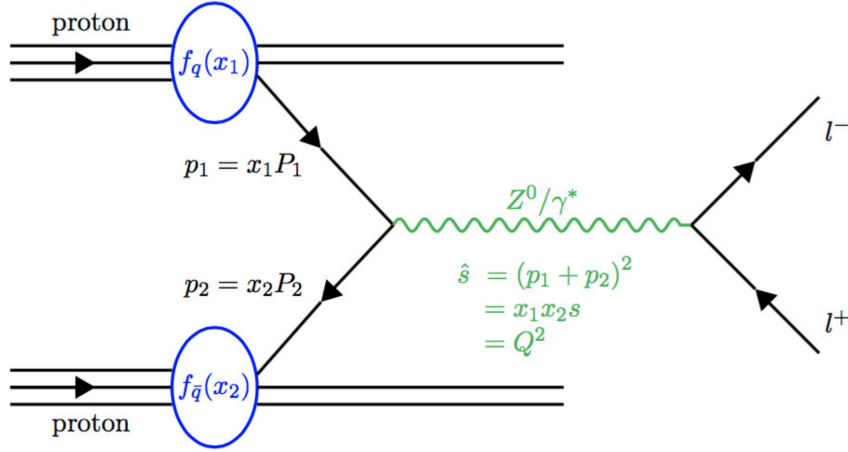


Figure 1.18. Leading order Feynman diagram for the Drell-Yan process. The four-momenta of the protons are labelled P_1 and P_2 , the relative four-momenta for the partons, p_1 and p_2 are scaled by the Bjorken fractions x_1 and x_2 .

protons four-vectors¹⁷ are

$$P_1 = \left(\frac{\sqrt{s}}{2}, 0, 0, \frac{\sqrt{s}}{2} \right) \quad P_2 = \left(\frac{\sqrt{s}}{2}, 0, 0, -\frac{\sqrt{s}}{2} \right), \quad (1.47)$$

while partons four vectors are obtained by scaling Eq. (1.47) for the Bjorken variables x_1, x_2

$$p_1 = \left(x_1 \frac{\sqrt{s}}{2}, 0, 0, x_1 \frac{\sqrt{s}}{2} \right) \quad p_2 = \left(x_2 \frac{\sqrt{s}}{2}, 0, 0, -x_2 \frac{\sqrt{s}}{2} \right), \quad (1.48)$$

From direct inspection of Eq. (1.48) the following relation is obtained for the partonic invariant mass

$$\sqrt{\hat{s}} = \sqrt{x_1 x_2} \sqrt{s}, \quad (1.49)$$

which is also equal to the di-lepton invariant mass $M_{\ell\ell}$ due to four-momentum conservation between initial and final state. In this process, the kinematics is determined once the gauge boson rapidity is specified. In fact, using rapidity definition and Eq. 1.48 one obtains

$$y = \frac{1}{2} \ln \left(\frac{E + p_z}{E - p_z} \right) = \frac{1}{2} \ln \left(\frac{x_1}{x_2} \right), \quad (1.50)$$

which substituted in Eq. (1.49) yields the partons momentum fractions

$$x_1 = \frac{M_{\ell\ell}}{\sqrt{s}} e^y \quad x_2 = \frac{M_{\ell\ell}}{\sqrt{s}} e^{-y}. \quad (1.51)$$

Analysing Eq. (1.51) one can recognise that when the gauge boson is emitted in the transverse plane ($y = 0$), partons momentum fractions are equal: $x_1 = x_2 = M_{\ell\ell}/\sqrt{s}$. Instead, when partons momentum fractions are maximal ($x_1 = 1$ or $x_2 = 1$), the gauge boson acquires the maximum rapidity value $y = \pm \ln(\sqrt{s}/M_{\ell\ell})$.

¹⁷We adopt the notation (E, p_x, p_y, p_z) for the four-vectors

The Drell-Yan hadronic cross section has to be calculated following the prescriptions described in Section 1.5.1, i.e. by evaluating the partonic quark-antiquark cross section via QFT methods and then integrating it applying the factorisation theorem. The baseline partonic cross section, in which only the γ^* mediator is considered, can be directly translated from the QED process $e^+e^- \rightarrow \mu^+\mu^-$ with the addition of the proper colour and charge factors

$$\hat{\sigma}(\bar{q}q \rightarrow e^+e^-) = \frac{4\pi\alpha^2}{3\hat{s}} \frac{1}{N} Q_q^2, \quad (1.52)$$

where Q_q is the quark charge, $Q_u = +2/3$, $Q_d = -1/3$, while the overall colour factor is $1/N = 1/3$ and is due to the fact that only when the quark colour matches the anti-quark colour annihilation into a colour-singlet final state can take place. The differential partonic cross-section can also be easily derived, the only difference being the selection of the phase space region compatible with quadri-momentum conservation with a δ -function

$$\frac{d\hat{\sigma}}{dM^2} = \frac{\hat{\sigma}_0}{N} Q_q^2 \delta(\hat{s} - M^2) \quad \hat{\sigma}_0 = \frac{4\pi\alpha^2}{3M^2}, \quad (1.53)$$

This has to be inserted into the factorisation theorem formula in Eq. 1.45 to get the hadronic differential cross section

$$\begin{aligned} \frac{d\sigma}{dM^2} &= \frac{\hat{\sigma}_0}{N} \int_0^1 dx_1 dx_2 \delta(x_1 x_2 s - M^2) \\ &\times \left[\sum_k Q_k^2 [f_q(x_1) f_{\bar{q}}(x_2) + f_{\bar{q}}(x_1) f_q(x_2)] \right]. \end{aligned} \quad (1.54)$$

Higher order corrections have to be inserted on top the leading order cross section calculation, evaluating the perturbative expansion coefficients in Eq. (1.46), which need to be regularised to avoid infrared, ultraviolet and collinear divergences.

The final di-lepton invariant mass spectrum is obtained considering that at centre of mass energies near the Z boson mass, also the Z -mediated diagram starts to contribute and the total cross section is given by the sum of three terms: γ^* exchange, Z exchange and interference term. Figure 1.19 represent each of the aforementioned contributions, together with their combination, for the Drell-Yan process happening at the LHC energy of 13 TeV. The bump structure at $M_{\ell\ell} \approx 90$ GeV is called the Z -peak and corresponds to a local enhancement of the Drell-Yan cross section due to the divergence of the Z boson propagator in the Z -mediated leading order diagram.

1.5.3 Searches of leptoquarks in the high mass tail

The Drell-Yan process with tau leptons in the final state has gained increasing interest among beyond-SM searches as it can be used as a probe to test exotic scenarios connected with the flavour anomalies of B mesons decays. As detailed in Section 1.3, theories which extend the SM in the flavour sector, like for example the “4321” model, predict new physics in the form of leptoquark particles more coupled to the third generation of leptons and quarks. Such particles are involved as mediators in the t -channel exchange diagram with two quarks in the initial state generating

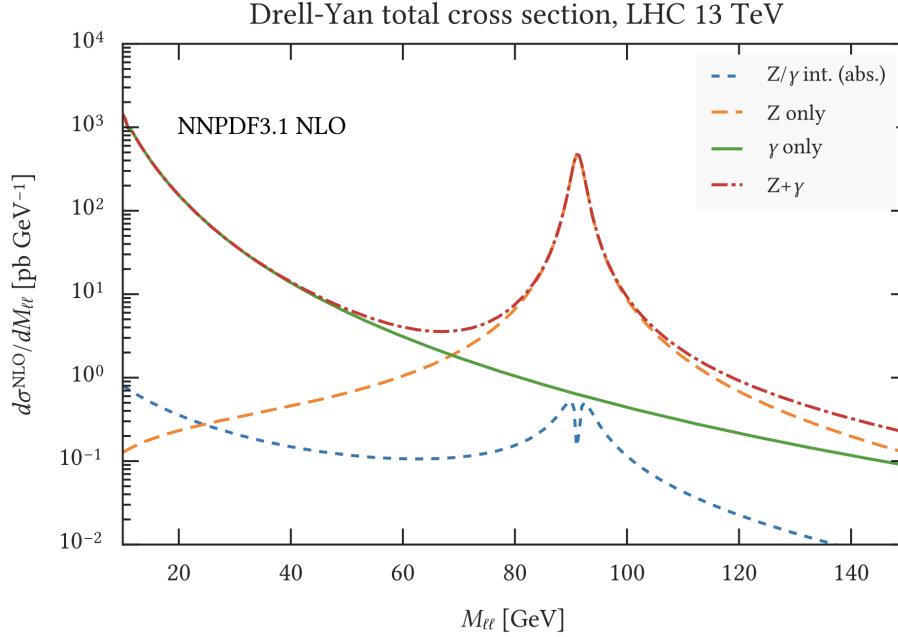


Figure 1.19. Total NLO Drell-Yan cross section $d\sigma/dM_{\ell\ell}$ at 13 TeV. The contributions arising from γ^* exchange, Z exchange, and the $\gamma^* - Z$ exchange are shown separately, together with their combination.

two taus in the final state, accompanied by two b -jets coming from the proton splitting in the initial state. This diagram is particularly effective in constraining leptoquarks models. Being the final state constituted of exactly two leptons (the additional b -jets are radiated in the *initial* state and propagated in the final state) an interference is generated between the exotic leptoquark t -channel and the SM Drell-Yan diagrams, which produces a variation in the events yields. If existing, leptoquarks would therefore be detected as anomalies in the Drell-Yan cross section precision measurement, which would show a deviation in the high-mass tail of the differential $d\sigma/dm_{\tau\tau}$ distribution.

The CMS experiment has exploited the aforementioned strategy performing a leptoquarks search with the di-tau Drell-Yan process [62], which is also complemented by measurements probing the single and pair leptoquark production. The search has been performed using 137 fb^{-1} data of pp collisions recorded at centre of mass energy $\sqrt{s} = 13 \text{ TeV}$, and selecting events both in the semi-leptonic and the hadronic channels. Results of exclusion limits are shown in Figure 1.20 for the scalar leptoquark case and in Figure 1.21 for the vector leptoquark case, distinguishing among two couplings scenarios. A global 3.4σ excess is detected, which is particularly evident in the limit set via the Drell-Yan production. The excess is jointly present in all channels and both in scalar and vector leptoquark interpretations, preventing the exclusion of the phase-space regions representing leptoquarks compatible with an explanation of low energy B -anomalies.

Although this result is quite interesting on its own, an independent analysis from the ATLAS experiment is necessary to get a confirmation or a denial of such evidence. ATLAS has performed such a search, consisting in the study of the same di-tau

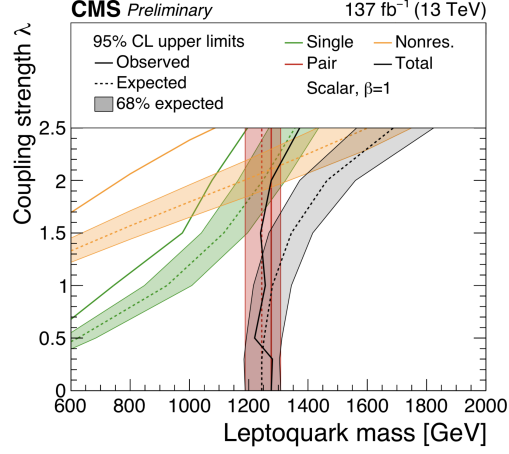


Figure 1.20. Exclusion contours in the mass versus coupling constant plane, for a scalar leptoquark model. Single production, pair production, Drell-Yan limits are shown, together with their combination [62].

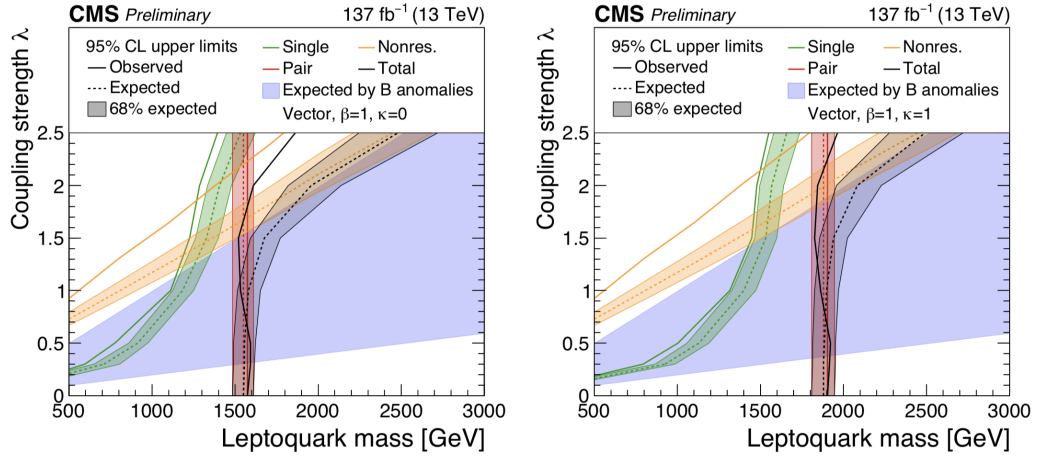


Figure 1.21. Exclusion contours in the mass versus coupling constant plane, for vector leptoquark models. Limits are calculated for different values of the coupling constant to right handed current: $k = 0$ (left), $k = 1$ (right). All production leptoquark modes are shown, together with their combination [62].

Drell-Yan process, with a selection inclusive in b -jets, and covering both semi-leptonic and fully hadronic channel. Results, together with a complete description of the analysis are outlined in Chapter 4 and constitute the main physics topic of this thesis.

Chapter 2

The experimental setup: LHC, ATLAS and objects reconstruction

In this summary chapter I outline all the information on the experimental infrastructure, which I collected from the study of published material and of the status of the art on object reconstruction.

The experimental infrastructure used to produce the results presented in this thesis is fully described in this chapter. Section 2.1 presents the Large Hadron Collider, the accelerating facility in which the ATLAS experiment is installed. A comprehensive overview of the ATLAS detector and its sub-systems is given in Section 2.2, while the reconstruction of physics objects is detailed in Section 2.3.

2.1 The Large Hadron Collider

The Large Hadron Collider (LHC) [63], installed at CERN laboratories at the Swiss-French border near Geneva, is the world's largest synchrotron. It is located between 45 and 175 m underground and has a circumference of about 27 km. The LHC accelerates protons, or heavy ions, to high energies and collides them to allow the study of particles produced in such collisions and their decay products in complex detector systems.

Four main experiments are located along the accelerator circumference, each of which is working on a characteristic physics program: ALICE [64], dedicated to the study of heavy ion collisions and quark-gluon plasma, LHCb [65], predominantly focusing on the study of heavy flavour physics, ATLAS [66] and CMS [67], which are general purpose detectors with a physics program covering both searches of exotic particles and Standard Model precision measurements.

In this thesis, only data from proton-proton collisions are analysed, therefore only pp collisions are discussed in the following. Protons travelling in the LHC are collected in two beams, separately running in opposite directions inside two independent vacuum beam pipes. The beams are themselves constituted of bunches of about 12×10^{10} protons which are accelerated by radio-frequency cavities, providing

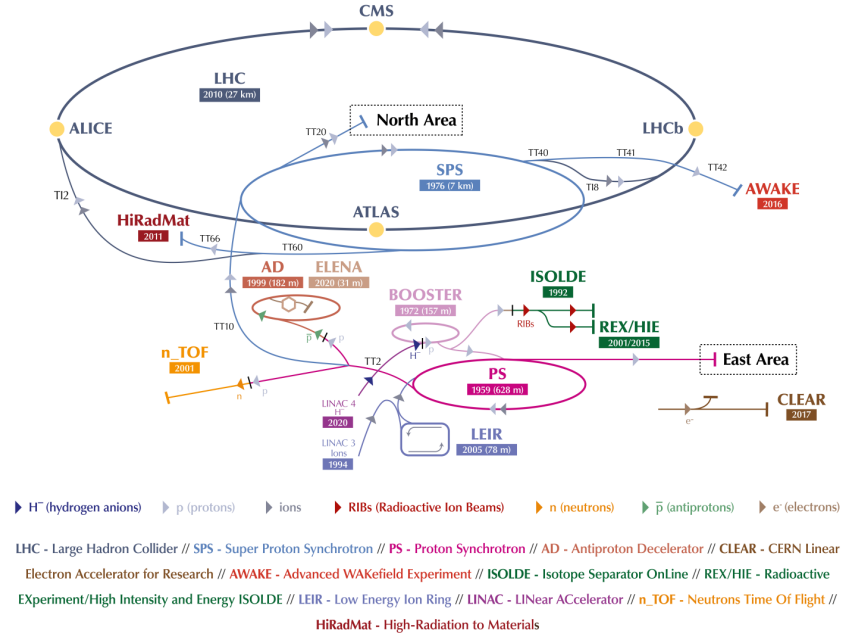


Figure 2.1. The CERN accelerators complex. Figure adapted from [68].

an oscillating electric field at a fixed frequency of 400 MHz. The proton bunches are kept at up to 7 TeV of energy on the LHC circular orbit by 1232 superconducting dipole magnets, able to provide a magnetic field up to 8.3 T, which bends their trajectories. Additional magnets, 858 quadrupoles and around 6000 correctors, are located along the accelerator ring and act on the beam characteristics, such as its focus.

Before protons can enter the LHC, they need to pass through a chain of pre-accelerators, as shown in Figure 2.1. The protons are extracted from a bottle of hydrogen gas, which is ionised using an electric field. A linear accelerator (Linac 2, replaced in 2020 by Linac 4) then speeds up the protons to energies of 50 MeV. This beam is then injected into the Proton Synchrotron Booster (PSB), which consists of four stacked synchrotron rings. The PSB accelerates the protons to 1.4 GeV, shapes the beam into bunches, and then injects it into the Proton Synchrotron (PS). The PS increases the beam energy to 25 GeV, followed by the Super Proton Synchrotron (SPS), which accelerates the protons to 450 GeV. Finally the beams are injected into the LHC, where they circulate at the highest achievable energy.

LHC operations started in 2008 and have been staged in Run and Long Shutdown (LS) periods. LHC Run 1 began in 2010 and lasted until the end of 2012. In this period pp collisions have been recorded with a centre of mass energy of $\sqrt{s} = 7$ and 8 TeV. The machine was then upgraded during LS1, followed by Run 2, which took place between 2015 and 2018, recording collisions at an energy of $\sqrt{s} = 13$ TeV. Then, after the LS2, Run 3 started in 2022 and it is still ongoing as of today.

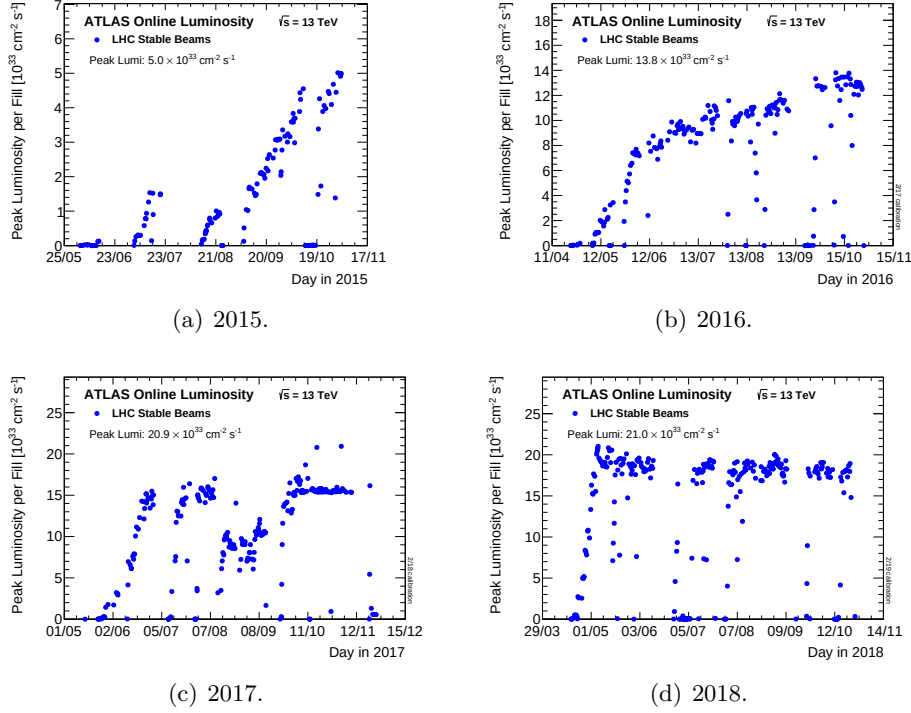


Figure 2.2. Peak instantaneous luminosity registered by the ATLAS experiment during the years of Run 2 of the LHC. Taken from [69].

2.1.1 Accelerator parameters and performance

The number of pp collisions per second at the LHC is proportional to the total proton-proton interaction cross section via the instantaneous luminosity

$$\frac{dN}{dt} = \mathcal{L} \sigma_{pp}^{\text{tot}}. \quad (2.1)$$

The instantaneous luminosity, measured in $\text{cm}^{-2}\text{s}^{-1}$, depends on the beam characteristics, and can be expressed as

$$\mathcal{L} = f(\alpha) \frac{k f n_1 n_2}{4\pi \sigma_x \sigma_y}, \quad (2.2)$$

where k is the number of bunches inside the ring, f is their revolution frequency, n_1 and n_2 are the number of protons in each bunch, σ_x and σ_y are the transverse amplitudes of the bunches, z being the propagation direction of the beams. The geometric factor $f(\alpha)$, lower than 1, accounts instead for non-collinearity of the beams, which cross each other in the interaction point with an angle $\alpha \neq 0$, and other intra- and extra-beam effects. Figure 2.2 shows the the instantaneous luminosity, as measured by the ATLAS experiment, for each year of Run 2. As can be seen, the luminosity was slowly increased during the data-taking, reaching the highest peak of $\mathcal{L} = 2.1 \times 10^{34} \text{cm}^{-2}\text{s}^{-1}$ [69].

In each collision between the bunches, multiple pp interactions take place. Among these, the most energetic head-on collision between protons is the one of interest, while

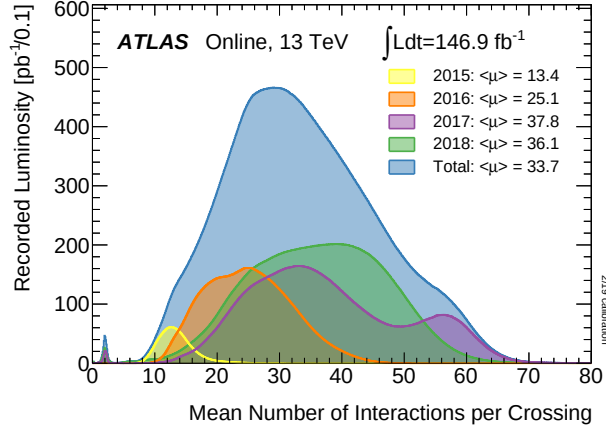


Figure 2.3. Number of interactions per crossing, recorded by the ATLAS experiment during Run 2 of the LHC. Taken from [69].

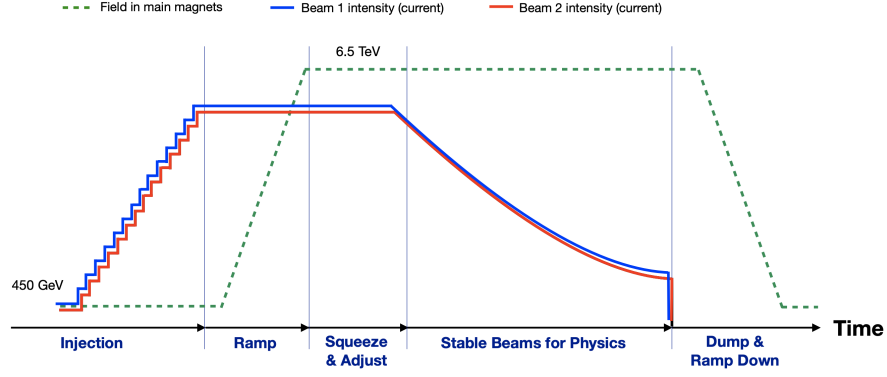


Figure 2.4. LHC filling cycle. Figure adapted from [80].

the others, known as *pile-up*, represent additional radiation which can deteriorate the reconstruction of the main hard scattering event. In particular, *in-time pile-up* is due to multiple collisions happening in the same bunch-crossing, while *out-of-time pile-up* is generated from residual energy deposits in the sub-detectors, lasting more than the separation time between two bunches. Pile-up can be quantified by the average number of interactions per bunch-crossing, which is related to the instantaneous luminosity $\mathcal{L}$, the total pp cross section σ_{pp}^{tot} , the number of bunches k and the revolution frequency f via the relation

$$\mu = \frac{\mathcal{L} \sigma_{pp}^{\text{tot}}}{k f} . \quad (2.3)$$

Figure 2.3 shows the distribution of the average number of interactions, measured by the ATLAS experiment for each year of the Run 2 data-taking. It can be seen that the number of interactions has been increased, due to the increase in instantaneous luminosity, reaching a total average value of $\langle \mu \rangle = 33.7$ [69].

During LHC operations, the instantaneous luminosity decreases, mainly due to collisions taking place in the interaction points (IPs) where the experiments are

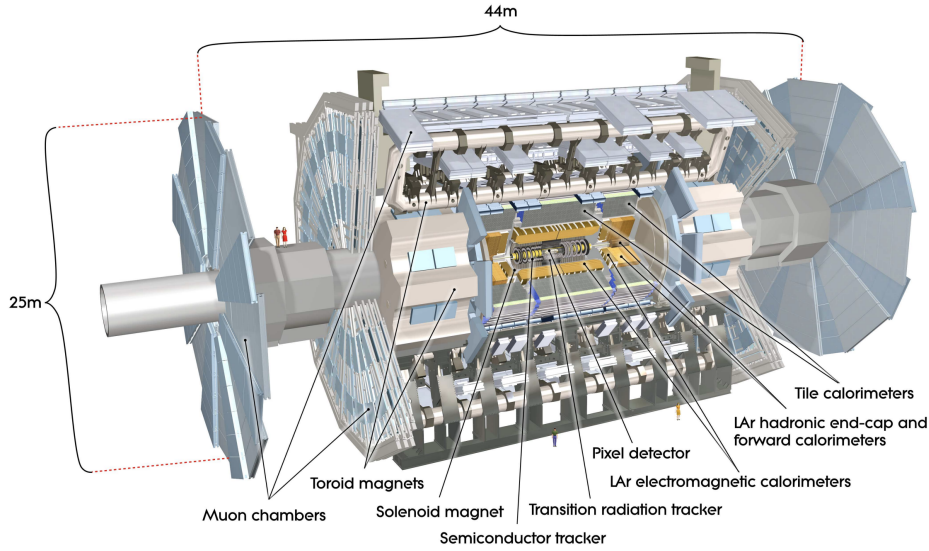


Figure 2.5. The ATLAS experiment. Figure taken from [66].

located, and, secondarily, due to degradation generated by intra-beam forces and interactions with residual gases in the beam pipe. Collisions are considered in *stable beams* condition for a time which typically lasts from 5 to 15 hours. When the luminosity is lower than a fixed threshold, beams are dumped via a system installed along the ring, and a new injection is performed. The fill of the rings with proton bunches and the ramping of the beam energy from 450 GeV to 6.5 TeV took between 90 and 120 minutes during Run 2. Figure 2.4 shows the LHC filling cycle, which is repeated several times during the data-taking.

2.2 A Toroidal LHC ApparatuS

ATLAS (A Toroidal LHC ApparatuS) [66] is a multi-purpose collider detector, located at the Interaction Point 1 (IP1) of the LHC. It is composed by a series of sub-detectors, placed in cylindrical symmetry around the beam axis and providing an almost hermetic coverage to reconstruct particles produced in the collisions. The experiment measures 44 m in length and 25 m in height and is divided into a *barrel* (or central) region and two *endcaps*. From the interaction point towards the outer part, the detector is constituted by a tracking system, an electromagnetic calorimeter, a hadronic calorimeter and the muon spectrometer (see Figure 2.5).

Superconducting magnets

Particles momentum is measured from their bending into a magnetic field, which is generated by four different superconductor magnets. The solenoid magnet, whose axis is parallel to the beam pipe, is located in the inner part of the detector. It is 5.8 m long, and has inner (outer) radius of 2.46 m (2.56 m) and provides a constant magnetic field of 2 T. The barrel toroid is made of 8 coils 25.3 m long. This toroid forms a cylindrical region of respectively 9.4 m and 20.1 m internal and external

diameters, in which a magnetic field of mean value of 0.5 T is provided in air. In the end-caps, two other toroids in a radial zone between 0.8 and 5.3 m around the beam pipe provide a magnetic field in the range 0.2 – 3.5 T. Hall probes are installed throughout the system to allow the online monitoring of the magnetic field, with a precision of 0.01 mT.

Coordinate system

A cylindrical coordinate system is adopted, centered in the middle of the experiment. The z -axis is defined along the beam pipe, the y -axis is vertical, and the x -axis is defined as pointing towards the LHC centre. In the (x, y) plane, transverse to the beam direction, the azimuth angle ϕ and the radius r are defined. The transverse momentum (p_T) of a particle is defined as the 2D projection of the momentum vector on this plane. In the (z, y) , or (z, r) , plane the polar angle θ is defined, with origin on the z axis. The rapidity, y , is defined as

$$y = \frac{1}{2} \ln \left(\frac{E + p_z}{E - p_z} \right) , \quad (2.4)$$

where p_z is the momentum component along the beam axis. It can be shown that the rapidity difference Δy is invariant under longitudinal boosts. In the ultra-relativistic limit, rapidity is approximated by pseudo-rapidity, defined as

$$\eta = -2 \ln \left(\tan \frac{\theta}{2} \right) . \quad (2.5)$$

This quantity allows for an expanded scale at low polar angles and is therefore preferred as polar kinematic variable and is used to report sub-detectors coverage. A geometrical distance in the transverse plane can also be defined in terms of pseudo-rapidity and azimuth angle as

$$\Delta R = \sqrt{\Delta \eta^2 + \Delta \phi^2} , \quad (2.6)$$

which is used to express separation between energy deposits, or between couples of reconstructed objects in the final state.

2.2.1 The sub-detector systems

Inner detector

The inner detector [71] is the closest sub-system to the beam pipe. Its purpose is to track charged particles from the interaction region until they reach the calorimeter and measure their momentum by determining the curvature of the tracks in the magnetic field. The ID covers a region of $|\eta| < 2.5$ and a radius between 3 cm and 1 m, and can reconstruct tracks with $p_T > 0.4$ GeV. The ID works in a high radiation density environment, requiring a good radiation tolerance as well as a fast readout and an excellent resolution on reconstructed tracks. The ID consists of three sub-systems: the pixel detector, the Semi-Conductor Tracker, the Transition Radiation Tracker (see Figure 2.6).

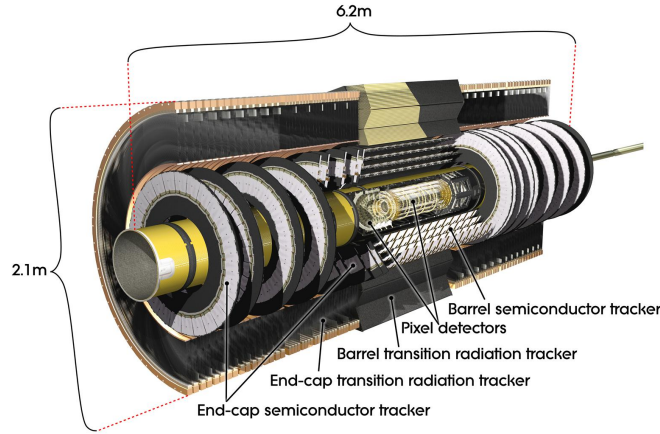


Figure 2.6. ATLAS inner detector. Figure from [72].

Pixel detector. The silicon pixel detector [73] is the innermost system. It consists of three barrel layers and three end-cap layers, and it is made of 1744 pixel modules with a total of 80 million pixels. The modules have a pixel pitch of $50 \times 400 \mu\text{m}^2$ and a sensor thickness of $250 \mu\text{m}$. During the LS1, an additional pixel detector has been inserted, the Insertable B-Layer (IBL) [74], meant to improve the flavour tagging performance as well as to compensate the radiation damage. The layer is located 33 mm away from the beamline and includes 12 million pixels with a pixel pitch of $50 \times 250 \mu\text{m}$. Globally, the pixel detector provides a spacepoint resolution of $10 \mu\text{m}$ in the (r, ϕ) plane and of $67 \mu\text{m}$ in the z -direction.

Semi-Conductor Tracker (SCT). The subsequent layer of the ID is the SCT [75], which consists of silicon microstrip modules, arranged into four concentric barrel layers and two end-caps with nine disks each. The pitch of the strips is $80 \mu\text{m}$, while the thickness of the detectors is $285 \mu\text{m}$. Strips are coupled with a stereo angle of 40 mrad, providing two dimensional hit reconstruction. The SCT modules have a total resolution of $17 \mu\text{m}$ in the (r, ϕ) plane and of $580 \mu\text{m}$ in the z -direction.

Transition Radiation Tracker (TRT). The outermost component of the ID is the TRT [76]. The TRT is a straw-tube tracker which consists of 300 thousand cylindrical drift tubes (straws), with a 4 mm diameter. The tubes are filled with a gas mixture Xenon- CO_2 - O_2 (70%, 27%, 3%), which is ionised by the energy deposited by passing particles, generating a signal. The TRT contributes not only to the momentum measurement of charged particles, but also to particle identification. The space between the straws is filled with polypropylene, which emits a transition radiation with an intensity dependent on the particles boost. The amount of radiation produced is used to determine the particle masses, and in particular to help discrimination between electrons and pions. The TRT provides a position resolution on ϕ of $130 \mu\text{m}$.

Combining the information of all the three sub-systems, the overall resolution

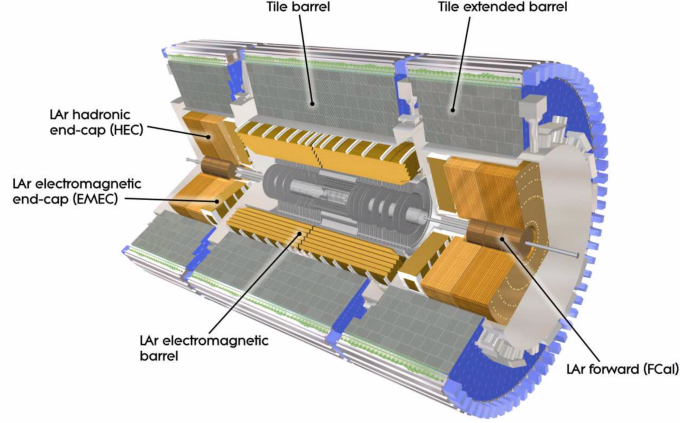


Figure 2.7. ATLAS calorimeter system. Figure taken from [66].

on the momentum a charged particle crossing the ID is

$$\frac{\sigma_{p_T}}{p_T} = 0.05\% p_T [\text{GeV}] \oplus 1\% ,$$

where p_T is the particle transverse momentum and $\oplus$ indicates a sum in quadrature.

Calorimeters

The ATLAS detector uses calorimeters to measure the energy of neutral and charged particles, as well as missing transverse momentum. The ATLAS calorimeters, shown in Figure 2.7, are hermetic along ϕ and cover a range of $|\eta| < 4.9$. All of them are *sampling* calorimeters, meaning that they consist of alternate layers of active and passive material. The passive material is usually dense and with a high atomic number, which induces cascades of particles (showers). The active layers, instead, measure the energy deposited by the showers, such as ionisation or scintillation light. A crucial point to correctly reconstruct the energy of the particles, is that the induced showers have to be fully contained in the calorimeters, while a negligible fraction of secondary particles has to escape and interact with the following detectors (a phenomenon called *punch-through*). To match these requirements, materials with a high radiation length (X_0) and interaction length (λ) are used.

Electromagnetic calorimeter. The ATLAS electromagnetic calorimeter [77] is shaped as an accordion. It is formed by lead slabs (passive material), which contains liquid Ar (active material) kept at a temperature of 88.5 K. The system has cylindrical symmetry around the interaction point and is divided in a barrel region, covering $|\eta| < 1.475$ and two end-caps, covering the range $1.375 < |\eta| < 2.5$. The separation region, in the range $1.37 < |\eta| < 1.52$ is called *crack-region* and is typically vetoed in the reconstruction of electrons and photons since it contains a large amount of inactive material. The barrel region extends for 6.4 m in total, and has inner and outer radii of 1.4 and 2 m. The total depth of the calorimeter is between $22 X_0$ and $33 X_0$, depending on the $|\eta|$ value. The end-caps are formed by two wheels of 63 cm of width and inner (outer) radius of 33 cm (2.1 m). A

total length between $24 X_0$ and $38 X_0$ is achieved, depending on the $|\eta|$ value. The energy resolution of the EMC was measured in test beams with electrons before the installation in ATLAS and was found to be

$$\frac{\sigma(E)}{E} = \frac{10.1\%}{\sqrt{E(\text{GeV})}} \oplus 0.17\% , \quad (2.7)$$

where the first term is stochastic and the second one is related to the non-uniformity of the detector response.

Hadronic calorimeter. The hadronic calorimeter is composed of a tile calorimeter, located in the central region behind the EMC, and a LAr hadronic end-cap calorimeter, located behind the LAr end-caps of the EMC. The tile calorimeter has an inner (outer) radius of 2.28 m (4.25 m) and is itself divided into a barrel region ($|\eta| < 1.0$) and two extended barrel regions ($1.0 < |\eta| < 1.7$). Tiles are alternatively formed by a steel absorber and scintillator, in a ratio of roughly 4.7 : 1. The UV light produced by scintillators is captured by wavelength shifter optic fibers and transferred to photo-multipliers (PMTs), used for the readout. The HC barrel is segmented radially in three layers, which cover globally a thickness of 7.4λ . The HC end-caps cover instead the range $1.5 < |\eta| < 3.2$, and are built with planar geometry. The sampling is obtained alternating copper plates and LAr with a pitch of 8.5 mm. The overall energy resolution of the HC is given by

$$\frac{\sigma(E)}{E} = \frac{52\%}{\sqrt{E(\text{GeV})}} \oplus \frac{1.6 \text{ GeV}}{E} \oplus 3\% , \quad (2.8)$$

where the first term is related to the stochastic nature of the shower development, the second is due to the read-out electronic noise, the third one is a constant related to effects in the calibration of the calorimeter.

Forward calorimeters. The forward calorimeter (FCal) is an additional subsystem, covering the region $3.1 < |\eta| < 4.9$. FCal is specifically designed to detect a high flux of particles, which is present in the forward region, since most of the collision happen with low transfer of momentum. It is divided into three sub-modules (FCal1, FCal2, FCal3), one electromagnetic and two hadronic, each 45 cm thick and adopting LAr as active material. The passive material depends instead on the sub-module: FCal1 uses copper, yielding a total thickness of $27.6 X_0$ and 2.66λ , while tungsten is used for FCal2 and FCal3, which allow to reach a total thickness of $90 X_0$ and 3.6λ . The read-out is fast and done in capacity way from the LAr gaps, whose width varies between $269 \mu\text{m}$ and $508 \mu\text{m}$.

Muon spectrometer

The ATLAS muon spectrometer (MS) [78], shown in Figure 2.8, is located in the outer part of the experiment and is used to track muons and measure their momentum as well as providing information for the muon trigger. Tracking is provided for muons in the interval $|\eta| < 2.7$ with momentum of at least 3 GeV. The momentum measurement is possible thanks to the magnetic field present around the spectrometer

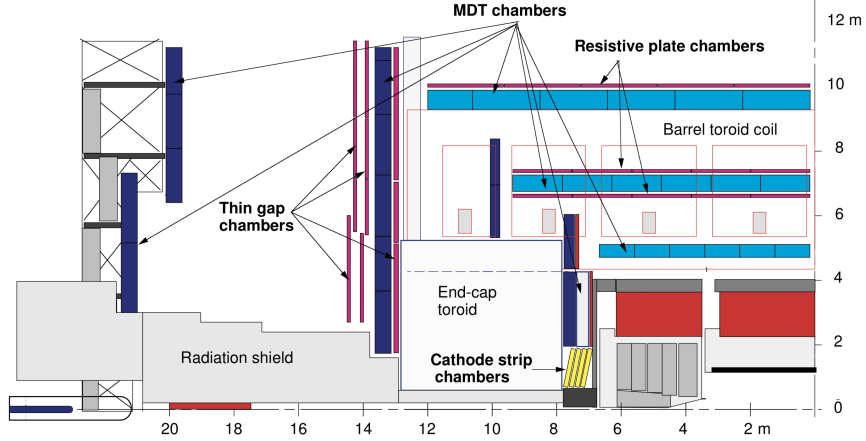


Figure 2.8. ATLAS muon spectrometer in the (z,r) plane. Figure adapted from [79].

chambers, which bends their trajectory allowing to measure the sagitta. Detectors are organised in 16 sectors, placed in cylindrical symmetry around the interaction point. In the barrel region, chambers are organised in three separate stations, located respectively at 5, 7.5, 10 m from the beam pipe. In the end-caps, detectors are mounted on wheels, located at $|z| = 7.4, 10.8, 14$ m. The innermost one is called *small wheel*, while the outer two are the *big wheels*.

Tracking chambers. Monitored tubes (MDT) are gas detectors, operating with a mixture of Ar : CO₂ (93%, 7%). They allow to measure the muon momentum through a sagitta measurement, which is performed with a precision of $\Delta s = 45 \mu\text{m}$. A laser system is monitoring online the chambers position, since the alignment error is the dominant source of uncertainty for high p_T muon ($p_T > 300$ GeV). For low p_T muons, instead, the leading source of uncertainty is the fluctuation of the energy deposited by the passing particle. MDT are installed on all MS stations, except for the small wheels, where for $|\eta| > 2$ cathode strip chambers (CSC) are installed, as they are able to manage the high rate of particles present in that region (150 Hz/cm^2). CSC chambers are installed on 8 sectors and are divided in pads. Along the $|\eta|$ direction a precision of $60 \mu\text{m}$ can be achieved, while on the ϕ direction the resolution is 5 mm. As part of the upgrade project in preparation for Run 3 the small wheels have been substituted by the New Small Wheels, as will be further detailed in Section 5.1.2 of Chapter 5.

Triggering chambers. The muon spectrometer provides also information to the trigger system, in charge of selecting interesting events during the data acquisition. Trigger chambers in the barrel region are based on Resistive Plate Chambers (RPC), installed on the middle and outer stations of the MS. These chambers provide a trigger in the region $|\eta| < 1.05$, with a spatial resolution of 10 mm both in the z and ϕ direction. The time resolution is very small, to support the precise timing of the triggers and is 1.5 ns. In the end-caps, thin-gap chambers (TGCs) are installed on the small wheel, while two TGC doublets are located on the big wheel, closer to the IP. These multi-wire proportional chambers operate in saturated mode and

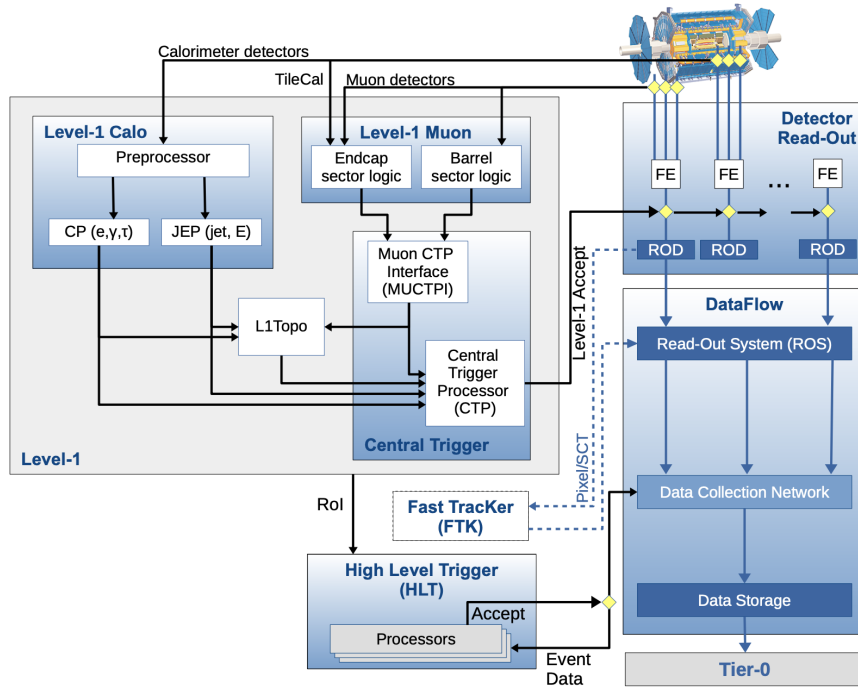


Figure 2.9. Scheme of the ATLAS trigger system during Run 2. Figure taken from [80].

provide trigger in the forward region $1.05 < |\eta| < 2.4$. The spatial resolution of TGCs is 2-6 mm on the radial coordinate, and 3-7 mm on the ϕ direction. The time resolution of these chambers is instead 4 ns.

The trigger system

The trigger system [80] is used in ATLAS to reduce the rate of incoming events selecting only a fraction of them. Only the selected events, considered interesting according to some criteria, are passed to the data-acquisition chain. During Run 2 the ATLAS trigger system was based on two levels (see Figure 2.9): a first hardware level (L1), in charge of reducing the events rate from the initial value of 40 MHz to 100 kHz, and the High Level Trigger (HLT), further reducing the rate of events to 1 kHz.

Level 1 trigger (L1). The L1 trigger performs the first level of selection and is the most hardware based sub-system, processing detector information directly with front-end electronics. This trigger level is divided into Level-1 Calo (L1Calo) and Level-1 Muon (L1Muon). L1Calo takes input signals from the calorimeters, makes analog-to-digital conversion using a reduced granularity and sends them to the Cluster Processor (CP) and the Jet Energy Processor (JEP), which identify the raw objects (electrons, photons, taus for the CP and jet and missing transverse momentum for the JEP). L1Muon uses instead the information coming from the muon spectrometer, complemented with information from the calorimeters, to identify muons and estimate their p_T . In particular, in the barrel region signals are received

from the RPCs, while in the end-caps signals are processed from the TGCs and the tile calorimeter. The muon p_T is computed using an algorithm based on the opening of coincidence windows centered in the central MS station. All reconstructed raw objects information is sent via the L1Topo and Muon CTP Interfaces to the central trigger processor (CTP), which takes the final decision whether to accept or reject the event, according to the trigger menu criteria and to the online status of the data acquisition chain. L1 trigger selection criteria are mainly based on the number of prompt muons and their p_T , on the total energy measured in the calorimeters or on the amount of missing transverse momentum. Additional triggers are based on more complex requirements, such as the angular distance between the energy deposits or the reconstructed invariant mass. Once the event is selected by the L1 trigger, regions of interest (ROI) in (η, ϕ) plane are identified and the corresponding data are transferred to the HLT. The latency of the L1 algorithm is $2.5 \mu\text{s}$.

High level trigger (HLT). The HLT integrates the ROI data with the complete information from all the sub-detector systems to perform a second level of events selection. The ROI data received from the front-end boards are transferred to the sub-detectors read-out system (ROS) via the read-out drivers (ROD). The ROS is interfaced with a farm of processors in which a full offline-like event reconstruction is executed and the HLT decision algorithm is run. HLT implements more complex decisions, involving different signatures and fully reconstructed objects (leptons, missing transverse momentum, b -jets).

Trigger menu and data streams. The final trigger decision is taken accounting for a series of requirements, which involve conditions on the number of reconstructed objects and their kinematics. Such requirements are encoded in the *trigger chains*, which can be combined in logical OR or AND to define the *trigger menu*. The trigger menu is decided before the data acquisition and evolves during the run to manage the changing conditions of the collisions performance. Trigger conditions are chosen to reduce the rate of events as needed and keep at the same time the thresholds on objects kinematic as low as possible, correspondingly keeping the kinematical phase space as wide as possible. A *prescaling* of $p > 1$ is applied in some conditions to further scale the events rate of a factor $1/p$ without requiring any particular condition. The typically used triggers in ATLAS data acquisition are the lowest un-prescaled triggers, with thresholds on p_T of the order of tens of GeV for the leptons and hundreds of GeV for the jets.

The data acquisition system uses streams to convey data during the data-taking. In particular, the *physics stream* is used to pipeline triggered data to the storage, to be analysed by physics analyses. The *debug stream* collects instead the events for which the HLT algorithms failed to run. These events are recovered offline. The *Trigger-Level Analysis (TLA) stream* saves data containing partial detector information (e.g. objects reconstructed by the HLT). These raw events have a smaller size than fully reconstructed events, hence lower trigger thresholds can be adopted on this stream, which are used for specific studies. A *calibration stream* is used instead to collect specific data to calibrate the trigger sub-systems, while the *express stream* saves specific samples of data, extracted from the physics stream to perform

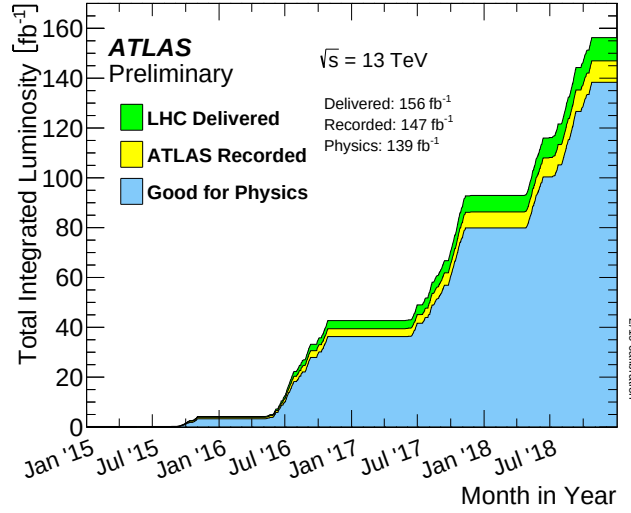


Figure 2.10. The total integrated luminosity during Run 2 as a function of time. The LHC delivered, ATLAS recorded and GRL values are displayed. Figure taken from [69].

quality checks during the data-taking. Finally, the *monitoring stream* is used to check online the status of the ATLAS sub-systems (e.g. in the control room during the run).

2.2.2 Data acquisition during Run2

The physics results presented in this thesis are based on Run 2 data, which took place in the years 2015-2018. During this period pp collisions happened with a centre-of-mass energy of $\sqrt{s} = 13$ TeV.

During the pp collisions, the luminosity is measured online by dedicated detectors located in the forward regions of the ATLAS experiment. The measurement is mainly done by LUCID2 Cherenkov detector [81], which consists in 16 PMTs, located along the beam pipe axis. Starting from the PMT counts, the luminosity value is calculated for all the luminosity blocks (LB), which are periods of around one minute in which luminosity is considered constant. From these values the instantaneous luminosity can be extrapolated (see Figure 2.2). The absolute luminosity scale is calibrated using the *Van der Meer scan*, which is a procedure performed during dedicated running periods in each year, and extrapolated to the physics data-taking regime using complementary measurements from the other luminosity-sensitive detectors.

Figure 2.10 shows the total integrated luminosity for Run 2. As can be seen from the figure, not all the delivered pp collisions from the LHC are recorded by ATLAS experiment due to inefficiencies. Moreover, only a fraction of recorded events is actually considered useful for physics analyses, if verifying the conditions to be added to the *good-run-list*. The total available luminosity for Run 2 is finally $140.1 \pm 1.2 \text{ fb}^{-1}$ [82].

2.2.3 Events simulation

ATLAS physics analyses are based on the comparison between real data, recorded by the experiment, and expected yields, evaluated from Monte Carlo simulations. The production of Monte Carlo samples describing both collision products and their interaction with the detector is therefore a task of crucial importance. The ATLAS simulation infrastructure [83] is based on status-of-the-art physics events generators, developed by theorists, integrated with the GEANT4 [84] model of the ATLAS detector.

Event generators simulate final state particles which are propagated into the GEANT4 model producing *hits* in the various sub-detectors (*simulation* stage). Afterwards, the simulated hits are merged with signals representing the cavern background and the detector noise, and a data stream is formed with the same format of the real data byte-stream (*digitization* stage). Pile-up is also considered and simulated events are re-weighted to correctly represent the average number of interactions measured in data. Reconstruction algorithms are finally applied to perform precise objects reconstruction and calibration. Being the data formats consistent, the same algorithms are applied both to the Monte Carlo files and to the data files. Since in the Monte Carlo simulation the interaction with the detector is fully computed and factorised with respect to the physics events generation, “truth level” information can be retained. This includes all the kinematics of the particles coming from the physics interaction both at generation and simulation stage, and is useful to quantify the performance of the objects reconstruction algorithms.

2.3 Physics objects reconstruction

Reconstruction algorithms run over raw signals from the detector to build the final physics objects used in the analyses. The reconstruction occurs in several steps. First of all, elementary objects are built, such as tracks, vertices and calorimeter clusters. Then, more complex objects, like leptons, photons and jets are constructed and additional identification and isolation criteria are applied. These objects are finally calibrated to fine-tune their estimated energy and momentum.

2.3.1 Tracking and vertexing

Particles travel in an helicoidal trajectory through the solenoid magnetic field in which the ATLAS ID is located. The helicoidal trajectory is described by five parameters, also shown in Figure 2.11: the magnitude of the transverse momentum p_T , the polar angle θ , the azimuth angle ϕ , the transverse impact parameter with respect to the beam direction, d_0 and the longitudinal impact parameter with respect to the nominal interaction point, z_0 . These last two parameters are evaluated referring to the point of closest approach of the trajectory with respect to the beam line. We summarise in the following the essential features reconstruction of tracks in ATLAS, the reader is referred to Ref. [85] for further details.

The reconstruction of tracks in the ID starts from the detection of hits in the pixel and SCT detectors. Hits are then grouped in *clusters* to form space-points. *Track seeds* are then formed by grouping three space-points. This approach maximizes

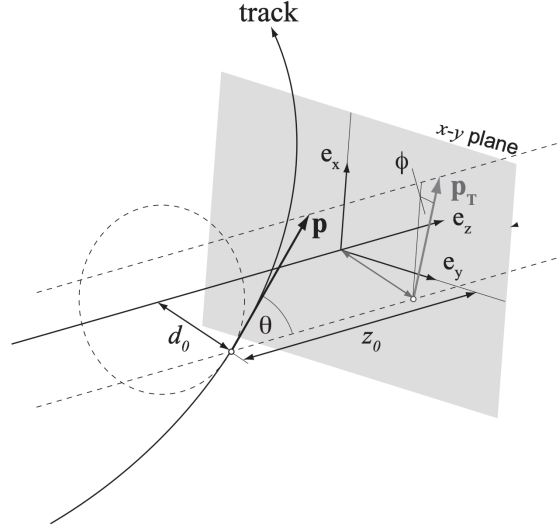


Figure 2.11. Scheme of the parameters for tracks description in ATLAS. The e_z base vector is placed along the beam pipe direction. Figure taken from [86].

the possible number of combinations while still allowing a first crude momentum estimate. A combinatorial Kalman filter [87] is then run to build track candidates from the chosen seeds by incorporating additional space-points from the remaining layers on the pixel and SCT detectors which are compatible with the preliminary trajectories. It can happen that more than one track is associated to the same space-point cluster. For this reason, an ambiguity solver algorithm is run to discard such kind of inconsistencies. The ambiguity solver selects tracks according to a score, that is assigned based on the χ^2 of the track fit, its p_T and the number of holes (i.e. layers with no hit in the predicted track). Moreover, clusters are also selected, checking that one cluster cannot be shared by more than two tracks and that a track cannot have more than two shared clusters. Highly ranked tracks are then extended to include the TRT hits. Moreover, tracks are further selected and removed if failing to meet one of the quality criteria reported in Table 2.1.

Table 2.1. Requirements for tracks selection during their reconstruction.

Requirement
$p_T > 400 \text{ MeV}$
$ \eta < 2.5$
≥ 7 pixel and SCT clusters (12 are expected)
≤ 1 shared pixel cluster or ≤ 2 shared SCT clusters on one layer
≤ 2 holes in pixel and SCT detectors
≤ 1 hole in the pixel detector
$ d_0 < 2.0 \text{ mm}$ with respect to the beam line
$ z_0 \sin \theta < 3.0 \text{ mm}$ with respect to the beam line

The accepted tracks are finally used to identify primary vertices, i.e. the locations where the interactions have occurred. The hard scatter (HS) is defined as the one

with the highest sum of the square of transverse momenta of the associated tracks.

2.3.2 Electrons and photons

Electron reconstruction

Electrons are high level objects, reconstructed in the central region of the detector ($|\eta| < 2.5$) by combining information from tracks and energy clusters. In the forward region ($2.5 < |\eta| < 4.9$) the tracks information is not available, hence electrons are reconstructed with the calorimetric information, exploiting also additional properties like the shape of the cluster. All details on electrons reconstruction in Run 2 are available in Refs. [88, 89] and are summarised in the following.

Electron reconstruction starts from the building of *topo-clusters*. These are variable-size topological clusters built combining information originating from the EM and hadronic calorimeters. Clusters are selected if the EM energy is above 400 MeV and the ratio between the EM and the total cluster energy is above 0.5. Tracks are instead reconstructed in the ID, also considering the energy losses due to bremsstrahlung. Using a sliding window algorithm tracks are loosely matched to the clusters. Tracks are then refitted with a Gaussian sum filter algorithm to improve the accuracy of the track parameters. Initial electron candidates are then built by matching at least one track to a calorimeter cluster and, in case of multiple tracks, the closest track to the cluster is chosen. Compatibility with the hard-scatter vertex is also checked in case of prompt electrons. It might happen that due to bremsstrahlung radiation an electron candidate is reconstructed as two clusters. To account for this effect, nearby clusters within $\Delta\eta \times \Delta\phi = 0.075 \times 0.125$ of their respective barycenters are merged within the initial cluster (*superclusters*). These clusters are finally used to repeat the track-cluster matching and build the final electron objects.

Electrons identification and isolation

After the reconstruction, an additional selection is performed to identify prompt electrons with respect to other objects. The electron identification algorithm uses a likelihood-based approach embedding several variables. The discriminating variables can be grouped in three types that are either related to the properties of the track, or the shower development in the different layers of the calorimeter, or the matching between the track and the calorimeter cluster. Three sets of identification selection requirement are defined, *Loose*, *Medium* and *Tight*, which correspond to increasingly restrictive selections. For each operating point, identification efficiencies are evaluated as a function of p_T and $|\eta|$, as can be seen in Figure 2.12(a).

Electron candidates are also requested to be isolated from additional tracks or energy deposits. Isolation variables can be defined, based on calorimeter energy deposits or tracks. The electron calorimeter isolation, E_T^{coneXX} , is calculated by summing the transverse energy of topological clusters whose barycentre falls in a cone centered around the electron cluster barycentre. The cone has a size of $\Delta R = \text{XX}/100$. The energy of the electron itself and contributions from pile-up activity are subtracted from the energy count, as described in Ref. [88]. The electron track isolation variable, p_T^{coneXX} is instead defined as the scalar sum of the transverse

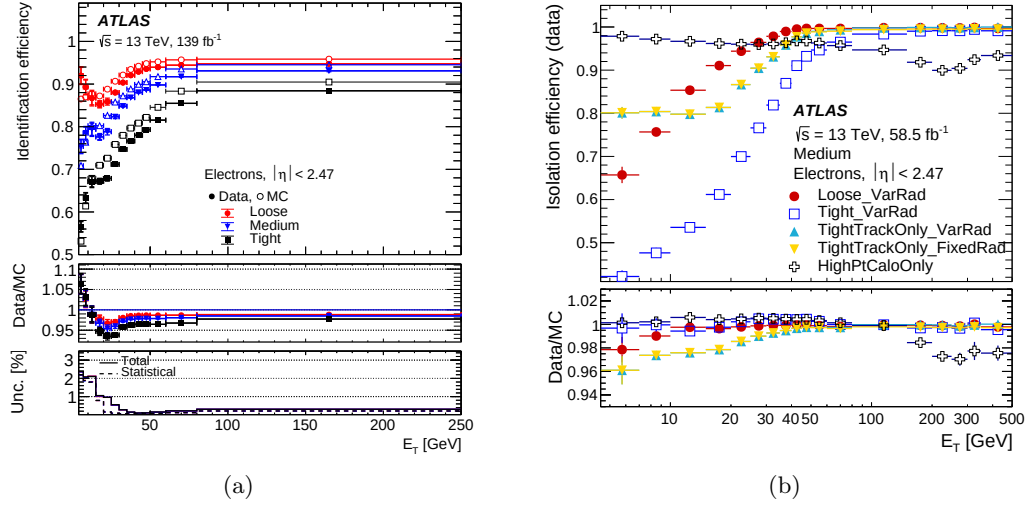


Figure 2.12. Electrons identification efficiency (a) and isolation efficiency (b) as a function of the transverse energy. The middle panel in (a) and lower panel in (b) show the ratio between the efficiencies measured in data and in MC. Figure taken from [88].

momenta of selected tracks within a cone of size $\Delta R = XX/100$ centered around the electron track direction. Tracks are required to fulfil minimum quality requirements and the electron track itself is excluded. For high-energy electrons, an alternative track isolation variable is used, $p_T^{\text{varconeXX}}$ in which the cone size is shrunk for larger transverse momentum

$$\Delta R = \min \left(\frac{10}{E_T [\text{GeV}]}, \Delta R_{\text{max}} \right),$$

where $\Delta R_{\text{max}} = XX/100$ is the maximum cone size. Table 2.2 shows different isolation criteria based both on calorimeter and tracks variables, of interest for the analyses presented in this thesis, while Figure 2.12(b) also shows the isolation selection efficiency for *Medium* electrons and the same selection criteria.

Table 2.2. Definition of main electron isolation selection criteria. Table adapted from [88].

Selection criteria	Calorimeter isolation	Track isolation
HighPtCaloOnly	$E_T^{\text{cone20}} < \max(0.015 \times p_T, 3.5 \text{ GeV})$	-
Tight_VarRad	$E_T^{\text{cone20}}/p_T < 0.06$	$p_T^{\text{varcone30}}/p_T < 0.06$
Loose_VarRad	$E_T^{\text{cone20}}/p_T < 0.20$	$p_T^{\text{varcone30}}/p_T < 0.15$

The total efficiency of reconstruction, triggering and selecting electrons can be factorised in different terms

$$\varepsilon_{\text{total}} = \varepsilon_{\text{cluster}} \times \varepsilon_{\text{reco}} \times \varepsilon_{\text{id}} \times \varepsilon_{\text{iso}} \times \varepsilon_{\text{trigger}}. \quad (2.9)$$

Each of these terms is measured both in data and Monte Carlo and *scale factors* (SF) are evaluated as ratios of the efficiencies in data and in MC, and are used to correct the MC simulation to better match the efficiencies observed in data.

Photons

The reconstruction of photons follows the same procedure as for electrons, except that in the photon case the energy cluster is not matched with a single track. Photons can be *unconverted* if they generate a e^+e^- pair in the ECAL, giving rise to the electromagnetic shower. Otherwise they are classified as *converted* photons, if they generate a pair before the ECAL, in some interaction with the ID layers. In the first case, photons are reconstructed as energy clusters not matched with any track, in the second case as clusters matched with pairs of tracks coming from a conversion secondary vertex. Identification criteria are based on the EM shower shape, considering that the energy deposit is wider for converted photons, due to the bending of the e^+e^- trajectories. Three identification working points are defined, *Loose*, *Medium*, *Tight*, and isolation criteria are also assigned, similarly to the electron case. Further details can be found in Refs. [88, 89].

2.3.3 Muons

Muons reconstruction

At the LHC energies, muons are minimum ionising particles (MIPs) passing through the inner detector and the calorimeters and leaving a track in the muon spectrometer. A complete description of muons reconstruction and identification in Run 2 is given in Refs. [90, 91]; the main features are summarised in the following. The ATLAS muon spectrometer (MS) is able to reconstruct standalone muons with $p_T > 7$ GeV, however the quality of the reconstruction is improved when using in combination information coming from the other sub-systems.

The reconstruction process begins from the generation of track candidates, starting from the track segments registered in the MS stations due to the passing muons. Candidate tracks are generated, loosely matched with the interaction point, and a χ^2 fit is executed. Additional hits are then considered among those nearest to each candidate track and the fit is repeated, yielding the final reconstructed muon tracks in the MS. Tracks from MS are combined with tracks measured in the ID and calorimetric information. Five different muon categories are defined, as described in the following:

- *Combined muons (CB)* are reconstructed by matching MS tracks to ID tracks and performing a combined fit, taking into account of the energy loss in the calorimeters. This is the standard reconstruction procedure and the majority of muons fall in this category. For $|\eta| > 2.5$ MS tracks may be combined with short track segments reconstructed from the pixel or SCT detectors: in this case muons are called *silicon-associated forward (SiF) muons*.
- *Inside-out combined muons (IO)* are reconstructed using a complementary algorithm, which matches the ID tracks to the MS tracks. This opposite procedure recovers some of the lost combined muons due to inefficiencies, for examples in regions of limited MS coverage.
- *Muon-spectrometer extrapolated muons (ME)* are obtained by standalone track measurements in the MS, which are not matched to any track in the ID. For

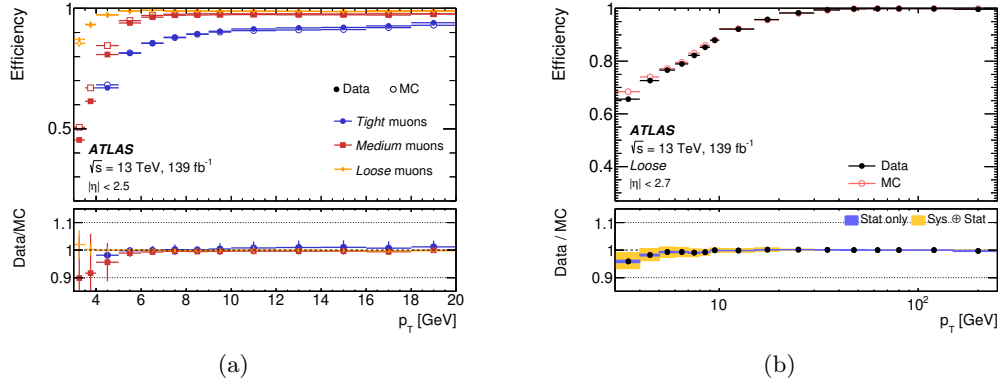


Figure 2.13. Muons identification efficiency (a) and isolation efficiency (b) as a function of p_T . The lower panels represent the ratio between efficiencies measured in data and in MC. Figure taken from [90].

these muons the track is extrapolated to the beamline and matched to the IP. With this category the full coverage of the MS till $|\eta| = 2.7$ is exploited.

- *Segment-tagged muons (ST)* are obtained by tracks in the ID, matched with a segment in the MS. The p_T reconstruction is obtained from the ID track fit only, while the segment in the MS is only needed to tag the track as a muon.
- *Calorimeter tagged muons (CT)* are similarly obtained by a track in the ID, matched with MIP energy deposit in the calorimeters. Also in this case p_T is only determined by the ID track and the calorimeter information serves as muon tagger.

Muons identification and isolation

Further requirements are applied on reconstructed muons to define different selection working points. The working points are constructed relying on two quality variables: the q/p compatibility, defined in Eq. (2.10a), and the ρ' variable, shown in Eq. (2.10b):

$$q/p \text{ compatibility} = \frac{|q/p_{\text{ID}} - q/p_{\text{MS}}|}{\sqrt{\sigma^2(q/p_{\text{ID}}) + \sigma^2(q/p_{\text{MS}})}} , \quad (2.10a)$$

$$\rho' = \frac{|p_{T,\text{ID}} - p_{T,\text{MS}}|}{p_{T,\text{CB}}} . \quad (2.10b)$$

In this notation, q is the muon electric charge, the suffix ID (MS) indicates that the p_T is measured in the inner detector (muon spectrometer), while CB indicates a combined measurement; $\sigma(q/p)$ indicates instead the uncertainty on the measurement. Using these variables and several other requirements on the number of hits and segments across the MS stations, the *Loose*, *Medium* and *Tight* working points are defined, yielding increased purity at the cost of lower efficiency, as shown in Figure 2.13(a). Two additional WPs, *low* and *high- p_T* are also developed, to provide

improved resolution and efficiency for analyses targeting extreme regions of the phase space.

Muons are also required to be isolated, to be distinguished with respect to secondary muons generated in hadronic jets or low energy activity. Isolation criteria are defined, based on discriminants constructed with tracks or calorimeter information. For the track-based isolation variable, $p_T^{\text{varcone30}}$ is used, defined as the scalar sum of the transverse momenta of the ID tracks associated with the primary vertex, included in a cone centered on the muon and with opening $\Delta R = \min(10 \text{ GeV}/p_T^\mu, 0.3)$. The calorimeter based variable, $E_T^{\text{topocone20}}$, is defined as the sum of the transverse energy of topological cell clusters in a cone of size $\Delta R = 0.2$ around the muon position, after subtraction of the muon energy itself and the contribution from pile-up. Several selection criteria are defined, based on these two variables. *Loose* and *Tight* isolation working points, of interest for the analyses presented in this thesis, are summarised in Table 2.3; the *Loose* efficiency curve is also shown in Figure 2.13(b).

Table 2.3. Definitions of some muon isolation selection criteria. Table adapted from [90].

Isolation WP	Definition	Track p_T requirement
Loose	$p_T^{\text{varcone30}} < 0.15 p_T^\mu$, $E_T^{\text{topocone20}} < 0.3 p_T^\mu$	$p_T > 1 \text{ GeV}$
Tight	$p_T^{\text{varcone30}} < 0.04 p_T^\mu$, $E_T^{\text{topocone20}} < 0.15 p_T^\mu$	$p_T > 1 \text{ GeV}$

Scale factors are also measured, to account for the differences in efficiencies measured in data and in the MC simulation, and are used to correct the simulated samples to correct for mis-modelling.

2.3.4 Jets

Jets are collimated sprays of particles, generated by the hadronisation of quarks and gluons induced by colour confinement. Jets are reconstructed using two different input types: topo-clusters constituted by energy deposits in the calorimeters cells, or algorithmic combinations of charged particles tracks with these topo-clusters. Jets reconstructed with the first type of inputs are called *EMTopo jets*, while the second type of inputs leads to the building of *PFlow jets*. The reader is referred to Ref. [92] for all the details on the jets reconstruction in Run 2; we report a summary in the following.

Jets reconstruction

Jets are reconstructed with the anti- k_T algorithm [93] starting from four-vector objects that may be stable particles defined by MC generators, calorimeter energy deposits, charged particle tracks, or an algorithmic combination of the latter two, as in the case of particle-flow reconstruction technique. The anti- k_T algorithm has the property of being *infrared and collinear (IRC) safe* and leads to the reconstruction of regular-shaped jets, made of hard particles surrounded by conical soft radiation, as shown in Figure 2.14.

The anti- k_T algorithm starts from an arbitrary seed object i , and considers each additional element j in an object list. Two distances are evaluated: the distance d_{ij}

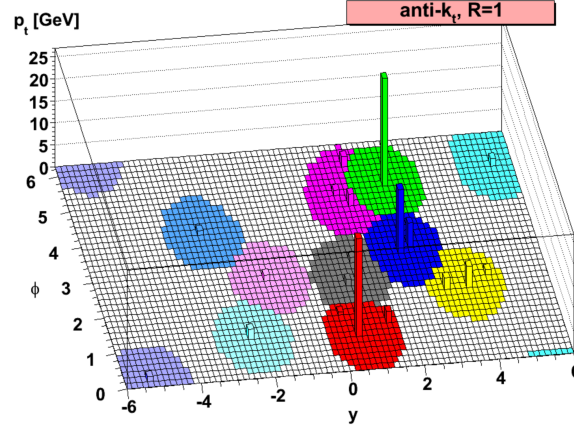


Figure 2.14. Reconstruction of jets with the anti- k_T algorithm on Herwig simulated events. Figure taken from [93].

between the the i, j objects and the reference distance d_{iB} between the i object and the *beam*, given by the following expressions:

$$d_{ij} = \min \left(\frac{1}{k_{Ti}^2}, \frac{1}{k_{Tj}^2} \right) \frac{\Delta R_{ij}^2}{R^2}, \quad d_{iB} = \frac{1}{k_{Ti}^2}, \quad (2.11)$$

where $\Delta R_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2$ is the angular distance between the two objects, y_i is the rapidity, ϕ_i is the azimuth angle of object i , and R is a parameter characteristic of the algorithm, representing in first approximation the jet cone maximum size. The two distances are compared: if $d_{ij} < d_{iB}$, objects i and j are merged together and the procedure is reiterated; if instead $d_{ij} > d_{iB}$ for each j object in the list, the object i is identified as a jet. A typical value of the parameter R for jets reconstruction in ATLAS is $R = 0.4$.

Jets energy scale calibration

The energy of the topo-clusters involved in the jet reconstruction is not fully representative of the actual jet energy, due to several effects that have to be compensated by an appropriate object calibration. These include detector effects, the presence of radiation coming from pile-up interactions, the hadronic interaction contained in the jets. The *Jet Energy Scale* (JES) calibration is a complex procedure that accounts for these effects and is divided into four main steps, summarised in the following:

- **Pile-up corrections.** Due to *in-time* and *out-of-time* pile-up present in the collisions environment an additional energy deposit is attributed to the jets, which has to be removed. A first pile-up correction is applied evaluating an energy density ρ in the event and subtracting an energy contribution proportional to the jet area. A residual dependence on pile-up is observed in jets, due to the fact that ρ is evaluated in low occupancy regions of the calorimeter and in limited region of the detector. An additional correction is then applied, which is a function of the number of primary vertices N_{PV}

and the pile-up parameter μ , sensitive respectively to in-time and out-of-time pile-up.

- **Absolute scale and η calibration.** The jet four-momentum is then corrected to account for non-compensating calorimeter response, energy losses in passive material, out-of-cone effects and biases in the jet η reconstruction. These biases are primarily generated by the sudden change of the calorimeter hardware technologies and variations of the cells granularity. Corrections are derived from Pythia8 MC simulation, by matching the jets with their truth particle-level counterpart. After these corrections jets are considered calibrated at the EM+JES scale.
- **Global sequential calibration.** Additional mismodellings are present due to the flavour and energy distribution of the jet constituents, their transverse distribution, the fluctuations in the jet development in the calorimeters. These are compensated by a sequence of corrections implemented by a series of multiplicative factors. Such corrections impact mainly the resolution on the jet response, while they do not change the jet energy scale. Corrections are derived with information from the first layer of the HCAL, the last layer of the LAr calorimeter, the number of tracks associated with the jet, the hits in the muon spectrometer chambers aligned with the jets.
- **In-situ calibrations.** Final corrections are derived to compensate residual difference in data and MC simulation, describing effects generated from mismodelling of the hard-scatter interactions and the underlying event or the jet formation process. Ratios are derived in Z +jets, γ +jets, multijet events comparing the response in p_T of the jet and of a well-reconstructed recoiling object (namely the Z , the γ or a system of well calibrated jets):

$$\mathcal{R}_{in\ situ} = \left\langle \frac{\text{jet } p_T}{\text{reference object } p_T} \right\rangle. \quad (2.12)$$

Ratios are derived both in data and in MC simulation and correction factors are evaluated from the double ratios:

$$c = \frac{\mathcal{R}_{in\ situ}^{\text{data}}}{\mathcal{R}_{in\ situ}^{\text{MC}}}. \quad (2.13)$$

The Z +jets events are used at low momenta ($20 < p_T < 500$ GeV), γ +jet events are used at intermediate momenta ($40 < p_T < 900$ GeV), while at very high momenta multijet events are used where the high energy jet is calibrated exploiting systems of low-energy jets, calibrated with one of the two preceding methods.

The JES calibration ratios are shown in Figure 2.15(a), while the fraction uncertainty on JES is shown in Figure 2.15(b). The dominant JES uncertainty contribution at low jet p_T is due to pile-up and the different detector response flavour, while at intermediate p_T JES absolute and in-situ calibrations play the leading role.

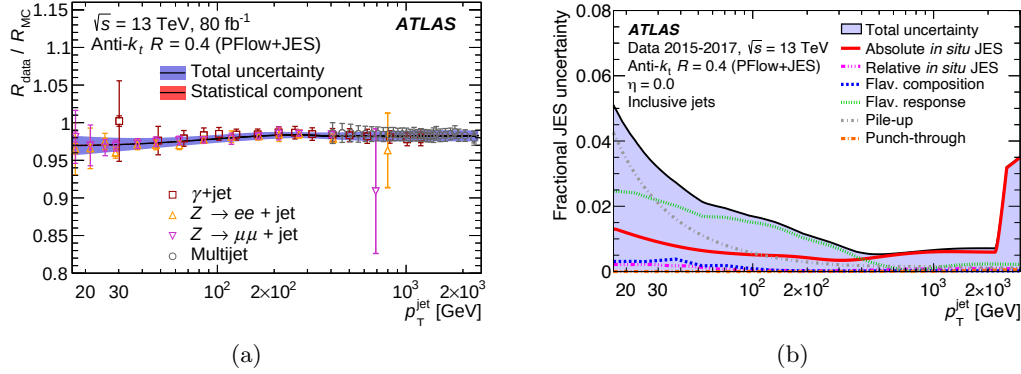


Figure 2.15. (a) Ratio of jets responses in data to that in MC for *in-situ* calibrations and (b) fractional jet energy scale uncertainty with its components. Figures taken from [92].

Jet energy resolution

The *Jet Energy Resolution* (JER) measures the precision at which the jet p_T can be estimated. It can be parameterised as the sum of three contributions:

$$\frac{\sigma(p_T)}{p_T} = \frac{N}{p_T} \oplus \frac{S}{\sqrt{p_T}} \oplus C, \quad (2.14)$$

where $\oplus$ indicates the quadrature sum. The noise (N) term is due to the contribution of the electronic noise to the signal measured by the detector front-end electronics, as well as due to pile-up. This term is expected to be significant in the low p_T region, below ~ 30 GeV. Statistical fluctuations in the amount of energy deposited are captured by the stochastic (S) term, which represents the limiting factor up to resolutions of several hundreds of GeV in jet p_T . The constant (C) term represents instead effects that are a constant fraction of the jet p_T , such as energy deposits in passive material, non-uniformity of the response across the calorimeters. This term dominates in the high- p_T region, above approximately 400 GeV. Figure 2.16 shows the jet energy resolution and its uncertainty, with ATLAS Run 2 jets reconstructed with both EM-topo clusters and PFlow objects.

Particle Flow jets

Particle-flow jets are reconstructed using the particle-flow algorithm [94]. Before the anti- k_T algorithm is run, jet cluster constituents are associated with tracks reconstructed in the ID. The energy contribution of the topo-cluster is subtracted from the reconstruction process and substituted with the particle p_T evaluated from the ID. A ghost energy cluster ($E_{\text{ghost}} \approx O(10^{-100})$) is added in order to fictitiously include the track among the list of objects on which the clustering algorithm is run. The substitution of a cluster with its corresponding track is not performed for high energy deposits, namely if the jet has $p_T > 100$ GeV.

The jet energy resolution is significantly improved by the particle-flow algorithm, as can be seen in Figure 2.16. The improvement is particularly localised at low jet energy, due to the fact that in this condition the track p_T is better measured

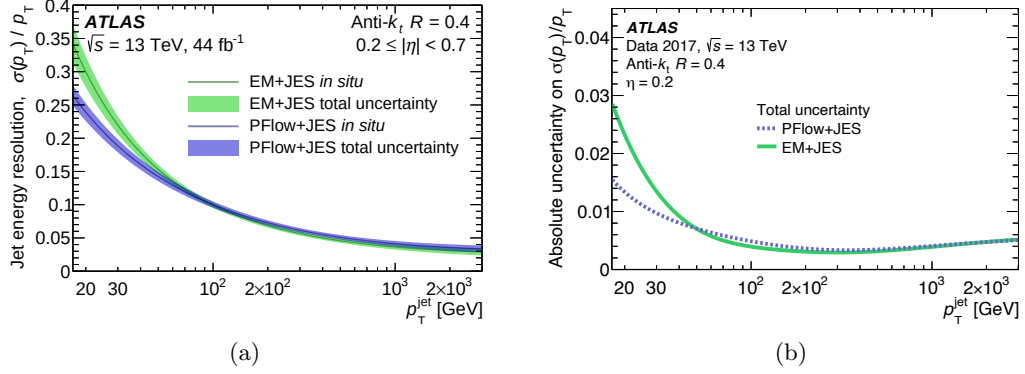


Figure 2.16. (a) Jet energy resolution for fully calibrated EM+JES and PFlow+JES jets and (b) their respective systematic uncertainty. Figure taken from [92].

than the corresponding cluster energy, due to the track bending. The particle-flow algorithm also yields improved management of the removal of additional pile-up radiation, since the track information enables to distinguish if radiation is coming from a secondary vertex or from the hard-scatter.

Pile-up jet tagging

Despite pile-up radiation is considered and removed from hard scatter jets reconstruction, it can nevertheless generate additional *pile-up* jets, due to local fluctuations of the average value of pile-up activity. The identification and removal of pile-up jets is crucial, especially when the average number of interactions per bunch-crossing is high. To achieve a good rejection *Jet Vertex Tagger* (JVT) algorithm [95] is used, based on a two-dimensional likelihood discriminant. More specifically, JVT exploits information from two variables: the corrected-JVF and R_{p_T} . The first one is the fraction of the scalar sum of transverse momenta associated with jet tracks belonging to the hard scatter, with respect to the scalar sum of transverse momenta of all available jet tracks, normalised to the number of pile-up vertices present in the event. The second one is the scalar sum of the p_T of the tracks associated with the jet and originating from the hard scatter, divided by the calibrated jet p_T . The efficiency of pile-up jet tagging is measured in Z +jets events and scale factors are calculated to correct for differences between data and MC simulations.

2.3.5 Flavour tagging of jets

Flavour tagging consists in the identification of the quark flavour from whose hadronisation the jet has been originated. In ATLAS a distinction is made between b -jets, c -jets and light jets. The first are originated from b -quarks, the second from c -quarks, the latter from light quarks, namely u -, d -, s -quarks. Also hadronically decaying τ leptons generate thin collimated hadronic jets; we postpone the discussion of this typology of jet to Section 2.3.7. A complete report on flavour tagging in ATLAS in Run 2 is given in Ref. [96], we report here a summary.

In simulated events, the flavour of an hadronic jet, is determined using truth MC

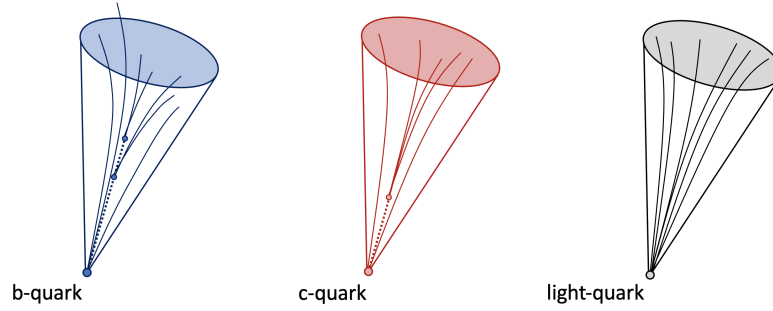


Figure 2.17. Illustration of different jets originating from a b -quark (left) a c -quark (centre) or a $light$ -quark (right).

information and looking at the flavour of the hadrons it contains. Jets are labelled as b -jets if at least one b -hadron with $p_T \geq 5$ GeV is found in a cone of size $\Delta R = 0.3$ around the jet axis. In case no b -hadrons are found, c -hadrons and τ leptons are searched for, leading to a c -tagged or a τ -tagged jet. In case neither c -hadrons nor τ leptons are found, the jet is tagged as light-jet. In real data, instead, flavour tagging is achieved by the simultaneous use of several algorithms, exploiting the different features characterising each type of jet.

Types of hadronic jets

Different flavour hadronic jets can be distinguished exploiting several features representing the different behavior of the hadrons generated at the beginning of the decay chain.

- **b -jets** originate from the hadronisation of a b -quark into a b -hadron. The b -hadron has on average a lifetime of ≈ 1.5 ps and is able to travel around ≈ 5 mm before decaying. For this reason b -jets show a secondary vertex, displaced with respect to the hard scatter. Typically the b -hadron decays into a c -hadron (via the $b \rightarrow c$ transition, which is more likely than $b \rightarrow u$ because $|V_{cb}|^2 > |V_{ub}|^2$). The c -hadron further propagates a few mm, then decays into secondary particles, generating the hadronic jet. This implies that the b -jets show in the majority of cases also a tertiary displaced vertex, corresponding to the c -hadron decay. Objects collected in a b -jet are hard and decay with a high multiplicity.
- **c -jets** originate from the hadronisation of a c -quark into a c -hadron. The c -hadron consists usually of a D -meson, decaying into a K -meson via the $c \rightarrow s$ transition. The D -meson has short lifetime, hence a small decay length (a few mm) separates the hard scatter from a secondary displaced vertex, where secondary particles are generated. The c -jet usually contains softer radiation with respect to the b -jet and its decay products have lower multiplicity.
- **light-jets** originate from the hadronisation of light quarks (u, d, s) or from a gluon. Light quarks decay almost instantly, hence no secondary vertex can be observed within ATLAS resolution and secondary hadrons are recognised as

originating directly from the principal vertex. Gluon jets are considered within this category in the context of flavour tagging. However, we acknowledge for completeness that gluon jets can be distinguished from quark jets due to a large number of constituents and a broader radiation pattern which can be exploited using specific techniques [97].

Figure 2.17 shows a graphical representation of the characteristics above mentioned, for b -, c - and light-jets.

Low level taggers

Low level taggers are algorithms whose aim is to analyse the jet to extract low level features, characterising the jet structure (e.g. information on the tracks, on the secondary vertex, on the decay chain). Such information is then used by a second stage of high-level algorithms which tag the jet according to the recognised flavour.

- **IP2D and IP3D [98].** The two algorithms aim at exploiting information on the impact parameter of each track. Tracks are considered as independent from each other. IP2D makes use of the signed transverse impact parameter significance to construct a discriminating variable. IP3D instead uses both the signed transverse and longitudinal impact parameters significance, accounting also for their correlation. Log-likelihood ratio (LLR) discriminants are then defined exploiting pdfs evaluated using truth jets in MC simulations. Three LLRs are defined, discriminating respectively b -jets from light-flavour jets, b -jets from c -jets and c -jets from light-flavour jets. These three LLR discriminants, evaluated for both IP2D and IP3D, are used as input for the high-level taggers.
- **RNNIP [99].** This algorithm is designed to exploit information encoded in the correlation between tracks. It is based on a recurrent neural network (RNN), which is suitable to learn sequential dependencies between the variables in sequences of arbitrary length. For each selected track the signed transverse (S_{d_0}) and longitudinal (S_{z_0}) impact parameter significances, the fraction of momentum carried by the track relative to the jet p_T , the angular distance between the track and the jet axis and the hit multiplicities in the ID are fed into the network. Tracks are ordered in $|S_{d_0}|$ to form a sequence. The network provides as output the probabilities of the jet of being a b -jet (p_b), a c -jet (p_c) or a light-flavour jet (p_{light}). Such probabilities are then combined into a b -tagging discriminant defined as:

$$D_{\text{RNNIP}} = \ln \left(\frac{p_b}{f_c \cdot p_c + (1 - f_c)p_{\text{light}}} \right),$$

where f_c denotes the c -jet fraction and is a parameter that can be optimised at analysis-level.

- **SV1 [100].** This algorithm aims at exploiting the information on the secondary vertex encoded in the jet tracks. The reconstruction starts by examining all the tracks and looking for a couple of tracks identifying the jet vertex. At the same time, all tracks compatible with K_s^0 , Λ decays, or photon conversions

with the detector material are discarded. Then **SV1** runs iteratively on all tracks and evaluates a χ^2 . The track with largest χ^2 is removed and the vertex fit is repeated until the total χ^2 is acceptable. Eight discriminant variables, including the jet p_T and η , the number of tracks associated with the vertex, the invariant mass of the secondary vertex, its energy fraction and the three-dimensional decay length significance, are used as inputs for the high-level taggers.

- **JetFitter** [101]. This algorithm aims at reconstructing the full decay chain inside the candidate b -jet. A modified Kalman filter [87] is used to find a common line on which the primary b - and c -hadron decay, approximating the flight path of the b -hadron as well the secondary and tertiary vertices positions. With this approach it is possible to identify the b - and c - decay vertex with one single track looking at the intersection with the flight path. The fitter releases as output eight discriminating variables, including track multiplicity, the invariant mass of the tracks associated with these vertices, their energy fraction, their average three-dimensional decay length significance, which are used as inputs for the high-level taggers.

High-level taggers

The outputs of low-level algorithms are fed into high-level taggers which finally classify the flavour of the jet. Currently high-level taggers are multi-layer feed-forward neural networks from the DL series and supersede the previously used algorithm **MV2c10** [102], which was a boosted decision tree.

The **DL1** algorithm [102], used at the beginning of Run 2, exploits **IP2D**, **IP3D**, **SV1**, **JetFitter** algorithms outputs. A more advanced implementation, **DL1r** [102], is used with full Run 2 dataset and exploits in addition **RNNIP** low-level tagger (see Table 2.4 for details). Large correlation is found in general between the outputs of **IP2D**, **IP3D**, **SV1**, **JetFitter**, which tend to decrease in light-flavour jets and at high- p_T values. Minor correlations are instead found with the output of **RNNIP**, yielding superior performances to the **DL1r** algorithm. The neural network training is performed using a sample of 70% $t\bar{t}$ events and 30% $Z' \rightarrow q\bar{q}$ events, which are re-sampled to be uniform in p_T and η among the flavour categories, to avoid possible biases.

DL1r releases as output the probabilities of one jet of being a b -jet, a c -jet or a light flavour-jet: p_b , p_c , p_{light} . Such probabilities are combined in a final discriminant to obtain a binary classification:

$$D_{\text{DL1r}} = \left(\frac{p_b}{f_c \cdot p_c + (1 - f_c) \cdot p_{\text{light}}} \right). \quad (2.15)$$

The jet is identified as b -tagged if the D_{DL1r} variable is higher than a fixed threshold. In this notation, f_c is a parameter representing the effective c -jet fraction in the background hypothesis and can be chosen a posteriori to optimise the algorithm performance at analysis level. Since all flavours are treated in the same way in the training of **DL1r**, the same neural network can be used also for c -tagging. A

Table 2.4. Input variables for the DL1 and DL1r taggers. Table adapted from [96].

Input	Variable	Description	DL1	DL1r
Kinematics	p_T	Jet p_T	x	x
	η	Jet $ \eta $	x	x
IP2D, IP3D	$\log(P_b/P_{\text{light}})$	Likelihood ratio of the b-jet to light-flavour jet hypotheses	x	x
	$\log(P_b/P_c)$	Likelihood ratio of the b-jet to c-jet hypotheses	x	x
	$\log(P_c/P_{\text{light}})$	Likelihood ratio of the c-jet to light-flavour jet hypotheses	x	x
RNNIP	P_b	b-jet probability		x
	P_c	c-jet probability		x
	P_{light}	light-jet probability		x
SV1	$m(\text{SV})$	Invariant mass of tracks at the secondary vertex assuming pion mass	x	x
	$f_E(\text{SV})$	Jet energy fraction of the tracks associated with the secondary vertex	x	x
	$N_{\text{TrkAtVtx}}(\text{SV})$	Number of tracks used in the secondary vertex	x	x
	$N_{2\text{TrkVtx}}(\text{SV})$	Number of two-track vertex candidates	x	x
	$L_{xy}(\text{SV})$	Transverse distance between the primary and secondary vertices	x	x
	$L_{xyz}(\text{SV})$	Distance between the primary and secondary vertices	x	x
	$S_{xyz}(\text{SV})$	Distance between the primary and secondary vertices divided by its uncertainty	x	x
	$\Delta R(\vec{p}_{\text{jet}}, \vec{p}_{\text{vtx}})(\text{SV})$	ΔR between the jet axis and the direction of the secondary vertex relative to the primary vertex	x	x
	$m(\text{JF})$	Invariant mass of tracks from displaced vertices	x	x
	$f_E(\text{JF})$	Jet energy fraction of the tracks associated with the displaced vertices	x	x
JetFitter	$\Delta R(\vec{p}_{\text{jet}}, \vec{p}_{\text{vtx}})(\text{JF})$	ΔR between the jet axis and the vectorial sum of momenta of all tracks attached to displaced vertices	x	x
	$S_{xyz}(\text{JF})$	Significance of the average distance between PV and displaced vertices	x	x
	$N_{\text{TrkAtVtx}}(\text{JF})$	Number of tracks from multi-prong displaced vertices	x	x
	$N_{2\text{TrkVtx}}(\text{JF})$	Number of two-track vertex candidates (prior to decay chain fit)	x	x
	$N_{1\text{-trk vert.}}(\text{JF})$	Number of single-prong displaced vertices	x	x
	$N_{\geq 2\text{-trk vert.}}(\text{JF})$	Number of multi-prong displaced vertices	x	x
	$L_{xyz}(2^{\text{nd}})(\text{JF})$	Distance of 2^{nd} vertex from PV	x	x
	$L_{xy}(2^{\text{nd}})(\text{JF})$	Transverse displacement of the 2^{nd} vertex	x	x
	$m_{\text{Trk}}(2^{\text{nd}})(\text{JF})$	Invariant mass of tracks associated with the 2^{nd} vertex	x	x
	$E(2^{\text{nd}})(\text{JF})$	Energy of the tracks associated with the 2^{nd} vertex	x	x
	$f_E(2^{\text{nd}})(\text{JF})$	Jet energy fraction of the tracks associated with the 2^{nd} vtx.	x	x
	$N_{\text{TrkAtVtx}}(2^{\text{nd}})(\text{JF})$	Number of tracks associated with the 2 vertex	x	x
	$\eta_{\text{trk}}(2^{\text{nd}})(\text{JF})$	Min., max. and avg. pseudorapidity of tracks at the 2^{nd} vertex	x	x

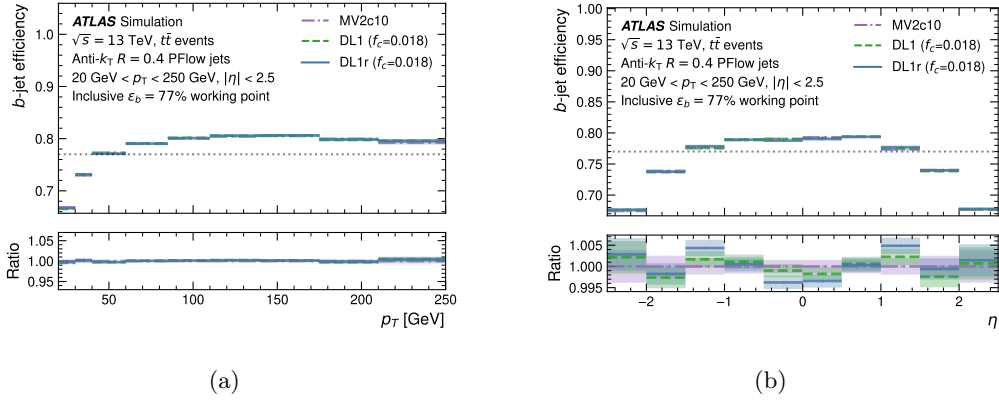


Figure 2.18. The b -tagging efficiency ε_b for DL1 and DL1r high-level taggers, as a function of (a) jet p_T and (b) jet η . Figures taken from [96].

c -tagging discriminant is built, using the same outputs probabilities:

$$D_{\text{DL1r}}^c = \left(\frac{p_c}{f_b \cdot p_b + (1 - f_b) \cdot p_{\text{light}}} \right), \quad (2.16)$$

where now f_b represents the effective fraction of b -jets in the background hypothesis, to be optimised at analysis level.

Single cut operating working points (OP) can be defined with efficiencies of 60%, 70%, 77% and 85%. The b -tagging efficiency is evaluated for each of these working points, and is shown in Figure 2.18 for the 70% OP and MV2c10, DL1 and DL1r taggers, as a function of jet p_T and η . A degradation of the efficiency at low p_T and high η can be observed, mainly due to particles multiple scattering in the detector and pile-up effects. Moreover the small decrease of the efficiency at high- p_T is due to the higher tracks collimation, caused by the decrease of their curvature. Scale factors are evaluated to compensate differences in data and MC simulation, and applied as correction factors at analysis level. Some MC-to-MC scale factors are also calculated, to compensate biases induced by the use of different MC simulations in flavour tagging calibration procedure and in the user analysis. Systematic uncertainties are also evaluated and propagated at analysis level. An eigenvector decomposition is performed to reduce the number of uncertainties based on the accuracy needed by the user analysis.

2.3.6 Missing transverse momentum

Neutrinos and elusive particles interact weakly with matter and do not leave specific signals in a general purpose detector like ATLAS. However, being ATLAS a hermetic detector, such particles can be detected via the measurement of the momentum imbalance in the transverse plane. In fact, in pp collisions the initial momentum of partons along the beam-axis is unknown, but its component in the transverse plane has to be zero. This implies that an eventually measured momentum imbalance in that plane has to be attributed to elusive particles. We report here the essential features of the reconstruction of missing transverse momentum, which is not exploited

among the objects necessary to perform the analyses presented in this thesis. The reader can refer to [103] for more details.

The missing transverse momentum is defined as

$$\begin{aligned}\vec{E}_T^{\text{miss}} &= - \left(\sum_{\text{hard}} \vec{p}_T + \sum_{\text{soft}} \vec{p}_T \right) \\ &= - \left(\sum_e \vec{p}_T^e + \sum_\gamma \vec{p}_T^\gamma + \sum_\tau \vec{p}_T^\tau + \sum_\mu \vec{p}_T^\mu + \sum_{\text{jets}} \vec{p}_T^{\text{jets}} + \sum_{\text{trk}} \vec{p}_T^{\text{trk}} \right),\end{aligned}$$

and is therefore the opposite of the vectorial sum of the transverse momentum of all reconstructed objects, as well as the momentum contribution of all spurious tracks reconstructed from the ID but not associated to any particular object. The momentum contribution coming from reconstructed objects, namely electrons, photons, taus, muons, jets, is called *hard term*. Instead, the momentum contribution coming from spurious tracks is called *soft term*. The magnitude and azimuthal angle of the missing transverse momentum are defined by

$$\begin{aligned}E_T^{\text{miss}} &= |\vec{E}_T^{\text{miss}}| = \sqrt{(E_x^{\text{miss}})^2 + (E_y^{\text{miss}})^2} \\ \phi^{\text{miss}} &= \tan \left(E_y^{\text{miss}} / E_x^{\text{miss}} \right)^{-1}.\end{aligned}$$

The procedures used in ATLAS to reconstruct each single component of the missing transverse momentum are independent. This implies that same detector signals can be used multiple times, for example a calorimeter energy deposit could be used both for a photon and a jet reconstruction. This can cause double counting of contributions in the missing transverse momentum, leading to a fictitious momentum imbalance in the event. To avoid this effect a *signal ambiguity resolution* algorithm is used [104], which removes double counted signals analysing all contributing objects. Objects are scrutinised in sequence following the list (from higher to lower priority): electrons, photons, τ -leptons, jets. Muons are reconstructed mainly from tracks in the ID matched with MS tracks, hence are considered as little overlapping with the reconstruction of other objects.

The resolution on E_T^{miss} is measured by the rms of the x and y components of $\vec{E}_T^{\text{miss}}$ with respect to the expected value. Performances are evaluated mainly exploiting events in which the expected value is zero ($Z \rightarrow \ell\ell$ events, with $\ell = \mu, e$), or in which E_T^{miss} is expected from a neutrino (e.g. W or top-quark decays). Systematic uncertainties on the E_T^{miss} reconstruction are provided for both scale and resolution. The hard-term uncertainty mainly comes from propagation to the E_T^{miss} of the uncertainties on the main constituting objects. Soft-term systematics are evaluated instead from MC, by looking at the components of $\vec{E}_T^{\text{miss,soft}}$ parallel and perpendicular to the hard term.

We report for completeness that in case the missing transverse momentum is evaluated using charged-particle tracks information only, the notation $\mathbf{p}_T^{\text{miss}}$ is used, instead of $\vec{E}_T^{\text{miss}}$.

2.3.7 Hadronic taus

Hadronically decaying tau leptons consist in low track-multiplicity jets, constituted mainly by charged and neutral pions, with small contamination from kaons and their decay products. The ATLAS Collaboration has not published a comprehensive paper in hadronic tau performance during Run 2, but the information on reconstruction, calibration and identification aspects is fully recovered in specific public notes, which will be cited along the discussion.

Reconstruction and energy calibration

The reconstruction and energy calibration of hadronic taus is reported in Ref. [105], to which the reader is referred for further details.

Tau candidates are seeded by hadronic jets, reconstructed with the usual procedure described in Sec. 2.3.4. Jets seeding tau candidates are additionally required to have $p_T > 10$ GeV and $|\eta| < 2.5$. Moreover, tau candidates are vetoed in the transition region between barrel and end-cap, $1.37 < |\eta| < 1.52$. A tau vertex is reconstructed as the vertex with the largest fraction of momentum from the tracks associated with the jet and verifying $\Delta R < 0.2$. Tracks involved in the tau reconstruction must pass additional requirements on the number of hits in the tracker, must have $p_T > 1$ GeV, should verify conditions on the shortest distance from the tau vertex in the transverse plane, $|d_0| < 1$ mm, and the shortest distance in the longitudinal plane, $|\Delta z_0 \sin \theta| < 1.5$ mm, where θ is the polar angle and z_0 is the point of closest approach along the longitudinal axis. The tau direction is reconstructed considering the vectorial sum of all the topo-clusters within $\Delta R < 0.2$ from the seed jet barycentre, using the tau vertex as origin. Finally, tracks are classified as belonging to the *core* cone if they have distance $0 < \Delta R < 0.2$ or to the *isolation* cone if they have distance $0.2 < \Delta R < 0.4$ from the tau axis.

The tau energy calibration starts from the evaluation of the energy of the local clusters, E_{LC} , given by the sum of the energies of all the topo-clusters within the tau core region. This energy is corrected by the baseline calibration procedure, described by the following expression

$$E_{\text{calib}} = \frac{E_{LC} - E_{\text{pileup}}}{\mathcal{R}(E_{LC} - E_{\text{pileup}}, |\eta|, n_p)} , \quad (2.17)$$

A first subtractive correction is applied to E_{LC} , which is decreased by a quantity E_{pileup} representing the effect of pile-up. It is found that pile-up contribution increases linearly with the number of primary vertices N_{PV} as

$$E_{\text{pileup}}(N_{PV}, |\eta|, n_p) = A(|\eta|, n_p) \times (N_{PV} - \langle N_{PV} \rangle) , \quad (2.18)$$

where the A coefficient depends on $|\eta|$ to represent the higher effect of pile-up at higher rapidities, and on the tau prongness n_p . Such correction vanishes when the number of primary vertices is equal to the average pile-up conditions of MC samples, $N_{PV} \approx 14$. A second multiplicative correction is applied by scaling $E_{LC} - E_{\text{pileup}}$ for the *response* $\mathcal{R}$, which is extracted from MC simulations as the Gaussian mean of the $(E_{LC} - E_{\text{pileup}})/E_{\text{true}}^{\text{vis}}$ distribution. Here $E_{\text{true}}^{\text{vis}}$ is the visible energy of the truth-tau in MC simulated events. Such correction accounts for effects like: decay

products not reaching the hadronic calorimeter, or not depositing sufficient energy to create topo-clusters, or not detected within $\Delta R < 0.2$.

The energy resolution corresponding to the baseline calibration is excellent at high p_T but quickly degrades at low- p_T . To avoid this effect a reconstruction method has been developed, known as Tau Particle Flow (TPF) [111], which is able to reconstruct the individual charged and neutral hadrons decays in the tau jet. The calibration procedure has correspondingly been improved, to exploit the better resolution yielded by the superior measurement of the pion tracks constituting the hadronic tau. The transverse component of the momenta of reconstructed charged hadron and neutral pion constituents is evaluated and referred as p_T^{TPF} , to be compared to the p_T^{LC} evaluated after the baseline calibration procedure. The p_T^{TPF} momentum yields a better resolution at low- p_T , while p_T^{LC} has better performance in the high- p_T regime. For this reason an interpolating quantity, p_T^{interp} , is defined as

$$p_T^{\text{interp}} = f_x \times p_T^{\text{LC}} + (1 - f_x) \times p_T^{\text{TPF}} , \quad (2.19)$$

where f_x is a weight between zero and one, given by

$$f_x(p_T^{\text{LC}}) = \frac{1}{2} \left(1 + \tanh \frac{p_T^{\text{LC}} - x \text{ GeV}}{20 \text{ GeV}} \right) . \quad (2.20)$$

The symbol x defines the transition point between the low- and high- p_T regimes and is set to $x = 250$. Finally the variables $p_T^{\text{LC}}/p_T^{\text{interp}}$, $p_T^{\text{TPF}}/p_T^{\text{interp}}$ and p_T^{interp} , together with additional information on topo-clusters (barycentre position, depth, second-moment, pre-sampler fraction, energy density and others), on the tau tracks and on pile-up conditions are given as input to a boosted regression tree (BRT) based on the TMVA package [107], which finally calculates a p_T with the improved BRT calibration.

Figure 2.19 shows the $\tau_{\text{had-vis}}$ energy resolution, corresponding to both baseline and BRT calibrations. As can be seen the two energy resolutions are comparable at high- p_T , but the BRT calibration yields better performances for $p_T < 100$ GeV.

Tau identification

The tau reconstruction algorithm provides no discrimination against particles with jet-like signatures and such particles are mistakenly reconstructed as fake hadronic taus. To prevent this, dedicated algorithms are used to apply identification constraints on the reconstructed hadronic taus. The identification algorithm used during Run 2 is based on a recurrent neural network (RNN), and is described in detail in Ref. [108].

The RNN uses a combination of low-level inputs from tracks and energy clusters associated to the $\tau_{\text{had-vis}}$ candidate, as well as high-level observables calculated from tracks and clusters information. All used variables, together with their description, are reported in detail in Table 2.5. Tau identification is separately implemented for the 1-prong and 3-prong cases, distinguishing if the $\tau_{\text{had-vis}}$ has 1 or 3 charged tracks.

The network architecture is depicted in Figure 2.20. It is split into three dedicated branches, processing respectively tracks, clusters and high-level variables. The high-level observables are processed through a sequence of three fully connected layers

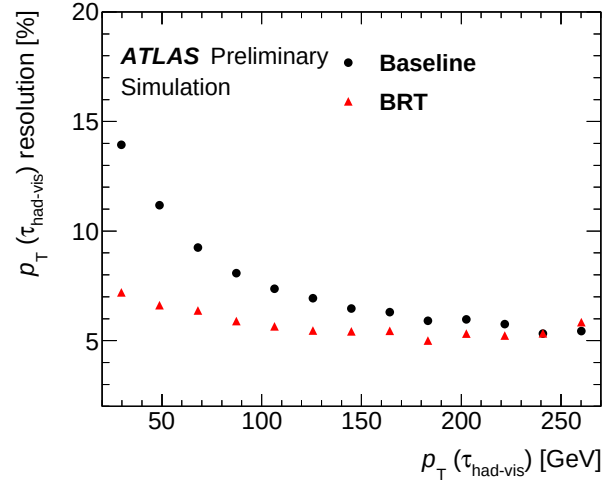


Figure 2.19. Resolution on p_T for reconstructed hadronically tau leptons, based on the baseline and BRT methods. Figure taken from [105].

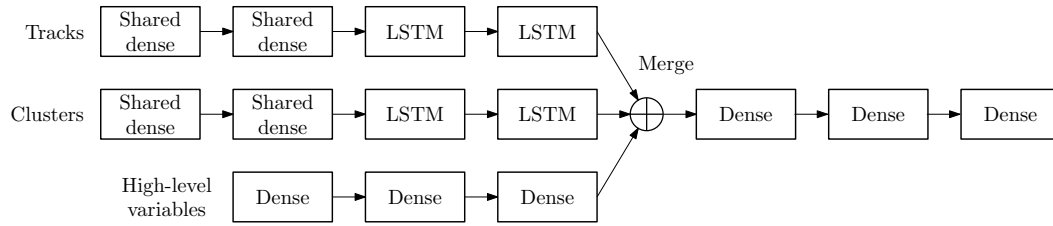


Figure 2.20. Schematic view of the recurrent neural network RNN used for tau identification. Figure taken from [108].

Table 2.5. List of observables used as inputs for the tau identification RNN. Details on which input is provided depending on the tau prongness are provided. Table adapted from Ref. [108]

Type	Variable	Description	1-prong	3-prong
Tracks	p_T^{track}	Track transverse momentum	X	X
	$\Delta\eta^{\text{track}}$	Angular distance between the track and the $\tau_{\text{had-vis}}$ axis	X	X
	$\Delta\phi^{\text{track}}$	Angular distance between the track and the $\tau_{\text{had-vis}}$ axis	X	X
	$ d_0^{\text{track}} $	Transverse impact parameter	X	X
	$ z_0^{\text{track}} \sin \theta $	Longitudinal impact parameter	X	X
	$N_{\text{IBL hits}}$	Number of hits in the innermost pixel detector layer	X	X
	$N_{\text{Pixel hits}}$	Number of hits in the pixel detector layers	X	X
	$N_{\text{SCT hits}}$	Number of hits in the microstrip detector layers	X	X
Clusters	E_T^{cluster}	Cluster transverse energy	X	X
	$\Delta\eta^{\text{cluster}}$	Angular distance between the cluster and the $\tau_{\text{had-vis}}$ axis	X	X
	$\Delta\phi^{\text{cluster}}$	Angular distance between the cluster and the $\tau_{\text{had-vis}}$ axis	X	X
	λ_{cluster}	Cluster depth	X	X
	$\langle \lambda_{\text{cluster}}^2 \rangle$	Second moment of the longitudinal distance	X	X
	$\langle r_{\text{cluster}}^2 \rangle$	Second moment of the radial distance	X	X
High-level	$p_T^{\text{jet seed}}$	Transverse momentum of the original seed jet	X	X
	$p_T^{\text{uncal.}}$	Transverse momentum at the LC scale	X	X
	f_{cent}	Central energy fraction	X	X
	$f_{\text{leadtrack}}^{-1}$	Inverse momentum fraction of the leading track	X	X
	ΔR_{max}	ΔR of the furthest track from the $\tau_{\text{had-vis}}$ axis	X	X
	$ S_{\text{lead track}} $	Transverse impact parameter significance of the leading track	X	
	S_T^{flight}	Transverse flight path significance		X
	$f_{\text{iso}}^{\text{track}}$	Momentum fraction of isolation tracks	X	X
	$f_{\text{track}}^{\text{EM}}$	Ratio of EM energy and track momentum	X	X
	$p_T^{\text{EM+track}}/p_T$	Fraction of track-plus-EM-system p_T	X	X
	$m^{\text{EM+track}}$	Mass of the track-plus-EM-system	X	X
	m^{track}	Mass of the track system		X

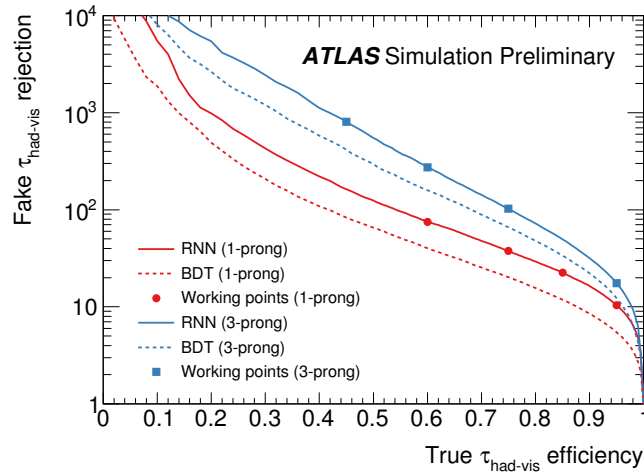


Figure 2.21. Rejection power of quark and gluon jets mis-identified as $\tau_{\text{had-vis}}$ as a function of true $\tau_{\text{had-vis}}$ selection efficiency. Curves for the RNN used in Run 2 and the previously used BDT are reported. The markers show the *Loose*, *Medium*, *Tight* operating points. Figure taken from [108].

with 128, 128, 16 units. Instead, the sequences of charged particles tracks and clusters in the calorimeters are ordered by decreasing p_T and E_T , and are passed through two *shared dense* layers which use the same set of shared weights to process the data. The output of shared dense layers is passed to two layers with *long short-term memory* (LSTM) architecture [109]. The first LSTM layer releases as output a sequence of the same length as the input sequence, while the second LSTM layer releases only the final element of the output sequence, summarising the input into a single vector. LSTM layers consist of 32 (24) units for the branch operating on particles tracks (calorimeter clusters). Results of the computation from the three branches are then merged into a single branch made of three fully connected layers with 64, 32, 1 unit(s) respectively. The LSTM layers use a sigmoid or hyperbolic tangent activation function. Instead all fully connected layers use a ReLU activation function, except for the last output layer which uses a sigmoid activation. The total model consists of 56000 free parameters which are determined during the training.

The RNN performance is evaluated using simulated events of $\gamma^* \rightarrow \tau\tau$ signal and dijet background, independently for the separate of 1-prong and 3-prong $\tau_{\text{had-vis}}$ candidates. Figure 2.21 shows the rejection power, defined as the reciprocal of the background selection efficiency, for misidentified $\tau_{\text{had-vis}}$ as a function of the true $\tau_{\text{had-vis}}$ signal selection efficiency. Four working points, *Very loose*, *Loose*, *Medium*, *Tight* are defined, corresponding to an increasingly higher rejection power and correspondingly lower signal selection efficiency, which are reported in detail in Table 2.6. The dependence of the algorithm performance with respect to tau p_T , $|\eta|$ and number of interaction vertices (μ) has also been studied. The signal selection efficiency is almost independent on $\tau_{\text{had-vis}}$ p_T , $|\eta|$ and μ . Instead, the rejection power shows a huge dependence on such parameters and increases at higher p_T and decreases at high $|\eta|$ and μ . For this reason it is important to point out that the signal efficiency and rejection power here reported are only an indication of the

Table 2.6. Operating working points for the tau identification RNN. Table taken from [108].

Working point	Signal efficiency		Background rejection	
	1 prong	3 prong	1 prong	3 prong
Tight	60%	45%	70	700
Medium	75%	60%	35	240
Loose	85%	75%	21	90
Very loose	95%	95%	9.9	16

expected performance, and the real performance could be different to some extent.

Discrimination against electrons

Aside from jets, electrons constitute also a substantial background to $\tau_{\text{had-vis}}$ identification. The RNN developed specifically to discriminate hadronic taus from jets does not provide sufficient rejection of electrons misidentified as $\tau_{\text{had-vis}}$ and the introduction of a separate e -veto is necessary. Despite the similarities between electrons and $\tau_{\text{had-vis}}$, several properties can be used to discriminate among them: the transition radiation, which is more likely to be emitted by an electron and causes a higher ratio f_{HT} of high-threshold to low-threshold track hits in the TRT for an electron than for a pion; the angular distance of the track from the calorimeter based direction of the tau, the fraction f_{EM} of the energy deposited in the ECAL with respect to the total energy in the calorimeters, the amount of energy leaking in the hadronic calorimeter and the ratio of energy deposited in the region $0.1 < \Delta R < 0.2$ with respect to the total core region $\Delta R < 0.2$. These different features are exploited in a BDT algorithm, referred to as eBDT, which is used in the physics analyses presented in this thesis as veto for electrons generating fake hadronic taus. Figure 2.22 shows the rejection power as a function of the selection efficiency for true taus, measured using simulated MC events. The same curve is reported for an old eBDT and a likelihood discriminator used during Run 1 and at the beginning of Run 2 respectively. Three working points are defined, *Loose*, *Medium* and *Tight*, yielding increasing rejection power.

Decay-mode classification

Hadronic taus decay mainly through five dominant modes, which yield one or three charged hadrons ($h^\pm$), up to two neutral pions (π^0) and a tau neutrino, which goes undetected. The hadrons $h^\pm$ are mainly charged pions $\pi^\pm$ with a minor contribution of kaons $K^\pm$, while the neutral pions decay into couples of photons. Decay mode classification in hadronic taus is described in Ref. [111], and summarised in the following.

The Tau Particle Flow [111] algorithm is able to reconstruct the individual components generated in hadronic tau decays. Such information can be exploited to obtain a decay mode classification. Five decay mode categories are considered: one hadron and no pions ($h^\pm$), one hadron and one pion ($h^\pm\pi^0$), one hadron and two or more pions ($h^\pm \geq 2\pi^0$), three hadrons and no pions ($3h^\pm$), three hadrons and

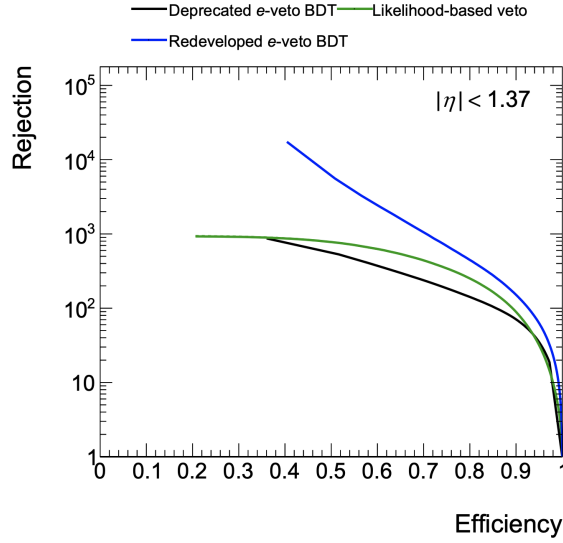


Figure 2.22. Rejection power for electrons misidentified as $\tau_{\text{had-vis}}$ as a function of signal selection efficiency. The blue curve is referred to the eBDT adopted in this thesis. Figure taken from [110]

one or more pions ($3h^\pm \geq 1\pi^0$). A first discrimination among these three categories is obtained exploiting tau particle flow information on the multiplicity and type of particles generated in the tau decay. This information is improved using a BDT discriminator which reconstructs the neutral pions decays exploiting information of the properties of the energy clusters in the ECAL. One additional BDT is used to collectively exploit information on charged particles tracks coming from Tau Particle Flow and on neutral pions decays. This BDT performs the final decay mode classification. The performance on decay mode classification is shown in Figure 2.23, which reports the probability of a given decay mode to be reconstructed as such or to be misidentified with another decay mode, among the five considered. As can be seen the major misidentifications happen between the $h^\pm\pi^0$ and $h^\pm \geq 2\pi^0$ cases, due to the merging of the energy clusters of photons coming from different pions into a single cluster, and between $3h^\pm$ and $3h^\pm \geq 1\pi^0$ cases, due to the merging of the EM energy cluster of the pion with the EM part of the hadronic energy deposit due to the charged hadrons.

ATLAS Simulation
Tau Particle Flow Diagonal fraction: 74.7% $Z/\gamma^* \rightarrow \tau\tau$

Reconstructed decay mode	$h^\pm$	$h^\pm \pi^0$	$h^\pm \geq 2\pi^0$	$3h^\pm$	$3h^\pm \geq 1\pi^0$
$3h^\pm \geq 1\pi^0$	0.2	2.5	3.6	5.3	56.6
$3h^\pm$	0.2	0.6	0.3	92.5	40.2
$h^\pm \geq 2\pi^0$	0.4	6.0	35.4	0.1	0.4
$h^\pm \pi^0$	9.4	74.8	56.3	0.9	2.5
$h^\pm$	89.7	16.0	4.3	1.2	0.3
Generated decay mode	$h^\pm$	$h^\pm \pi^0$	$h^\pm \geq 2\pi^0$	$3h^\pm$	$3h^\pm \geq 1\pi^0$

Figure 2.23. Decay mode classification efficiency matrix, showing the probability of a given decay mode to be reconstructed as any of the available decay modes. Figure taken from [111].

Chapter 3

The Fake Factors method for the estimate of fake hadronic taus

This chapter presents original work I have performed in characterising the misidentification of hadronically decaying tau leptons with hadronic jets via the Fake Factors method. After learning this methodology from the ATLAS Fake Tau Task Force, I provided a validation of the method in final states with two taus. I also delivered a comprehensive analysis of all the possible sources of uncertainty to be attributed to the methodology, and proposed an alternative and faster way of assessing some uncertainty components.

Hadronically decaying tau leptons are complex objects to reconstruct and generate a detector signature very similar to hadronic jets. For this reason, physics analyses exploiting final states with tau leptons are typically limited by a huge background of hadronic jets misidentified as fake hadronic taus. The Fake Factors method is currently the baseline methodology in ATLAS to measure the background of fake taus with a data-driven approach, and is described in this chapter. After a brief summary on tau hadronic decays in Section 3.1, a complete overview of the Fake Factors method is given in Section 3.2, together with the measurement of the *primitive* Fake Factors (Section 3.3), constituting the basic ingredients of the method. A complete analysis of all sources of uncertainty for the fake taus background is reported in Section 3.4, while the validation of the method is described in detail in Section 3.5 and 3.6 for single-tau and di-tau final states respectively.

3.1 Tau leptons and their decays

The tau lepton is the heaviest known lepton and has a mass of $m = 1.777$ GeV and a lifetime of about $\tau = 2.9 \times 10^{-13}$ s, corresponding to proper decay length of $c\tau = 87$ μm [112]. The tau lepton decays leptonically into an electron or a muon, or hadronically into charged and neutral hadrons. A detailed list of its main decays in both channels is given in Table 3.1: leptonic decays represent the 35% of all cases, while hadronic decays cover the 65% of all cases. High energy neutrinos are emitted

in all decays, generating non-null missing transverse momentum in the relative events. Neutrinos are generally highly collinear with the original tau direction. Final states with tau leptons play an important role in the physics programme of the ATLAS experiment and are involved in precision measurements [113, 114], studies of the Higgs boson properties and di-Higgs production [115, 116], searches for lepton flavour violation [117] as well as searches for exotic particles (heavy Higgs, supersymmetric particles, leptoquarks) [118, 119].

Leptonically decaying taus generate electrons and muons which cannot be distinguished with respect to prompt light leptons, within the ATLAS experiential resolution. Thus, this kind of decays can only be identified within a collective analysis of events, exploiting the fact that light leptons coming from a tau lepton are accompanied by missing transverse energy. To give an example, the reconstruction of the $Z \rightarrow \tau\tau$ invariant mass spectrum would yield a distribution peaked at $m_{\tau\tau} \approx 60$ GeV, while the analogue process $Z \rightarrow ee$ would be measured as peaked at $m_{ee} \approx m_Z = 91$ GeV.

Hadronically decaying tau leptons generate instead hadronic secondaries, grouped in thin and highly collimated jets. Among the hadronic decays, only one or three charged hadrons are produced, in 72% and 22% of all cases respectively. The first type of decays is called *one-prong*, while the second type *three-prong*. The charged hadrons typically interact with the detector before decaying and are therefore considered stable particles. They could be charged pions ($\pi^\pm$), or with very little probability, charged kaons ($K^\pm$) and no attempt is made in ATLAS to distinguish between the two. Charged hadrons can be accompanied by ≥ 1 neutral pions (π^0). Neutral pions decay into couples of photons which usually convert into e^+e^- pairs in the interaction with matter of the inner detector. The neutral and charged hadrons produced in the tau lepton decay make up the visible part of the tau lepton, which is referred to as $\tau_{\text{had-vis}}$. Hadronic decays with more than three charged hadrons are also possible, as shown in Table 3.1, but since their branching fraction is very small they are usually not considered in ATLAS.

3.2 Overview of the Fake Factors method

Hadronically decaying taus generate signatures in the detector very similar to hadronic jets. For this reason, jets misidentified as hadronic taus are a dominant source of background in analyses involving taus in the final state, which has to be carefully estimated to obtain successful measurements. The Monte Carlo (MC) simulation cannot estimate this background within the required precision, hence a proper data-driven approach has to be deployed. The *Fake Factors method* is one of the most effective methods to achieve this in the ATLAS experiment, and is described in the following.

3.2.1 The general idea: the Fake Factors as transfer factors

Given a physics analysis with its defined signal region (SR) selecting final states with one tau, the goal of the Fake Factors method is to provide an estimate of the number of fake events ($N^{\text{SR,fake}}$) in which taus have been generated by misidentification of an hadronic jet. Such yield can be evaluated defining a control region (CR), enriched

Table 3.1. Summary of the main tau leptons decays, in the leptonic and hadronic modes. Branching fractions are reported, whose numerical values are taken from [112].

Channel	Decay	Branching ratio [%]
leptonic	$\tau^- \rightarrow \mu^- \bar{\nu}_\mu \nu_\tau$	17.39 ± 0.04
	$\tau^- \rightarrow e^- \bar{\nu}_e \nu_\tau$	17.82 ± 0.04
hadronic 1-prong	$\tau^- \rightarrow \pi^- \nu_\tau$	10.82 ± 0.05
	$\tau^- \rightarrow K^- \nu_\tau$	$(6.96 \pm 0.10) \times 10^{-3}$
	$\tau^- \rightarrow \pi^- \pi^0 \nu_\tau$	25.49 ± 0.09
	$\tau^- \rightarrow K^- \pi^0 \nu_\tau$	$(4.33 \pm 0.15) \times 10^{-3}$
	$\tau^- \rightarrow \pi^- 2\pi^0 \nu_\tau$	9.26 ± 0.10
	$\tau^- \rightarrow K^- 2\pi^0 \nu_\tau$	$(6.5 \pm 2.2) \times 10^{-4}$
	$\tau^- \rightarrow \pi^- 3\pi^0 \nu_\tau$	1.04 ± 0.07
	$\tau^- \rightarrow K^- 3\pi^0 \nu_\tau$	$(4.8 \pm 2.1) \times 10^{-4}$
hadronic 3-prong	$\tau^- \rightarrow \pi^- \pi^+ \pi^- \nu_\tau$	9.31 ± 0.05
	$\tau^- \rightarrow \pi^- \pi^+ \pi^- \pi^0 \nu_\tau$	4.62 ± 0.05
	$\tau^- \rightarrow K^- \pi^+ \pi^- \nu_\tau$	$(3.45 \pm 0.07) \times 10^{-3}$
	$\tau^- \rightarrow K^- \pi^+ \pi^- \pi^0 \nu_\tau$	$(1.31 \pm 0.12) \times 10^{-3}$
	$\tau^- \rightarrow K^- K^+ \pi^- \nu_\tau$	$(1.435 \pm 0.027) \times 10^{-3}$
	$\tau^- \rightarrow K^- K^+ \pi^- \pi^0 \nu_\tau$	$(6.1 \pm 1.8) \times 10^{-5}$
	$\tau^- \rightarrow K^- K^+ K^- \nu_\tau$	$(2.2 \pm 0.8) \times 10^{-5}$
	$\tau^- \rightarrow K^- K^+ K^- \pi^0 \nu_\tau$	$< 4.8 \times 10^{-6}$
other hadronic decays	$\tau^- \rightarrow 3\pi^- 2\pi^+ \nu_\tau$	$(8.27 \pm 0.31) \times 10^{-4}$
	$\tau^- \rightarrow K^+ 3\pi^- \pi^+ \nu_\tau$	$< 5.0 \times 10^{-6}$
	$\tau^- \rightarrow K^+ K^- 2\pi^- \pi^+ \nu_\tau$	$< 4.5 \times 10^{-7}$
	other	$\simeq 4.2$

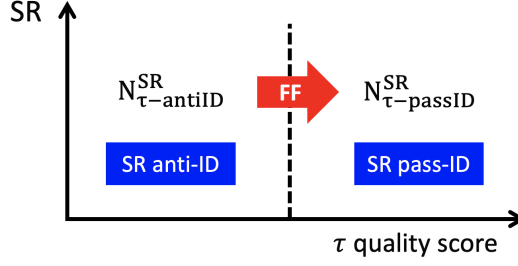


Figure 3.1. Graphical representation of the conceptual Fake Factors methodology. The Fake Factor is a transfer factor from the SR antiID to the SR passID.

in events with jets misidentified as taus, and multiplying the number of fake events in the CR ($N^{\text{CR},\text{fake}}$) by a Fake Factor FF, proportional to the probability of a jet of being misidentified as a tau

$$N^{\text{SR},\text{fake}} = N^{\text{CR},\text{fake}} \times \text{FF} . \quad (3.1)$$

The CR is usually defined by the same set of selections as the SR, but requiring that the tau is failing the identification (ID) criterion rather than passing it. For this reason the CR is typically denoted as SR anti-ID, while the aforementioned SR is denoted as SR pass-ID, to stress that the ID requirement is verified. In this notation we will write

$$N_{\text{passID}}^{\text{SR},\text{fake}} = N_{\text{antiID}}^{\text{SR},\text{fake}} \times \text{FF} . \quad (3.2)$$

As can be noticed, the FF plays the role of *transfer factor* from the SR anti-ID to the SR pass-ID, as also shown graphically in Figure 3.1. Obviously, the Fake Factor has to be measured, and this can be in principle done in another CR to be properly defined

$$\text{FF} = \frac{N_{\text{passID}}^{\text{CR},\text{fake}}}{N_{\text{antiID}}^{\text{CR},\text{fake}}} \quad (3.3)$$

We will see in the discussion in Section 3.2.2 that such control region is in practice hard to be constructed and how the Fake Factors method solves this issue.

Until now, we have treated the Fake Factor as if it was a constant number. The most realistic case is that in which the FF depends on some tau properties which are correlated with the probability of misidentifying a hadronic jet with a hadronic tau. The FF usually depends strongly on the tau transverse momentum p_T , its reconstructed decay mode, and weakly depends also on tau pseudorapidity η

$$\text{FF} = \text{FF}(p_T, \eta, \text{dm}) , \quad (3.4)$$

where we denote with dm the decay mode, usually varying among the 1-prong and 3-prong categories. The FF dependence shown in Eq. (3.4) is managed splitting the analysis phase space into bins in which the relative FFs can be considered constant and applying the FF method separately in each of such bins. This approach also enables to estimate the fakes background in binned distributions, typical of the ATLAS analyses. The fakes background is evaluated bin-by-bin in the considered spectrum, weighting the contributions in each bin by the FFs to the proper value of p_T , η , decay mode.

Subtraction of events with truth matched taus

The Fake Factors method has been designed to estimate the number of events in which a fake tau is generated by the misidentification of a hadronic jet. For this reason the yields in Eqs. (3.2) and (3.3) should count only the fake taus strictly verifying this request. In particular, we want to avoid that events with real taus or electrons and muons misidentified as fake hadronic taus enter in such yields. Unfortunately, such events will inevitably enter both in the SR and in the CR and will contribute to the yields $N_{\text{antiID}}^{\text{SR,fake}}$, $N_{\text{passID}}^{\text{CR,fake}}$ and $N_{\text{antiID}}^{\text{CR,fake}}$. However, this contamination can be estimated via MC simulation and subtracted from the aforementioned yields. Equations (3.2) and (3.3) therefore become

$$N_{\text{passID}}^{\text{SR,fake}} = \left(N_{\text{antiID}}^{\text{SR,Data}} - N_{\text{antiID}}^{\text{SR,MC}} \right) \times \text{FF} \quad (3.5)$$

$$\text{FF} = \frac{N_{\text{passID}}^{\text{CR,Data}} - N_{\text{passID}}^{\text{CR,MC}}}{N_{\text{antiID}}^{\text{CR,Data}} - N_{\text{antiID}}^{\text{CR,MC}}} \quad (3.6)$$

where the superscripts Data and MC denote an event yield in Data and an yield of events with a truth-matched tau in MC, respectively. Let's specify what truth-matched means here. We want to remove events with real taus, i.e. reconstructed taus matched with taus at truth-level. We also want to remove events with electrons and muons misidentified as taus, i.e. reconstructed taus matched with electrons and muons at truth-level. Therefore, we have to consider as truth-matched every tau that is matched with either a tau, or an electron, or a muon at truth-level. The process of removal of events with truth-matched taus is called *truth-subtraction*, and will be addressed as such in the following.

3.2.2 Combined Fake Factors evaluation

Let's now focus on the problem of measuring FFs to be used to apply the method. As previously mentioned, the definition of a proper control region CR to be used to apply Eq. (3.3) is in general very difficult. The reason for this is that several types of hadronic jets exist, which could originate a fake hadronic tau. Most importantly we can distinguish among light-quark-originated (q), gluon-originated (g), *b*-quark-originated (b) and pile-up (p) jets. These types of jets have different characteristics, and therefore have a different probability of being misidentified as a hadronic tau. Hence, each of these types of jet is described by a different FF.

The signal region will include fake taus originated by misidentified hadronic jets in a certain composition among the four categories q/g/b/p. Such composition results basically from the cuts and requirements which constitute the SR definition. A suitable control region for the FF measurement has to hold exactly the same q-/g-/b-/p-jets relative abundance. The closer the q-/g-/b-/p-jets compositions in the CR is to the one of the SR, the more applicable are the measured FFs to the SR itself. One possibility to verify this requirement is to make the definitions of the SR and the CR very similar to each other. However, even a small difference in the definition could yield FFs leading to an unsatisfactory estimate of the fakes background.

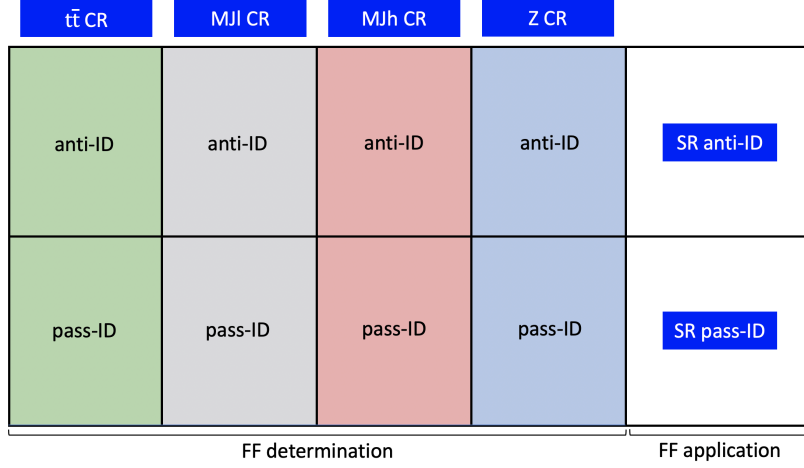


Figure 3.2. Graphical scheme representing the signal region (SR) and the auxiliary control regions (CR) used to the primitive FFs measurement.

Template fits and combination of primitive Fake Factors

To solve the issue of finding a proper control region for the FF measurement, a combinatorial approach can be used. Instead of finding a single fake enriched CR with similar composition as the anti-ID SR, we can alternatively proceed to determine the anti-ID SR composition and estimate a combined FF, suitable for this particular composition. This is the main idea at the basis of the Fake Factors method: we aim at estimating the fractions of q-/g-/b-/p-originated fake taus in the anti-ID SR and to use these fractions to make a combination of FFs representative of each of these types

$$\text{FF}_{\text{comb}} = \mu_q \text{FF}_q + \mu_g \text{FF}_g + \mu_b \text{FF}_b + \mu_p \text{FF}_p, \quad (3.7)$$

where μ_x stands for the fraction of x -originated fakes in the anti-ID SR and FF_x is the relative FF.

The Fake Factors $\text{FF}_{q/g/b/p}$, also referred to as *primitive FFs*, have to be measured in specific regions highly enriched in q-/g-/b-/p-jets respectively. A suitable set of measurement regions is (see also Figure 3.2):

- $Z\mu\mu$ region, selecting events coming from $Z \rightarrow \mu\mu$ decays. Jets misidentified as taus in this region are mainly quark-jets;
- MJh region, selecting multijet events with high score of the JVT tagger [95]. This region is enriched in gluon jets;
- MJl region, selecting multijet events with low score of the JVT tagger [95]. This region is enriched in pile-up jets;
- $t\bar{t}$ region, selecting top-antitop events. Since the top-quark decays into b -quarks, this region is enriched in b -jets.

Using these regions for the measurement of the primitive FFs, Eq. 3.7 becomes

$$\text{FF}_{\text{comb}} = \mu_Z \text{FF}_Z + \mu_{\text{MJh}} \text{FF}_{\text{MJh}} + \mu_{\text{MJl}} \text{FF}_{\text{MJl}} + \mu_{t\bar{t}} \text{FF}_{t\bar{t}}, \quad (3.8)$$

The fractions μ_x in Eq. (3.8) can be determined from data in the anti-ID SR with a template fit. The variable used in the fit should have a high discriminating power between the different types of jets. Examples of such variables are quantities representing features highly correlated with the shape of the tau, such as the tau-width, or multivariate variables, such as the score of a BDT-based q/g tagger algorithm developed in the ATLAS performance groups [120]. Typically multivariate scores have a less intuitive definition, but yield higher performances, since they are more informative. The fractions μ_x are determined as the values yielding the best fit of the combined template

$$h_{\text{comb}} = \mu_Z h_Z + \mu_{\text{MJh}} h_{\text{MJh}} + \mu_{\text{MJl}} h_{\text{MJl}} + \mu_{t\bar{t}} h_{t\bar{t}} \quad (3.9)$$

to the template of data in the anti-ID SR, $h_{\text{SR antiID}}$. Here h_x denotes the template histogram of the considered variable (q/g tagger score or tau-width), measured in the region x and applying the anti-ID requirement. It is worth remembering that all histograms involved in the template fit (namely: $h_{\text{SR antiID}}$, h_Z , h_{MJh} , h_{MJl} , $h_{t\bar{t}}$) can be contaminated by counts originating from true taus or electrons and muons misidentified as fake taus. Such contamination can be negligible but, in general, has to be estimated via MC simulation and subtracted from the templates.

3.2.3 Extension of the method to di-tau final states

The previous discussion was focused on how to implement the Fake Factors method in analyses in which the final state contains only one tau. We want now to extend this procedure to the more complex case in which the final state contains two taus.

The first step is to define an ordering criterion among the two taus. The simplest strategy is to order them by decreasing p_T : we will therefore identify as “first” tau the leading one and as “second” tau the subleading. An intuitive approach to build a fakes estimate in this case is to run the FF method twice, independently for the “first” and the “second” tau and to sum the relative contributions

$$N_{\text{passID1,passID2}}^{\text{SR,fake}} = \left(N_{\text{antiID1,passID2}}^{\text{SR,Data}} - N_{\text{antiID1,passID2}}^{\text{SR,MC}} \right) \times \text{FF}_1 \\ + \left(N_{\text{passID1,antiID2}}^{\text{SR,Data}} - N_{\text{passID1,antiID2}}^{\text{SR,MC}} \right) \times \text{FF}_2, \quad (3.10)$$

where the subscripts indicate whether the leading or subleading taus are required to pass or fail the ID cut, and different FFs are used for the two contributions, each one referred to the tau verifying the anti-ID cut. This generalisation is straightforward, but can work only if the source of fake taus were events with one real tau and one fake tau (i.e. single fake events). Events of this kind come, for example, from the W +jets process.

Let’s now consider also events in which two fake taus can be present (i.e. double fake events). Events of this kind are generated, for example, via the multijet process. In this case Eq. (3.10) is incorrect. In fact, as fake taus can in general verify both the anti-ID and the pass-ID requirements, double fake events will be counted in the yields of both first and second term of Eq. (3.10) and therefore such contribution will be double-counted. To correct for this, we need to subtract a term equal to the double fake events contribution in the SR pass-ID, which can be estimated as

$$N_{\text{passID1,passID2}}^{\text{SR,double fake}} = \left(N_{\text{antiID1,antiID2}}^{\text{SR,Data}} - N_{\text{antiID1,antiID2}}^{\text{SR,MC}} \right) \times \text{FF}_1 \times \text{FF}_2. \quad (3.11)$$

Including also this contribution, the final combinatorial expression for the fake-tau event yield in the di-tau SR is

$$\begin{aligned}
N_{\text{passID1,passID2}}^{\text{SR,fake}} = & \left(N_{\text{antiID1,passID2}}^{\text{SR,Data}} - N_{\text{antiID1,passID2}}^{\text{SR,MC}} \right) \times \text{FF}_1 \\
& + \left(N_{\text{passID1,antiID2}}^{\text{SR,Data}} - N_{\text{passID1,antiID2}}^{\text{SR,MC}} \right) \times \text{FF}_2 \\
& - \left(N_{\text{antiID1,antiID2}}^{\text{SR,Data}} - N_{\text{antiID1,antiID2}}^{\text{SR,MC}} \right) \times \text{FF}_1 \times \text{FF}_2 ,
\end{aligned} \tag{3.12}$$

Further check of the combinatorial formula

To gain a deeper understanding of the combinatorial expression in Eq. (3.12), let's rephrase it from a different perspective. Using the short notation $N^{\text{SR}} = (N^{\text{SR,Data}} - N^{\text{SR,MC}})$ we can re-write it as

$$\begin{aligned}
N_{\text{passID1,passID2}}^{\text{SR,fake}} = & N_{\text{antiID1,passID2}}^{\text{SR}} \times \text{FF}_1 \\
& + N_{\text{passID1,antiID2}}^{\text{SR}} \times \text{FF}_2 \\
& - N_{\text{antiID1,antiID2}}^{\text{SR}} \times \text{FF}_1 \times \text{FF}_2 ,
\end{aligned} \tag{3.13}$$

The first term in the sum can be rewritten as

$$\begin{aligned}
N_{\text{antiID1,passID2}}^{\text{SR}} \times \text{FF}_1 = & \left(N_{\text{antiID1,passID2-T}}^{\text{SR}} + N_{\text{antiID1,passID2-F}}^{\text{SR}} \right) \times \text{FF}_1 \\
= & N_{\text{antiID1,passID2-T}}^{\text{SR}} \times \text{FF}_1 + N_{\text{antiID1,antiID2}}^{\text{SR}} \times \text{FF}_1 \times \text{FF}_2 .
\end{aligned} \tag{3.14}$$

where we have explicitly factorised the two contributions in which the pass-ID tau is either a true or a fake tau, and we have used the FF definition for the second tau. A similar expression can be obtained for the second term of Eq. (3.13). Substituting these expressions into Eq. (3.13) one obtains

$$\begin{aligned}
N_{\text{passID1,passID2}}^{\text{SR,fake}} = & N_{\text{antiID1,passID2-T}}^{\text{SR}} \times \text{FF}_1 \\
& + N_{\text{passID1-T,antiID2}}^{\text{SR}} \times \text{FF}_2 \\
& + N_{\text{antiID1,antiID2}}^{\text{SR}} \times \text{FF}_1 \times \text{FF}_2 ,
\end{aligned} \tag{3.15}$$

which estimates the fake tau background more intuitively as the *addition* of three contributions corresponding to the cases in which the first tau is anti-ID *and the second is true*, the second tau is anti-ID *and the first is true*, both taus are anti-ID.

3.2.4 Benefits of the Fake Factors method

The Fake Factors method provides two major advantages to the physics analyses, with respect to the direct computation of FFs in a proper control region.

The first advantage is merely technical. The FF method provides a unified approach for the fake tau background estimate, which can be used by all ATLAS analyses. The primitive FFs and the relative templates can be measured centrally only one time, and shared between all physics analyses. The analysers working on a specific measurement will only have to determine the templates in the anti-ID SR and perform the template fit to measure the q-/g-/b-/p- jet composition, obtaining the combined FFs from the already provided primitive FFs.

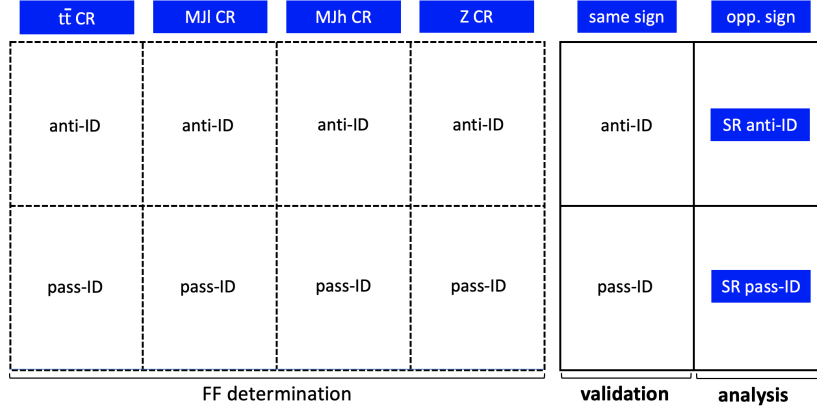


Figure 3.3. Scheme of the regions in an example analysis, using a same sign SR and validating the FF method with an opposite sign validation.

The second advantage is related to the physics and is the most important. An analysis measuring FFs with direct determination in a CR usually has no region left for validation of such FFs. The FF method, instead, provides FFs using the additional auxiliary regions $Z\mu\mu$, MJh, MJl, $t\bar{t}$ and therefore has the potential to “free” regions that would be used for the FFs measurement. Such regions can be employed as validation regions for the method, providing an important check for the correctness of the extrapolated fakes background.

Let’s discuss this in a real example. Let’s consider the physics analysis presented in this thesis in Chapter 4. The analysis is based on a di-tau signal region and the two taus have opposite sign (OS) charge. A fake enriched auxiliary region can be defined, using exactly the same cuts as the SR, but requiring that the two taus have charge of the same sign (SS). If we use the SS region as a CR to get a direct measurement of the FFs, then no region is left to validate the correctness of the FFs extrapolation from the OS region to the SS region. If, instead, we evaluate the FFs using the FF method, then the SS region will be “freed” and can serve as validation region. In fact, we can apply the FF method both in the SS and OS regions, and we will end up with two fakes background estimates. The fakes background in the OS region is used for the physics analysis, while the fakes background in the SS region, which is unblinded, is used to cross-check the agreement between data and MC, providing a validation of the fakes background in the OS region. A graphical representation of the regions used in this discussion is provided in Figure 3.3.

3.2.5 Towards a Universal Fake Factor method

Let’s now deepen the discussion and enlight a feature of generality of the Fake Factors method. We have seen that the combined FFs can be obtained as a combination of primitive FFs, measured in auxiliary regions enriched in q-/g-/b-/p-jets. We want to address the following question: is it really necessary that the composition of the auxiliary regions is *pure* in q-/g-/b-/p-jets?

To simplify the discussion let’s assume that only q-/g-jets exists. Equation (3.7)

reduces then to

$$\text{FF}_{\text{comb}} = \mu_q \text{FF}_q + \mu_g \text{FF}_g . \quad (3.16)$$

Let's now consider two general auxiliary regions, labelled by indices 1 and 2, which verify the only requirement of having different q/g composition. We can generally write

$$\text{FF}_1 = \mu_{q1} \text{FF}_q + \mu_{g1} \text{FF}_g \quad (3.17)$$

$$\text{FF}_2 = \mu_{q2} \text{FF}_q + \mu_{g2} \text{FF}_g , \quad (3.18)$$

where μ_{q1} , μ_{g1} and μ_{q2} , μ_{g2} are the fractions of q-/g-originated fakes in the anti-ID regions of samples 1 and 2. Inverting the system of Eqs. (3.17) and (3.18) one obtains

$$\text{FF}_q = \frac{\mu_{g2} \text{FF}_1 - \mu_{g1} \text{FF}_2}{\mu_{g2} \mu_{q1} - \mu_{g1} \mu_{q2}} \quad (3.19)$$

$$\text{FF}_g = \frac{-\mu_{q2} \text{FF}_1 + \mu_{q1} \text{FF}_2}{\mu_{g2} \mu_{q1} - \mu_{g1} \mu_{q2}} \quad (3.20)$$

Substituting Eqs. (3.19) and (3.20) into Eq. (3.16) one obtains

$$\text{FF}_{\text{comb}} = \frac{\mu_q \mu_{g2} - \mu_g \mu_{q2}}{\mu_{g2} \mu_{q1} - \mu_{g1} \mu_{q2}} \text{FF}_1 + \frac{-\mu_q \mu_{g1} + \mu_g \mu_{q1}}{\mu_{g2} \mu_{q1} - \mu_{g1} \mu_{q2}} \text{FF}_2 \quad (3.21)$$

The coefficients in front of FF_1 and FF_2 denote the fractions of fakes in the anti-ID SR that have the same q-/g- composition as fakes in samples 1 and 2. If we denote them with μ_1 and μ_2 we obtain

$$\text{FF}_{\text{comb}} = \mu_1 \text{FF}_1 + \mu_2 \text{FF}_2 , \quad (3.22)$$

which is exactly analogue as Eq. (3.16). This means that the FF method is even more general and it is not required that the regions in which the primitive FFs are measured are pure each respective source of fakes. It is sufficient that these regions have a different q/g composition from each other, such that the primitive FFs are independent (i.e. they constitute a “basis” of primitive FFs). We can call this more broadened version of the method *Universal Fake Factors method*.

3.3 Measurement of Fake Factors in jets enriched regions

As mentioned in Section 3.2.2, the combined Fake Factors FF_{comb} of the user analysis are evaluated as a combination of primitive FFs, measured in regions enriched in q-/g-/b-/p-jets. We describe in what follows the primitive FFs measurement, obtained with pp collision data recorded by the ATLAS experiment in 2015-2018.

3.3.1 Data and simulated samples

Data

The analysis uses $\sqrt{s} = 13$ TeV pp collisions data, recorded by the ATLAS experiment during Run 2 in 2015-2018. The dataset corresponds to an integrated luminosity of 139 fb^{-1} with an uncertainty of 1.7% [121]. Only the luminosity blocks subscribed to the Good Run List (GRL) for Run 2 are considered.

Simulated samples

The Monte Carlo (MC) simulation is used to model processes leading to tau production. The generated events are interfaced with a detailed simulation of the ATLAS detector's response to particles, based on GEANT4 [84]. The effect of multiple interactions due to pile-up is modelled combining the hard scatter event with a simulation of the underlying event generated via PYTHIA 8.186 [122] using the NNPDF2.3LO set of parton distribution functions (PDF) [123] and the A3 set of tuned parameters [124]. The MC events are reweighted properly to reproduce the distribution of the average number of interactions per bunch crossing $\langle\mu\rangle$ observed in data. Information on the MC generators used, the PDF sets, the tune and the order of precision for the cross-section generation are reported in Table 3.2. Further details on each single process are given in what follows.

Table 3.2. Details on MC generators used in the analysis. The acronyms ME and PS stand for matrix element and parton shower respectively. The cross-section order stands for the order of cross-section calculation in QCD, with ((next-to-)next-to-)leading order ((N)N)LO and ((nex-to-)next-to-)leading-logarithm ((N)N)LL, respectively.

Process	ME generator	ME PDF	PS and hadronis.	Tune	Cross-section
V+jets	Sherpa 2.2.1	NNPDF3.0NNLO	Sherpa 2.2.1	Default	NNLO
Di-jet di-lep.	Sherpa 2.2.1	NNPDF3.0NNLO	Sherpa 2.2.1	Default	NNLO
ttbar	PowhegBox v2	NNPDF3.0NLO	Pythia 8.230	A14	NNLO, NNLL
single top <i>s</i>	PowhegBox v2	NNPDF3.0NLO	Pythia 8.230	A14	NLO
single top <i>t</i>	PowhegBox v2	NNPDF3.0NLO	Pythia 8.230	A14	NLO
single top <i>Wt</i>	PowhegBox v2	NNPDF3.0NLO	Pythia 8.230	A14	NLO, NNLL
Diboson	Sherpa 2.2.1-2	NNPDF3.0NNLO	Sherpa 2.2.1-2	Default	NNLO
<i>t</i> $\bar{t}$ V	MG5 2.3.3	NNPDF3.0NLO	Pythia 8.210	A14	NLO

V+jets. Vector boson production in association with jets is simulated with SHERPA 2.2.1 [125] generator. The matrix element (ME) is calculated with next-to-leading order (NLO) accuracy for events with emission of 0, 1, 2 partons and to leading order (LO) accuracy for events with emission of 3, 4 partons. Parton hard-scatter processes are matched with the parton showering [126] according to the MEPS@NLO prescription [127, 128, 129, 130]. The NNPDF3.0NNLO set of PDFs [131] is used. These samples are normalised to a next-to-next-to-leading order (NNLO) precision [132].

Dijet and di-lepton production. The electroweak of di-jet plus di-lepton final states ($\ell\ell jj, \ell\nu jj, \nu\nu jj$) is simulated with SHERPA 2.2.1 [125] generator. Similarly as for V+jets samples, LO matrix elements with up to two additional partons emitted are evaluated and merged with the SHERPA parton shower. The NNPDF3.0NNLO PDFs set is used [131].

Top production. Top quark pair production is simulated with POWHEGBOX v2 [133, 134, 135, 136] with NLO ME accuracy. The NNPDF3.0NLO [131] PDF set is

used. The damping parameter h_{damp} is set to 1.5 top quark masses [137]. The parton showering and hadronisation processes are modelled with the PYTHIA 8.230 generator [138], while heavy-flavour quark decay is simulated with EVTGEN 1.6.0 [139]. The lower statistics of the high- p_T tails are compensated by additional samples inclusive in top quark pair events. Single top quark production is modelled in the three possible modes: s -channel, t -channel and Wt -channel. These processes are simulated with POWHEGBOX v2 [133, 134, 135, 136] generator with NLO accuracy. The NNPDF3.0NLO PDFs set is adopted. The generated events are interfaced with PYTHIA 8.230 [123] using the A14 [140] tune.

Diboson. Diboson processes are simulated with SHERPA 2.2.1 and SHERPA 2.2.2 [125]. MEs are calculated with NLO accuracy for up to one additional parton and LO accuracy for up to three additional parton emissions. The MEs are matched and merged with SHERPA parton shower using the MEPS@NLO prescriptions [127, 128, 129, 130]. The NNPDF3.0NNLO set [131] is used for PDFs, to set parton shower tuning parameters.

$t\bar{t}V$. The $t\bar{t}V$ process is simulated with MADGRAPH5 AMC@NLO 2.3.3 [141] generator at NLO. The NNPDF3.0NLO [131] PDF set is used. Events are interfaced with PYTHIA 8.210 [138] using the A14 [140] tune. The bottom and charm hadron decays are simulated using the EVTGEN 1.2.0 generator [139].

3.3.2 Events pre-selection

This section outlines the baseline selections applied to the events and the requirements to physics analysis objects.

Objects selection

The analysis is based on jets, taus, electrons, muons and photons. These objects are reconstructed as detailed in Section 2.3. To be considered in the analysis, the reconstructed objects need to verify additional requirements, which are detailed in what follows.

Jets. Jets are reconstructed using the anti- k_T clustering algorithm [93] run on Particle Flow objects [94]. The radius parameter is set to $R = 0.4$. Jets are required to be in the rapidity range $|\eta| < 4.5$ and are classified as *central* jets if they have $|\eta| < 2.5$ or *forward* jets if they have $2.5 < |\eta| < 4.5$. A cut on missing transverse momentum $p_T > 20$ GeV is applied, both on central and forward jets. Flavour tagging algorithms are run on jets to discriminate whether they are b -tagged or not. The b -jets need to be central jets ($|\eta| < 2.5$) and have to satisfy the 85% efficiency working point of DL1r tagger [96].

Taus. Hadronic tau leptons [105] are reconstructed in the rapidity range $|\eta| < 2.5$, excluding the transition region between the barrel and end-cap of the electromagnetic calorimeter $1.37 < |\eta| < 1.52$. They must have $p_T > 20$ GeV, unitary electric charge

$|q| = 1$ and should have one or three tracks. A baseline requirement on the RNN identification score is required $\text{RNN} > 0.01$.

Electrons. Electrons are reconstructed from ID tracks matched with energy clusters in the electromagnetic calorimeter [88]. All electrons are required to have $p_T > 15$ GeV and $|\eta| < 2.47$. They must verify the *Loose* identification criteria and the *Tight* isolation criteria. Additional requirements are assigned on the transverse impact parameter significance, $|d_0|/\sigma_{d_0} < 5$, and on the longitudinal impact parameter $|z_0 \sin \theta| < 0.5$.

Muons. Muons are reconstructed from tracks in the ID matched with the corresponding tracks in the muon spectrometer [90]. All muons are required to verify $p_T > 7$ GeV and $|\eta| < 2.5$. The *Loose* quality working point and the *Tight* isolation working point are chosen. Additional requirements are assigned on transverse impact parameter significance, $|d_0|/\sigma_{d_0} < 5$ and longitudinal impact parameter $|z_0 \sin \theta| < 0.5$.

Photons. Photons are reconstructed from energy clusters in the electromagnetic calorimeter [88]. All photons have to verify $p_T > 15$ GeV and $|\eta| < 2.47$. Photons reconstructed in the transition region between barrel and end-cap $1.37 < |\eta| < 1.52$ are vetoed. Isolation requirements have to be verified with *Tight* working point. Moreover photons are vetoed when reconstructed starting from calorimeter cells with dead high-voltage.

The overlap removal (OLR) is applied to reconstructed objects, after selecting them with the aforementioned requirements. All couples of objects reconstructed in the same region of (η, ϕ) space are considered and one of the two is rejected according to a defined priority list with specified selection criteria. The *Standard* working point of the OLR is used.

Tau selection and truth subtraction

In each event exactly one tau is required to be present. Moreover, in MC the taus are required to be matched either to a truth tau or to a truth electron or to a truth muon. As detailed in Section 3.2.1, the reason for this matching is that true taus as well as fake taus originating from electrons or muon sources are not treated in the FF method. Hence, such contributions are estimated via MC simulation and subtracted from data yields.

Real tau suppression

The removal of true taus is already performed via the subtraction of yields estimated with the MC simulation (the truth-subtraction). However, this procedure introduces some dependence on the MC simulation, which is in general preferable to avoid. For this reason, further cuts are applied on E_T^{miss} to reject true taus contamination directly in data. The cuts are the following:

- $E_T^{\text{miss}} < 50$ GeV. Fake events have a low or null E_T^{miss} , since fictitious missing transverse momentum can only be originated from miscalibration of objects and is expected to be within the object resolution (for example, fake E_T^{miss} coming from miscalibrated jets, will be of the order of the JER). Instead, real taus have a high associated E_T^{miss} , generated by the neutrinos originated in the tau decay.
- Significance on E_T^{miss} lower than 2. True taus are associated with real E_T^{miss} , while fake taus are associated with fake E_T^{miss} , which has a low significance.
- $\Delta\phi(\tau, E_T^{\text{miss}}) > 1$. Real taus decay in neutrinos emitted almost collinearly with the original tau direction. Therefore, a small angle between the tau and E_T^{miss} is expected. Instead, E_T^{miss} associated with fake tau decays is randomly oriented.

3.3.3 Measurement regions for the primitive Fake Factors

Events passing the pre-selection requirements are categorised in four regions, used for the measurement of the primitive Fake Factors. Such regions are enriched in q-/g-/b-/p-jets to allow the measurement of the relative FFs. The selection requirements are summarised in Table 3.3, and are listed below.

$Z\mu\mu$ region

The $Z\mu\mu$ region is constructed to select events coming from the $Z \rightarrow \mu\mu$ electroweak process. The presence of a tau is additionally required, hence selecting fake taus mainly originating from quark-jets. A muon trigger is required on the leading lepton, with a threshold on the muon p_T depending on the year of data-taking. Exactly two muons are required, having opposite electric charge and verifying the *Tight* ID working point. The leading muon should have $p_T > 28$ GeV, while the sub-leading $p_T > 15$ GeV. Moreover, the invariant mass of the di-muon system has to assume values around the Z -boson mass, $76 < m_{\mu\mu} < 106$ GeV. Events with electrons or photons are vetoed from this region. Finally, the required additional tau lepton needs to have seed jet $JVT > 0.8$ [95].

MJh region

The MJh region is defined to select multijet events enriched in jets coming from QCD activity and matched with the hard-scatter. The presence of an hadronic tau is also required, leading to the reconstruction of fake taus originated from gluon jets. Jet triggers are used, with thresholds varying with the year of data-taking. At least two hadronic jets are required in the event, in the rapidity range $|\eta| < 3$ and with jet timing less than 12.5 ns. The leading jet is required to have $p_T > 450$ GeV. This threshold is decreased to $p_T > 390$ GeV in 2015 data. The two leading jets should have a back-to-back topology: they need to show high angular separation $\Delta\phi(j_0, j_1) > 2.7$ and should have dominant average p_T with respect to the fake tau transverse momentum, $p_T^\tau < 0.25 (p_T^{j_0} + p_T^{j_1})/2$. If the event has more than two jets, additional jets should have sub-dominant momentum $p_T^{j_2} < p_T^\tau$, where j_2 is the third

Table 3.3. Summary of the requirements the events selection in the $Z\mu\mu$, MJh, MJl, $t\bar{t}$ regions, used for the measurement of the primitive Fake Factors.

$Z\mu\mu$ region	
Trigger	leading muon
Muons	two muons with $p_T > 15$ GeV and <i>Tight</i> ID Leading muon $p_T > 28$ GeV $76 < m_{\mu\mu} < 106$ GeV opposite electric charge
Electrons and photons	veto
Tau	one tau with seed jet JVT > 0.8
MJh region	
Trigger	jet
Jets	≥ 2 jets with $ \eta < 3$ $ \text{Timing} < 12.5$ ns Leading jet $p_T > 450$ GeV (> 390 GeV for 2015) $\Delta\phi(j_0, j_1) > 2.7$ $p_T^\tau < 0.25 (p_T^{j_0} + p_T^{j_1})/2$
Third jet veto	either exactly two jets or $p_T^{j_2} < p_T^\tau$
Light leptons, photons	veto
Tau	one tau with seed jet JVT > 0.8
MJl region	
All cuts	same as MJh region, except for tau seed jet JVT
Tau	one tau with seed jet JVT < 0.8
$t\bar{t}$ region	
Trigger	jet and b -jet unprescaled triggers in OR
Jets	≥ 5 jets with $p_T > 20$ GeV ≥ 1 jet b -tagged $ \text{Timing} < 12.5$ ns <i>Medium</i> JVT and FJVT working point
Light leptons, photons	veto
Tau	one tau

jet in the p_T -ordered collection. Moreover, events with either an electron or a muon or a photon are vetoed from this region. The tau jet seed is required to have Jet Vertex Tagger [95] score $JVT > 0.8$. This requirement ensures that the fake tau is not originated from a pile-up jet.

MJl region

The MJl region definition follows exactly the same requirements as the MJh region, with the exception that the cut on the tau jet seed JVT score is reversed. The tau jet seed is required to have $JVT < 0.8$. Since the JVT score measures the fraction of tracks associated with the hard scatter vertex, this requirement ensures that the fake tau is originated from a pile-up jet.

$t\bar{t}$ region

The $t\bar{t}$ region is defined to select fake taus originated from b -jets. Events are triggered with a complex logical OR of several unprescaled jet and b -jet triggers. At least five jets are required, with $p_T > 20$ GeV, and at least one jet has to be b -tagged. Jets must have timing less than 12.5 ns and should verify the *Medium* JVT and FJVT working points. Events with either electrons or muons or photons are vetoed. One tau is required, which will be most likely a fake tau.

3.3.4 Results

The results of the primitive Fake Factors measurement in the $Z\mu\mu$, MJh, MJl, $t\bar{t}$ regions are shown in Figure 3.4. The FFs have been measured in bins of tau p_T , and separating the decay mode in the 1-prong and 3-prong categories. The p_T binning has been chosen to be sufficiently thin to be utilised by the user analyses, and at the same time sufficiently large to preserve high statistics in the bins. If, in the user analyses, a tau has momentum not falling within the FFs p_T binning, the FF relative to the nearest bin is attributed. The *Loose* tau ID working point has been used for this measurement, hence FFs are calculated as ratios of event yields verifying (pass-ID) and not verifying (anti-ID) this working point requirement (see Eq. (3.6)). The slight dependence on tau rapidity η has been neglected in this measurement, and FFs have been considered constant in all the rapidity range. The 1-prong category includes tau decays with one hadron and no pion ($h^\pm$), one hadron and one pion ($h^\pm\pi^0$), one hadron and two or more pions ($h^\pm \geq 2\pi^0$), while the 3-prong category includes decays with three hadrons and no pion ($3h^\pm$), three hadrons and one or more pions ($3h^\pm \geq 1\pi^0$). The tau rapidity is binned in three bins, $[0, 1]$, $[1, 1.37]$, $[1.52, 2.5]$, which we denote with the numerals 0, 1, 2 respectively. Notice that the transition region between barrel and end-cap $1.37 < |\eta| < 1.52$ is removed from the bins definition. Since the primitive FFs dependence on tau rapidity is neglected, events corresponding to different η bins have been merged into a single inclusive bin.

Figures 3.5 and 3.6 show the yields for data and MC events in the anti-ID subregion for each of the four measurement regions. In particular, Figure 3.5 shows yields for events passing the *Loose* tau ID requirement (pass-ID), while Figure 3.6 shows the same yields for events failing the same ID requirement (anti-ID). Such yields correspond to the event counts $N_{\text{passID}}^{\text{CR,Data}}$, $N_{\text{passID}}^{\text{CR,MC}}$, $N_{\text{antiID}}^{\text{CR,Data}}$, $N_{\text{antiID}}^{\text{CR,MC}}$ in

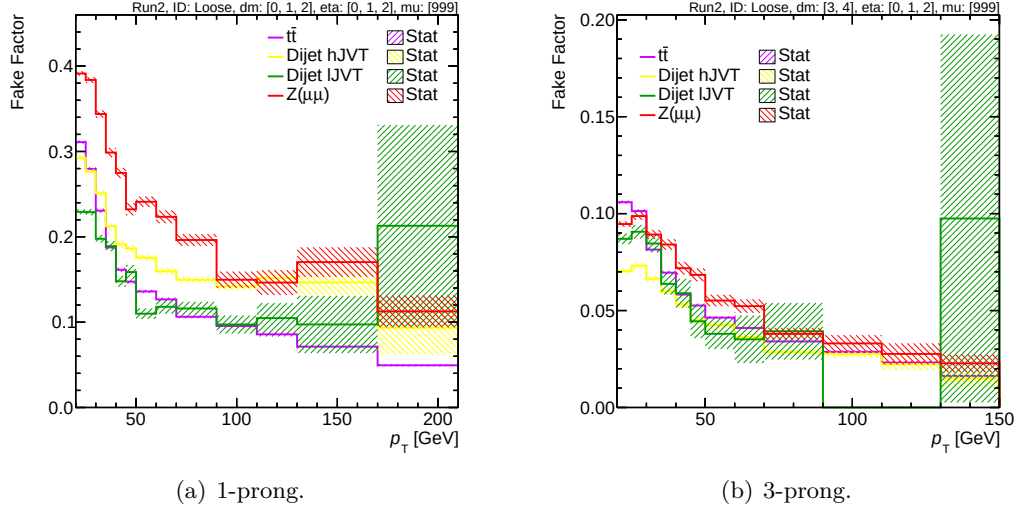


Figure 3.4. Primitive FFs for (a) 1-prong and (b) 3-prong tau decays, measured in the $Z\mu\mu$, MJh, MJl and $t\bar{t}$ regions. The shaded bands display the statistical uncertainty on FFs.

Eq. (3.6). It can be noticed that the real tau contamination is mostly present in the yields of pass-ID subregions, but it is below 10% of the data yield in the large majority of cases. Only in some cases, namely in the high- p_T tails of the distributions in the MJh region, the truth component reaches values up to 30% of the data yield. Instead, in the anti-ID subregions the truth component is negligible, as expected due to the required fail of the ID condition.

All the uncertainty bands in the FFs and events yields plots represent statistical uncertainties evaluated starting from the event counts in each bin and their propagation through the ratios. More detailed information on how to attribute an uncertainty to the FFs evaluated through the FF method will be provided in Section 3.4

3.4 Uncertainty assessment in the Fake Factors method

The extrapolated tau fakes background needs to be accompanied by an estimation of its uncertainty. Several strategies are available, since the uncertainty estimation also depends on the characteristics of the user analysis. The aim of this section is to provide guidelines for such uncertainty estimation, based on the author's experience in the Fake Factors method implementation. Examples of usage of these guidelines will be provided in the validation analyses, presented in Sections 3.5 and 3.6.

According to Eq. (3.5), the extrapolated fakes background will show a total uncertainty which is the combination (i.e. quadrature sum) of three independent sources of uncertainty:

- the *statistical* uncertainty on the extrapolated histogram. The extrapolated fakes background will concretise in an histogram with counts b_i in each of its bins. The usual poissonian uncertainty $\Delta b_i \sim \sqrt{b_i}$ has to be attributed to each

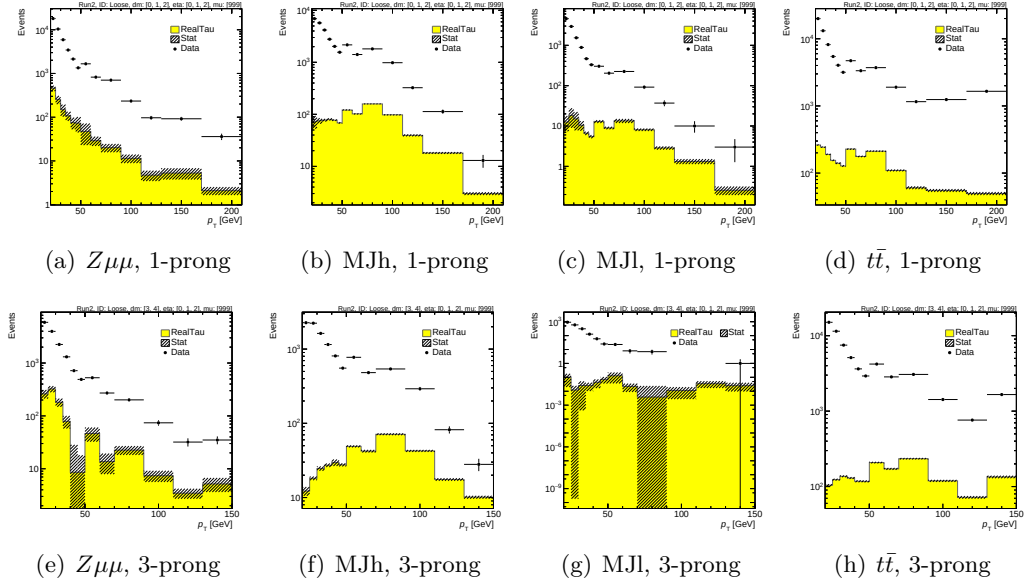


Figure 3.5. Data and MC yields for events passing the *Loose* tau ID requirement in the four measurement regions $Z\mu\mu$, MJh, MJl, $t\bar{t}$, separated in the 1-prong and 3-prong cases. MC yields measure the truth tau component in each region.

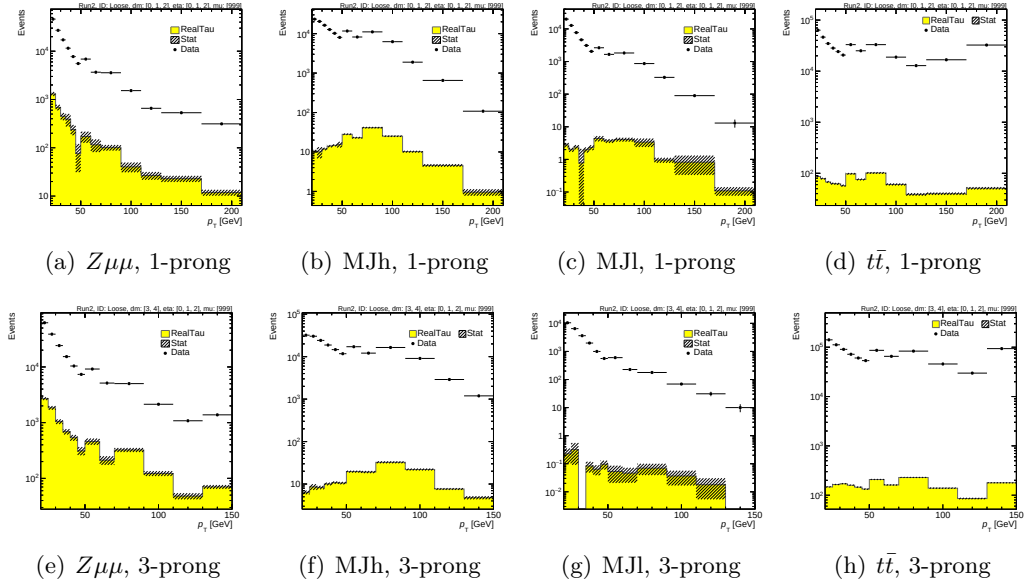


Figure 3.6. Data and MC yields for events *not* passing the *Loose* tau ID requirement in the four measurement regions $Z\mu\mu$, MJh, MJl, $t\bar{t}$, separated in the 1-prong and 3-prong cases. MC yields measure the truth tau component in each region.

bin of the histogram, representing the statistical fluctuations of the bin counts. This uncertainty decreases with the increasing statistics of the background histogram, which is proportional to the events statistics in the SR anti-ID.

- the *systematic* uncertainty associated to the combined Fake Factor FF_{comb} . This FF is not a pure number and is known within an uncertainty $\Delta\text{FF}_{\text{comb}}$ which has to be properly estimated. We will discuss this in the following paragraphs.
- the *modelling* uncertainty associated to the choice of MC generator to perform the truth-subtraction. The events containing true taus (or electrons and muons misidentified as taus) are simulated via MC and removed. The choice of the MC generator to be used for this purpose is arbitrary, and different generators could lead to different results. Hence, a modelling uncertainty should be added representing the potential variability of the truth-subtraction, due to a change of choice of MC generator.

The statistical uncertainty on the extrapolated background is taken into account attributing to bins a band representing the poissonian fluctuation of their content. The modelling uncertainty associated to the choice of MC generators is usually small, since the truth component yields are typically sub-dominant. Hence, we will neglect this uncertainty component in what follows.

Let's then discuss how to attribute an uncertainty to the combined Fake Factors, which is a non-negligible component to be carefully estimated. According to FF_{comb} definition in Eq. (3.8) and recalling that the fractions μ_x are evaluated through the template fit in Eq. (3.9) we can recognise four uncertainty sources contributing to the systematic uncertainty on FF_{comb} :

1. uncertainty originating from the limited statistics of the fitted data template $h_{\text{SR antiID}}$. The statistical uncertainty of the fitted histogram generates an uncertainty on the fit parameters μ_x , which is propagated to FF_{comb} ;
2. uncertainty originating from the limited statistics of the primitive templates h_x . Also the primitive templates used to define the fitting formula in Eq. (3.9) are subject to statistical fluctuations. This effect should enlarge the uncertainty of the fractions μ_x (and therefore also the final uncertainty on FF_{comb}).
3. uncertainty originating from statistical uncertainty on the primitive FFs, FF_x . The primitive FFs have an associated uncertainty ΔFF_x , resulting from propagation of templates statistics in the measurement regions across the ratio in Eq. (3.6). This uncertainty is also propagated to FF_{comb} .
4. uncertainty on FF_{comb} originated from the neglected dependence of the primitive FFs on variables other than p_T , η and decay mode.

The first three sources of uncertainties have a statistical nature (i.e. they decrease with increasing statistics of the templates). They are statistical sources for the systematic uncertainty on FF_{comb} . The fourth source is intrinsically systematic depending from a reductive assumption and cannot be decreased with increasing statistics. We discuss in the following sections how to estimate these four uncertainty components.

3.4.1 Statistical sources of uncertainty on FF_{comb}

Let's first focus on the first three components of the FF_{comb} uncertainty (namely, components (1) (2) (3) in the previous list), which originate from limited statistics.

Baseline procedure based on uncertainty propagation

The baseline strategy to estimate and combine the uncertainties on FF_{comb} coming from statistical sources is to use the standard error propagation formula. Starting from FF_{comb} definition in Eq. (3.8) we can write

$$\begin{aligned} \Delta \text{FF}_{\text{comb}}^2 &= \sum_i \left(\frac{\partial \text{FF}_{\text{comb}}}{\partial \text{FF}_i} \right)^2 \text{Var} [\text{FF}_i] \\ &+ \sum_{i,j} \left(\frac{\partial \text{FF}_{\text{comb}}}{\partial \mu_i} \right) \left(\frac{\partial \text{FF}_{\text{comb}}}{\partial \mu_j} \right) \text{Cov} [\mu_i, \mu_j] \end{aligned} \quad (3.23)$$

where the i index runs over the FF measurement regions $Z\mu\mu$, MJh, MJl, $t\bar{t}$ and we have used that primitive FFs are uncorrelated (as they are measured in independent regions). Evaluating the partial derivatives and expliciting the FFs variance we obtain

$$\Delta \text{FF}_{\text{comb}}^2 = \sum_i \mu_i^2 \Delta \text{FF}_i^2 + \sum_{i,j} \text{FF}_i \text{FF}_j V_{ij} \quad (3.24)$$

where we denoted with V_{ij} the covariance matrix of the fitted fractions μ_x .

For the sake of clarity we explicit that the source (1) of uncertainty has been taken into account and is encoded in the second term of Eq. (3.24), namely in the covariance matrix, which is evaluated via the template fit. Similarly source (3) of uncertainty has been taken into account and is encoded in the first term of Eq. 3.24. To account for source (2) some nuisance parameters λ can be introduced in the template fit representing the statistical fluctuations in the bins of the primitive templates. These nuisance parameters will decrease the constraining power of the fit, hence will increase the elements of the covariance matrix V_{ij} . Also the source (2) of uncertainty is therefore encoded in second term of Eq. 3.24.

A proposal for an alternative and faster procedure: uncertainty assessment based on variance sampling

The procedure presented above can be complex to implement from a technical point of view. This is because the implementation of the FF method in a real analysis requires to run several template fits, and some of them can show singularities in the covariance matrix. Moreover, the addition of nuisance parameters to account for the finite statistics of the primitive templates increases a lot the fit complexity. Such complexity can be an overkill, especially for physics analyses in which the uncertainty on the fakes background plays a sub-leading role in the full set of experimental uncertainties.

I propose here an alternative method, which can be used to sample the uncertainty $\Delta \text{FF}_{\text{comb}}$ via multiple fit runs. The proposed procedure is practically a translation to this context of the Bootstrap method for the uncertainties assessment, which has

been described by the ATLAS Collaboration in Ref. [142] and is typically used to evaluate the statistical uncertainties of the unfolded distributions in Standard Model precision measurements.

I give the details of the proposed procedure in what follows. For simplicity, let's restrict to the most simple case in which we have only two sources of tau fakes: quark- and gluon-originated jets. In this hypothesis the combined FF expression in Eq. (3.8) reduces to

$$\text{FF}_{\text{comb}} = \mu_q \text{FF}_q + \mu_g \text{FF}_g , \quad (3.25)$$

while the fit model in Eq. (3.9) reduces to

$$h_{\text{comb}} = \mu_q h_q + \mu_g h_g , \quad (3.26)$$

and is used to fit the data histogram in the SR anti-ID, $h_{\text{SR antiID}}$.

To account for the uncertainty originating from the statistics of the data template in the SR anti-ID we generate N variations of the $h_{\text{SR antiID}}$ histogram. Each $h_{\text{SR antiID}}^i$ histogram ($i = 1, \dots, N$) is generated varying randomly each bin content, according to a poissonian distribution with parameter equal to the bin content of the nominal histogram. N template fits are performed, each one corresponding to a different $h_{\text{SR antiID}}^i$ histogram, with the model

$$h_{\text{comb}}^i = \mu_q^i h_q + \mu_g^i h_g , \quad (3.27)$$

The resulting coefficients μ_q^i, μ_g^i are used to obtain N values of the combined FF

$$\text{FF}_{\text{comb}}^i = \mu_q^i \text{FF}_q + \mu_g^i \text{FF}_g . \quad (3.28)$$

The standard deviation of these values provides a sampling of the uncertainty coming from source (1)

$$\Delta \text{FF}_{\text{comb}}^{(1)} = \sqrt{\frac{1}{N} \sum_i \left(\text{FF}_{\text{comb}}^i - \text{FF}_{\text{comb}} \right)^2} \quad (3.29)$$

To account for the uncertainty originating from the limited statistics of the primitive templates (i.e. source (2)) a similar procedure is used. Two series of M variated templates are generated, h_q^i, h_g^j , with $i, j = 1, \dots, M$. $2M$ template fits are performed with the models

$$\begin{aligned} h_{\text{comb}}^i &= \mu_q^i h_q^i + \mu_g^i h_g , \\ h_{\text{comb}}^j &= \mu_q^j h_q + \mu_g^j h_g^j , \end{aligned} \quad (3.30)$$

all of them referred to the nominal template in the SR anti-ID $h_{\text{SR antiID}}$. Using expressions similar to Eqs. (3.28) and (3.29) the dispersion $\Delta \text{FF}_{\text{comb}}^{(2)}$ is evaluated. Notice that $\Delta \text{FF}_{\text{comb}}^{(2)}$ will be the quadrature sum of two independent contributions, each one referred to the respective set of variations of the two primitive templates.

Finally, to account for the uncertainty originating from primitive FFs uncertainty (i.e. source (3)) we simply evaluate the impact on FF_{comb} of the variations on primitive FFs, using nominal values of the fractions μ_x .

$$\Delta \text{FF}_{\text{comb}}^{(+)} = \mu_q \Delta \text{FF}_q^{(+)} + \mu_g \Delta \text{FF}_g^{(+)} \quad (3.31)$$

where the apex (+) indicates the positive variation. A similar expression holds for the negative variation. Symmetrising the two variations we obtain

$$\Delta\text{FF}_{\text{comb}}^{(3)} = \frac{\Delta\text{FF}_{\text{comb}}^{(+)} + \Delta\text{FF}_{\text{comb}}^{(-)}}{2} \quad (3.32)$$

The total uncertainty is calculated combining in quadrature the three contributions $\Delta\text{FF}_{\text{comb}}^{(1)}$, $\Delta\text{FF}_{\text{comb}}^{(2)}$, $\Delta\text{FF}_{\text{comb}}^{(3)}$ and is equivalent to what is provided by Eq. (3.24). The actual values of the M , N parameters have to be optimised within the user analysis. To give a reference, acceptable values, optimising both the processing time and the precision of the samplings are $M = O(10)$ and $N = n \times M$, where n is the number of primitive templates used.

3.4.2 Systematic sources of uncertainty on FF_{comb}

Let's now discuss the last component of the FF_{comb} uncertainty, denoted as (4) in the list in Section 3.4. This uncertainty is due to the fact that we are considering primitive FFs as depending only on tau p_T , $|\eta|$ and decay mode, while in general they could show dependence also with respect to other variables. Due to these neglected dependences the FFs are averaged across the bins of such additional variables, and this induces an additional component of uncertainty. Examples of variables with respect to which the primitive FFs can show a dependence are:

- the number of interaction vertices per bunch crossing μ , representing pile-up activity;
- the ratio between the transverse momentum of the tau to that of the tau seed jet $p_T^\tau/p_T^{\text{seed jet}}$, quantifying how much the energy is located in the inner part of the fake-tau structure;
- the energy fraction deposited in the electromagnetic calorimeter, f_{EM} , probing the electromagnetic fraction of the fake-tau decay products.

These variables can indirectly influence the probability of a jet of being misidentified as a tau, and therefore can modify the FFs values.

To attribute an uncertainty to FF_{comb} representing these effects one can split into sub-bins each bin in $(p_T \times |\eta| \times \text{dm})$ phase space, in which the FFs are assumed constant. In each of the sub-bins, the combined FFs can be evaluated and an uncertainty component $\Delta\text{FF}_{\text{comb}}^{(4)}$ is attributed equal to the difference between the FFs in the sub-bins and the nominal FFs in the original bins. This procedure is repeated for all the variables inducing neglected FFs variability, and all the corresponding uncertainties are summed in quadrature. We explicitly notice that the aforementioned list of variables is not exhaustive and the dependence with respect to other variables has to be investigated specifically in each user analysis and cross-checked via closure tests in the validation regions.

3.5 Validation with single-tau final state events

The Fake Factors method needs to be validated in order to be considered reliable for its usage in physics analyses. The most simple way to provide a validation is to

estimate the fakes background in some exemplary analyses based on regions enriched in fake taus. We report here two validation analyses, based on $\mu + \tau$ and $\gamma + \tau$ final states. In both cases the analysis selection has been constructed to select processes in which real taus are not present in the final state, hence the required taus are very likely fake taus. For both validation analyses we are probing a single-tau final state, hence we are validating the FF method in the case in which there is only one single fake tau.

Both the $\mu + \tau$ and $\gamma + \tau$ analyses are performed using the dataset described in Section 3.3.1 and applying the events pre-selection and objects definitions reported in Section 3.3.2 with the only exception that cuts for the real taus suppression are not applied. The q-/g-/b-/p- fractions for the combined FFs evaluation are calculated via a template fit exploiting the BDT-based q/g tagger score described in Ref. [120] as discriminating variable. This score is computed starting from the characteristics of the nearest hadronic jet matched with the fake tau. The matching condition is based on the angular distance between the two objects

$$\Delta R(j, \tau) = \sqrt{(\eta_j - \eta_\tau)^2 + (\phi_j - \phi_\tau)^2}, \quad (3.33)$$

and the two objects are considered matched if $\Delta R < 0.4$.

3.5.1 The $\mu + \tau$ validation analysis

Event selection

The $\mu + \tau$ analysis is based on the selection of final states with one true muon and one fake tau. Single muon triggers are required as baseline events selection, with thresholds depending on the year of data-taking. Exactly one muon is required, which has to verify the *Medium* ID working point and must have $p_T > 27.3$ GeV. Moreover, the muon is required to be trigger matched. Events with electrons are vetoed, to avoid contamination from this type of leptons. The presence of one tau is required, having the same charge of the muon. The choice of having the muon and the tau with the same charge ensures that the tau is most likely a fake. In fact, this requirement rejects all events in which a $\mu\tau$ final state could originate from a true di-tau couple, with one tau decaying in the muonic channel. Most likely, the selected events are originating from the $Z + \text{jets}$ production, where the Z boson decays into a pair of muons, one muon is lost and one jet is misidentified as a fake tau lepton. The events selected in the analysis signal region (SR) are split into the SR pass-ID and SR anti-ID according to whether the tau verifies or not the *Loose* identification criteria. A summary of the discussed selections is provided in Table 3.4.

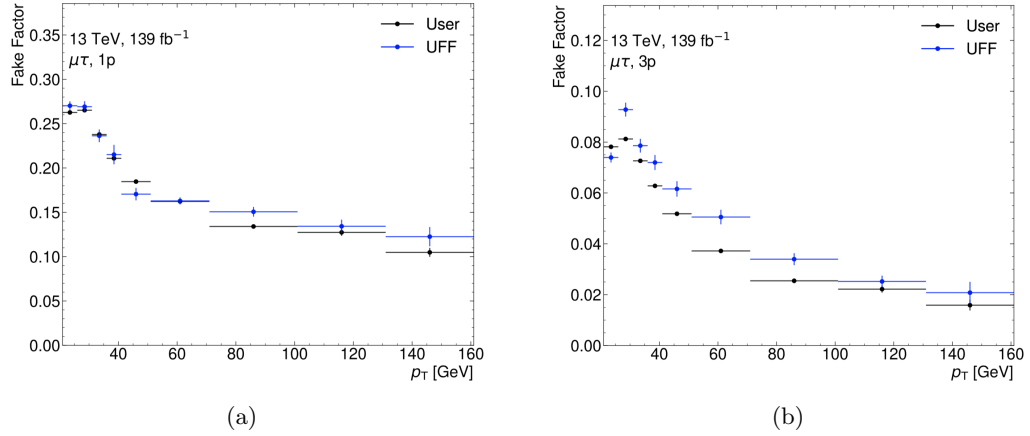
Combined Fake Factors and template fits

The combined FFs are evaluated using the FF method, as described in Section 3.2. FFs are computed as a function of p_T , separating the decay modes into the 1-prong and 3-prong categories, and are assumed constant with respect to the tau rapidity η . Figure 3.7 shows the resulting FFs for both the 1-prong and 3-prong decay modes.

Figure 3.8 shows instead the q/g tagger score templates involved in the fit. The data template in the SR anti-ID and the post-fit combined template are compared,

Table 3.4. Summary of the $\mu + \tau$ analysis selections for events in the signal region (SR).

$\mu + \tau$ analysis	
Trigger	single muon
Muon	exactly one muon with <i>Medium</i> ID $p_T > 27.3$ GeV trigger matched
Tau	exactly one tau same charge of the muon
Electrons	veto

**Figure 3.7.** FFs for the $\mu + \tau$ analysis SR, evaluated with the FF method (UFF) and via a direct ratio (user). The FFs are provided in bins of p_T for (a) 1-prong decays, (b) 3-prong decays.

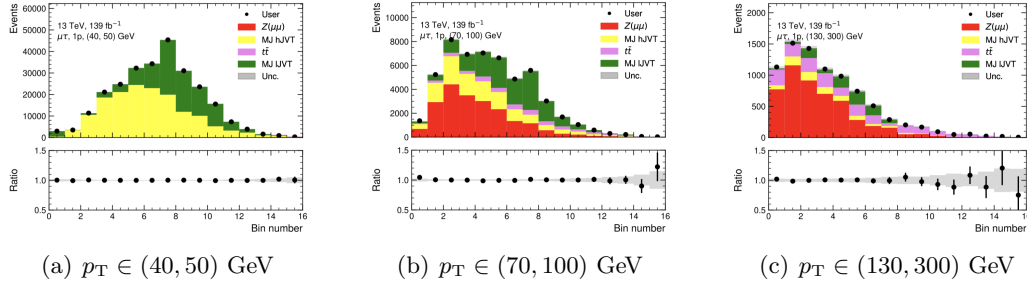


Figure 3.8. Comparison of data and the post-fit combined templates in the $\mu + \tau$ analysis SR anti-ID. The colored areas represent the primitive templates multiplied by the post-fit q -/g-/b-/p-fractions. The distributions refer to fits in different bins of p_T for the 1-prong case.

in some exemplary p_T bins and for the 1-prong case. The colored areas filling the combined template are equal to the primitive templates, scaled by the post-fit q -/g-/b-/p- fractions. As can be noticed from the relations between the areas, at low p_T the MJl and MJh templates play the leading role in the combination, manifesting that the majority of fake taus are originating from misidentified pile-up jets and gluon jets. Conversely, at high p_T the $Z\mu\mu$ template is dominant, hence the majority of fake taus are originating from quark-jets.

The uncertainty evaluation for the FFs follows the guidelines provided in Section 3.4. In particular, the uncertainty originating from the SR anti-ID statistics as well as the primitive FFs uncertainty are taken into account, and are evaluated using the propagation formula in Eq. (3.24). Instead, the uncertainty originating from primitive templates statistics as well as the systematic uncertainty generated from neglected FFs dependence on other variables are not considered here.

Since this is a validation analysis the SR is unblinded and therefore also a “direct” calculation of FFs is possible, applying the definition as reported in Eq. (3.6). Figure 3.7 shows also a comparison between the FFs calculated with the FF method and the ones calculated as a direct ratio. A fair agreement is observed between the two within the respective uncertainty bands, even if we notice the presence of a systematic shift which has to be investigated. We also notice that the uncertainties associated with the FFs evaluated with the FF method are larger than the ones of the FFs evaluated via direct ratio, pointing to the necessity to further improving the uncertainties estimation strategy.

Results

The fakes background extrapolation from the SR anti-ID to the SR pass-ID is performed, following the expression in Eq. 3.5 and using the evaluated FFs. The fakes background is stacked with the MC prediction for the other backgrounds involved in the analysis and compared with the data. Figure 3.9 shows the spectra for the tau and muon p_T and η variables. Data show good agreement with the background predictions within the uncertainty band attributed to the background. Such uncertainty band is obtained, following the guidelines in Section 3.4, by combining the statistical uncertainty due to the limited yields in the SR pass-ID

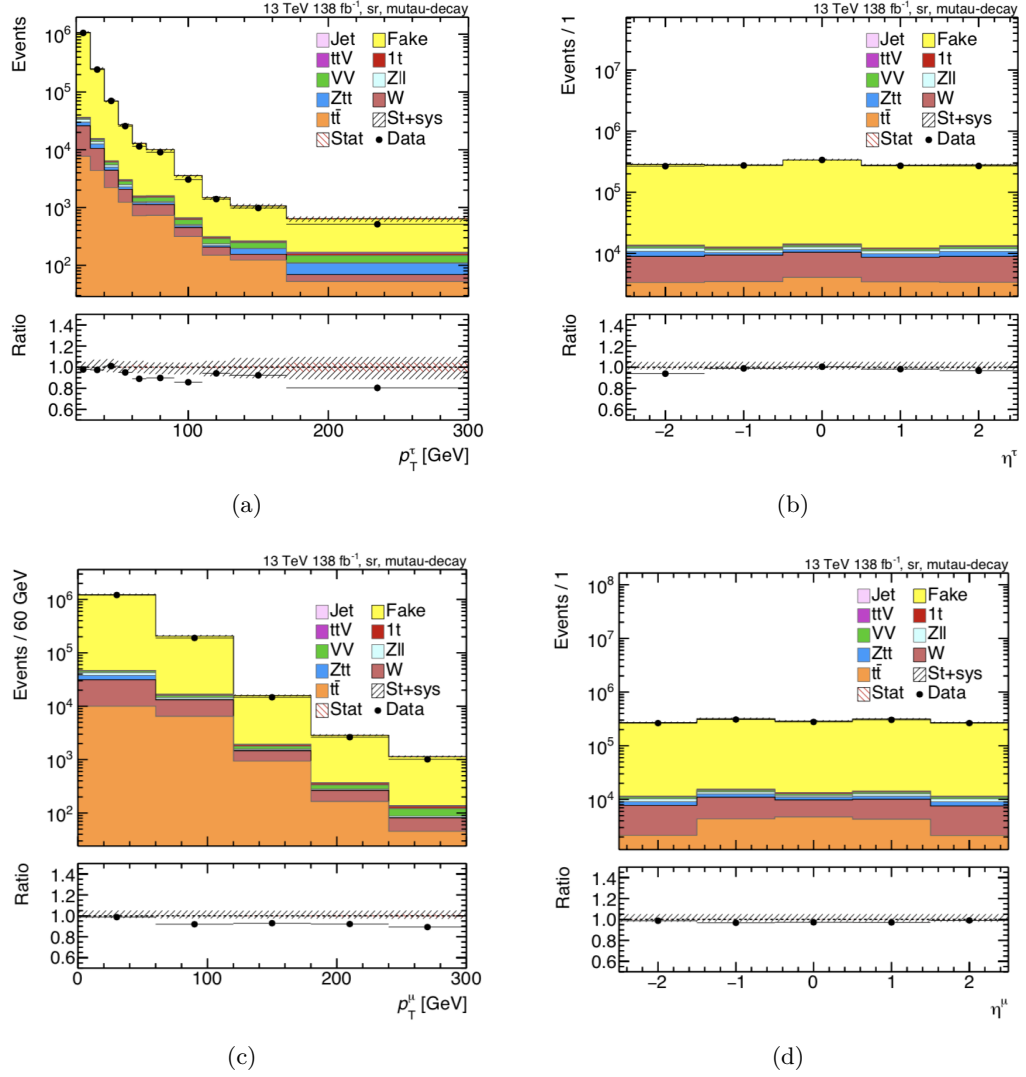


Figure 3.9. Comparison of data with the total predicted backgrounds in the $\mu + \tau$ analysis. Distributions are shown for the (a) tau p_T , (b) tau η , (c) muon p_T , (d) muon η .

Table 3.5. Summary of the $\gamma + \tau$ analysis selections for events in the signal region (SR).

$\gamma + \tau$ analysis	
Trigger	single photon
Photon	exactly one photon with $p_T > 145$ GeV $\Delta R > 0.2$ between photon and tau $\Delta R > 0.5$ between tau and nearest jet
Light leptons	veto
Tau	exactly one tau

together with the uncertainty on the combined FFs. A slight overestimation of the total background can be noticed, caused by a $\sim 10\%$ overestimation of the fakes background. We notice that such discrepancy reflects the slight difference present in the comparison between the FFs obtained with the “direct” calculation and the ones obtained via the FF method (see Figure 3.7). Therefore, the background estimate slight discrepancy is most likely attributed to a limited evaluation of the combined FFs, which is not completely covered by the considered systematic uncertainties.

3.5.2 The $\gamma + \tau$ validation analysis

Events selection

The $\gamma + \tau$ analysis is based on the selection of final states with one true photon and one fake tau. A single photon trigger is required, with a constant threshold, independent of the year of data-taking. The presence of exactly one photon is needed, with a transverse momentum $p_T > 145$ GeV. The photon should have angular separation $\Delta R > 0.2$ from the final state tau, while the tau should have $\Delta R > 0.5$ from the nearest jet. These requirements ensure that the same energy clusters are not shared in the reconstruction between the photon, the tau and hadronic jets. Events with electrons and muons are vetoed, to avoid contamination from these types of leptons. The selections of this analysis are constructed to target events generated in QCD activity. Most likely then, the selected tau leptons will be fake taus originating from misidentified gluon jets. The SR is further separated in SR pass-ID and SR anti-ID, according to whether the reconstructed tau passes or not the *Medium* identification criteria. A summary of all the aforementioned cuts is given in Table 3.5.

Combined Fake Factors and template fits

The combined FFs are evaluated using the FF method, and are computed as a function of p_T , separating the decay modes into the 1-prong and 3-prong categories. As in the $\mu + \tau$ validation analysis, FFs are assumed constant with respect to the tau rapidity η . Figure 3.10 displays the resulting FFs, for both 1-prong and 3-prong tau decays. The uncertainties associated with the FFs follow the guidelines discussed in Section 3.4 and include the uncertainty originating from the SR anti-ID template statistics and the primitive FFs uncertainty, evaluated using Eq. 3.24. FFs evaluated through the “direct” calculation are also provided in Figure 3.10, and show compatibility with the ones calculated via the FF method.

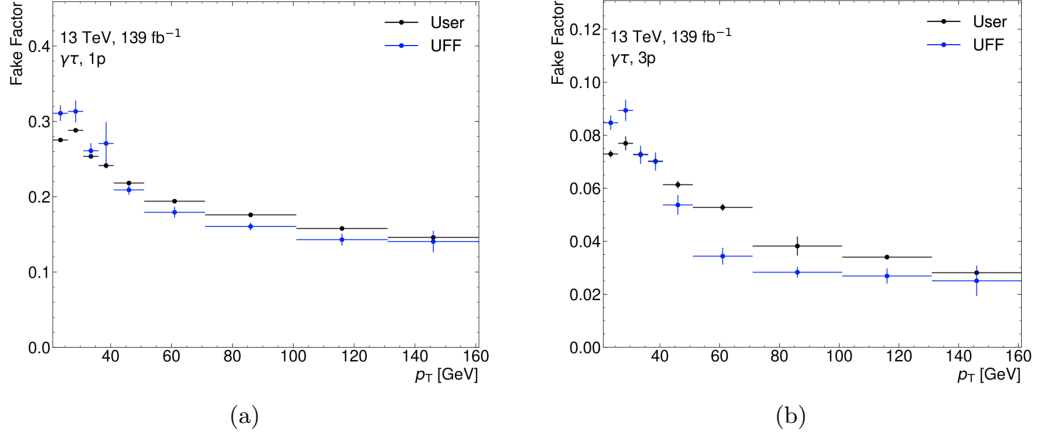


Figure 3.10. FFs for the $\gamma + \tau$ analysis SR, evaluated with the FF method (UFF) and via a direct ratio (user). The FFs are provided in bins of p_T for (a) 1-prong decays, (b) 3-prong decays.

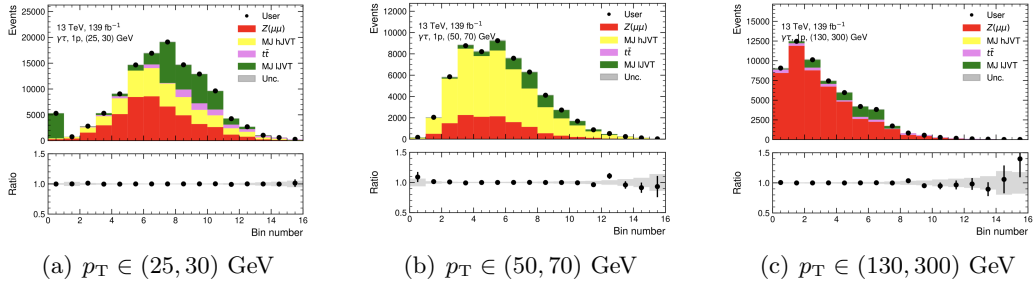


Figure 3.11. Comparison of data and the post-fit combined templates in the $\gamma + \tau$ analysis SR anti-ID. The colored areas represent the primitive templates multiplied by the post-fit q-/g-/b-/p-fractions. The distributions refer to fits in different bins of p_T for the 1-prong case.

Figure 3.11 shows the templates of the q/g tagger score used in the fits, referred to some particular p_T bins and 1-prong decays. It can be noted how the MJl and MJh templates are playing the leading role in the combinations at low and intermediate p_T values, meaning that the majority of fake taus are originating from pile-up and gluon jets in this p_T range. At high p_T values, instead, the $Z\mu\mu$ template gives the leading contribution, hence quark-jets generate the majority of fake taus.

Results

Figure 3.12 shows the results of the background extrapolation in the SR pass-ID, using the FFs evaluated for the $\gamma + \tau$ analysis. Agreement between data and the total background prediction is achieved in the large majority of the phase space, within the uncertainty attributed to the background. It is worth noting some localised discrepancies: background yields are overestimated at low p_T and underestimated at high p_T . Similarly to the $\mu + \tau$ validation analysis, this discrepancy reflects the difference between the FFs obtained via the FF method and the ones

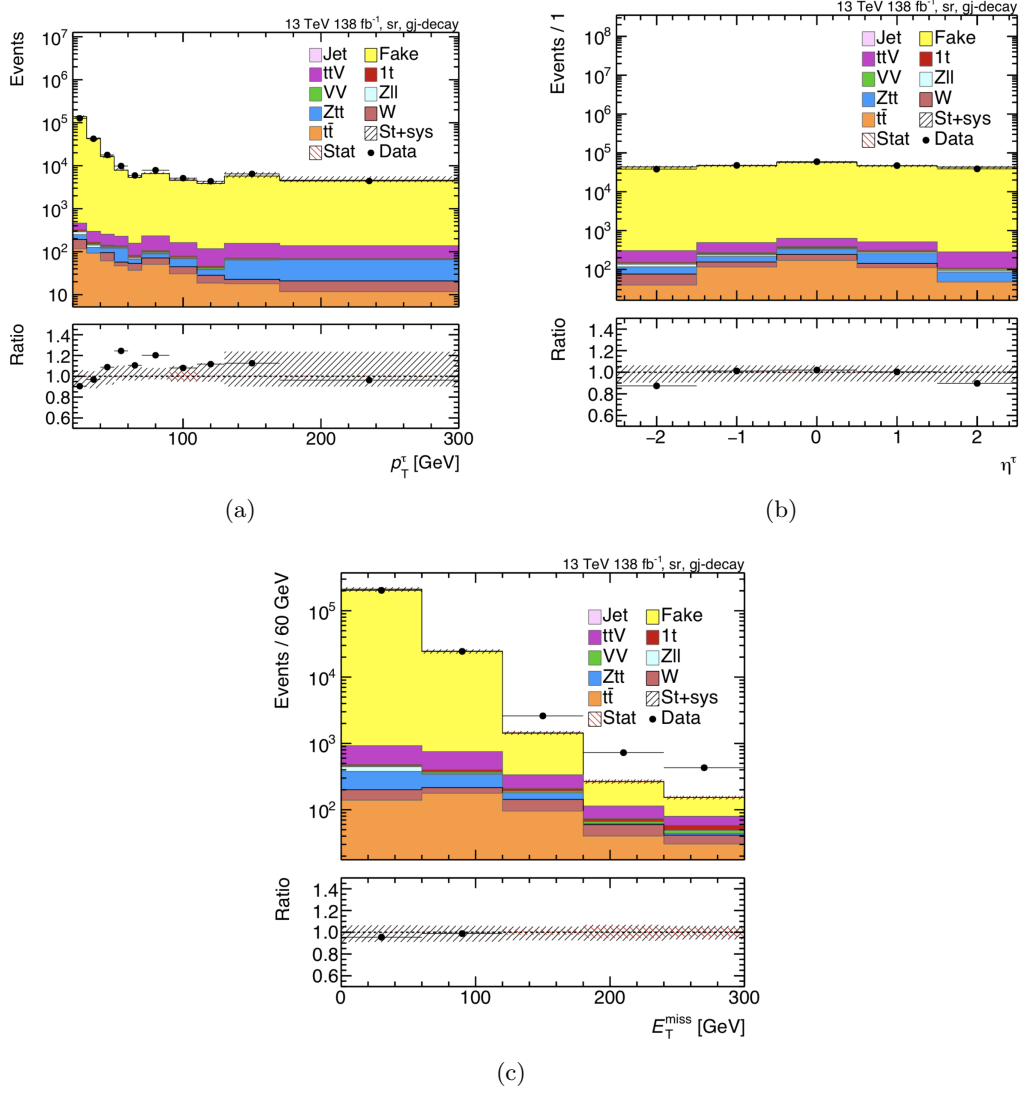


Figure 3.12. Comparison of data with the total predicted backgrounds in the $\gamma + \tau$ analysis. Distributions are shown for (a) tau p_T , (b) tau η , (c) missing transverse momentum.

evaluated through the “direct” calculation (see Figure 3.10), and can therefore be attributed to the limited precision of the combined FFs calculation. Some mismodelling is also evident in the missing transverse momentum distribution, shown in Figure 3.12(c). Recalling that true taus generate missing momentum through their decays in neutrinos, while fake tau in general do not generate E_T^{miss} , we can attribute this mismodelling to an incorrect estimate of the subtracted true taus component via MC simulation.

3.6 Validation with di-tau final state events

This section presents the author’s personal contribution in the validation of the FF method with di-tau final states. This validation is based on the High Mass Drell-Yan (HMDY) analysis, performed by ATLAS to search for leptoquark particles in the high mass tail of the Drell-Yan process with tau leptons, and presented in this thesis in Chapter 4. A validation region is constructed starting from the analysis signal region and requiring that the two tau leptons in the final state have the same electric charge, instead of opposite charge. This requirement ensures that at least one of the two taus is a fake, since couples of real taus generated from a neutral initial state should necessarily have opposite charge. It is worth mentioning that the validation with di-tau final states is different and complementary to the validation with single tau final states, provided through the $\mu + \tau$ and $\gamma + \tau$ analyses in Section 3.5. In the di-tau case, in fact, we are validating the combinatorial expression for background extrapolation, provided in Eq. 3.12, whose correctness could not be demonstrated with single tau final states.

The dataset and the analysis objects selections for this validation are the same as in HMDY analysis, and are described in Section 4.3 and Section 4.4 respectively. Fake taus originating from b -jets are neglected in this study, hence only q -/ g -/ p -jets will be considered as possible sources of fake taus. The q -/ g -/ p -fractions for the combined FFs evaluation are determined in template fits, performed on the tau jet width variable, which provides a performance comparable to the q/g tagger score used for the $\mu + \tau$ and $\gamma + \tau$ analyses. This validation is performed both in the fully hadronic channel, in which both final state taus decay hadronically, and in the semi-leptonic channel, in which one tau decays leptonically in e or μ and the other decays hadronically.

3.6.1 Validation in the fully hadronic channel

Events selection

The validation region (VR) for the fully hadronic channel is defined following exactly the same requirements used for the corresponding High Mass Drell-Yan analysis signal region, with the only exception that the two taus should have the same electric charge, instead of opposite charge. All selection criteria are described in detail in Section 4.5 and listed in Table 4.5.

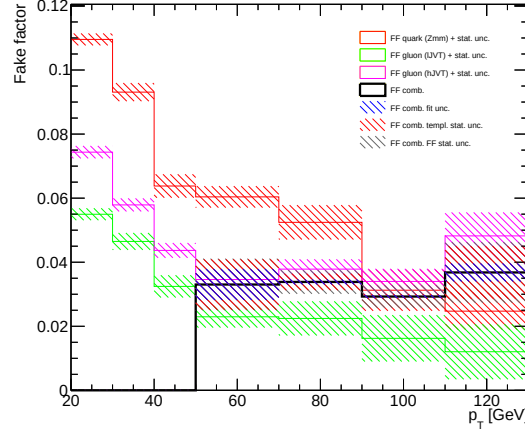


Figure 3.13. FFs for the High Mass Drell-Yan analysis VR in the fully hadronic channel. FFs are provided as a function of p_T , for 1-prong decays and $|\eta| \in [0, 1]$. The primitive FFs are also displayed.

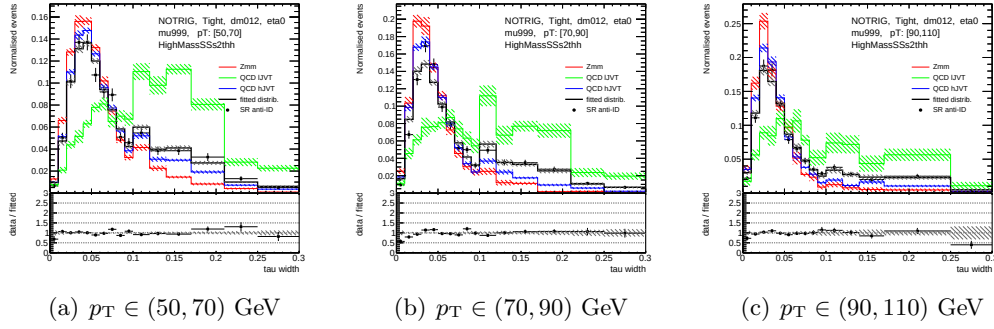


Figure 3.14. Comparison of data and the post-fit combined template in the High Mass Drell-Yan analysis VR anti-ID, for the had-had channel. The distributions refer to fits in different p_T bins for $|\eta| \in [0, 1]$ and 1-prong decays. The primitive templates are also displayed.

Combined Fake Factors and template fits

The combined FFs are evaluated following the procedure described in Section 3.2.2. FFs are computed as a function of tau p_T separating the 1-prong and 3-prong decay modes and using three bins of tau rapidity $|\eta| \in [0, 1]$, $[1, 1.37]$, $[1.52, 2.5]$. Figure 3.13 shows the resulting combined FFs, compared to the corresponding primitive FFs, as a function of p_T for the particular case of 1-prong decays with $|\eta| \in [0, 1]$.

The FFs uncertainty is calculated following the guidelines described in Section 3.4. The alternative approach based on variance sampling described in Section 3.4.1 has been followed. In particular, the uncertainty due to the limited statistics of the anti-ID data template has been taken into consideration, generating $N = 30$ variations of the nominal template (see Eq. 3.27) and the uncertainty originating from primitive templates statistics has been evaluated via $M = 10$ variations of each primitive template (see Eq. 3.30). The N, M values have been determined through several

attempts, optimising jointly the processing time and the samplings precision. The uncertainty on the primitive FFs has also been taken into account. The error bands in Figure 3.13 show separately all these three components.

Figure 3.14 shows instead the data tau width templates, overlaid with the fitted combined templates and pre-fit primitive templates, for some p_T bins and the choice of 1-prong decays with $|\eta| \in [0, 1]$.

Results

The fakes background extrapolation from the anti-ID to the pass-ID region has been done, using the combinatorial formula reported in Eq 3.12: the event yields with first, second or both tau fakes have been considered and combined after being weighted for the proper FF. Figure 3.15 shows the comparison between data and the total background prediction for the di-tau invariant mass spectrum $m_{\tau\tau}$ as well as for the leading tau p_T and η . The uncertainty on the total background prediction accounts for the statistical uncertainty on the event yields in the pass-ID region, as well as the total uncertainty on the FFs. The systematic uncertainty band also includes all the experimental systematic effects considered in the HMDY analysis, for which details are given in Section 4.7. As can be seen from direct inspection of the plots the total predicted background correctly agrees with data within the total uncertainty band, providing a validation of the fakes background for the HMDY analysis and also a confirmation of the correctness of the combinatorial expression for di-tau final states in Eq. 3.12

3.6.2 Validation in the semi-leptonic channel

Events selection

Also for the semi-leptonic channel, selection requirements are the same as the ones used in the High Mass Drell-Yan analysis signal region, with the exception of changing the sign of the charge product of the two final state taus. In this channel final states constituted by one electron or one muon in association with one hadronic tau are selected. The electron (muon) is a true light-lepton originating from the leptonic tau decay in the electronic (muonic) channel, while the reconstructed hadronic tau is most likely a fake, due to the same charge requirement. A detailed description of the events selection is provided in Section 4.5 and Table 4.5.

Combined Fake Factors and template fits

The combined FFs are evaluated following the same procedure as the fully hadronic channel. The same separation in tau p_T bins is adopted as well as the categorisation in 1-prong and 3-prong decays and the separation in tau rapidity bins $|\eta| \in [0, 1]$, $[1, 1.37]$, $[1.52, 2.5]$. FFs are evaluated separately for the e-had and μ -had channel, as shown in Figure 3.16, which is reporting results for the particular choice of 1-prong decays and $\eta \in [0, 1]$.

The uncertainty on the FFs is evaluated exactly as in the fully hadronic channel, using the approach based on variance sampling discussed in Section 3.4.1 and

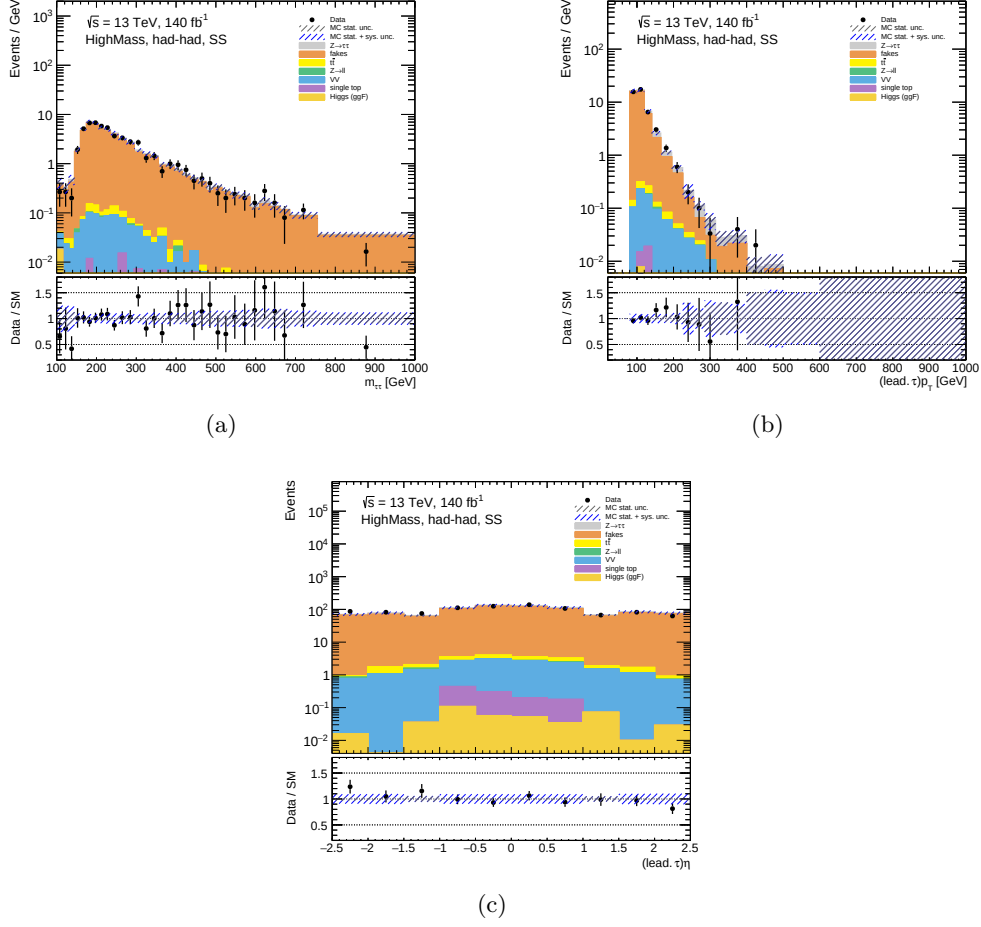


Figure 3.15. Comparison of data with the total predicted background in the High Mass Drell-Yan analysis VR, for the had-had channel: (a) $m_{\tau\tau}$, (b) leading tau p_T , (c) leading tau η .

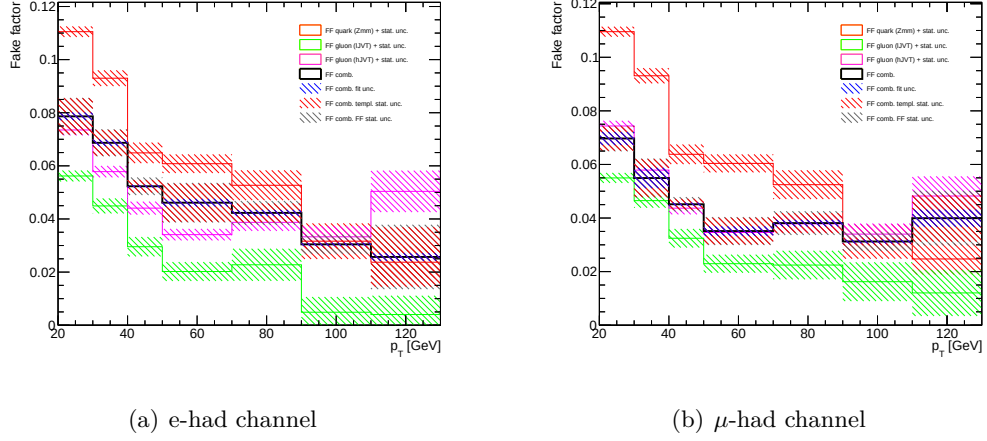


Figure 3.16. FFs for the High Mass Drell-Yan analysis VR in the semi-leptonic channel. FFs are provided as a function of p_T , for 1-prong decays and $|\eta| \in [0, 1]$. The primitive FFs are also displayed.

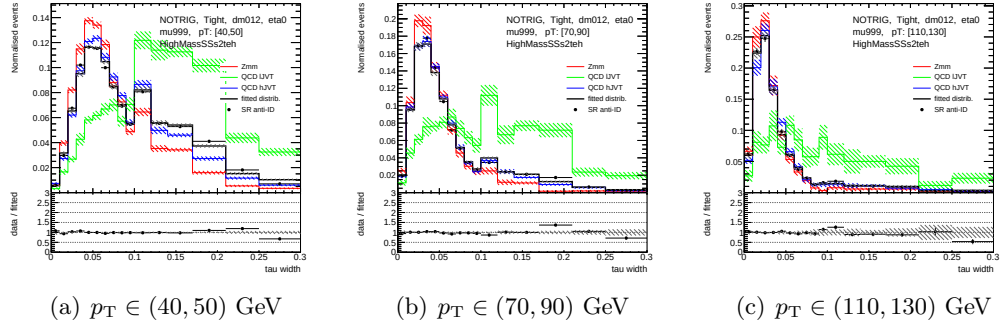


Figure 3.17. Comparison of data and the post-fit combined template in the High Mass Drell-Yan analysis VR anti-ID, for the e-had channel. The distributions refer to fits in different p_T bins for $|\eta| \in [0, 1]$ and 1-prong decays. The primitive templates are also displayed.

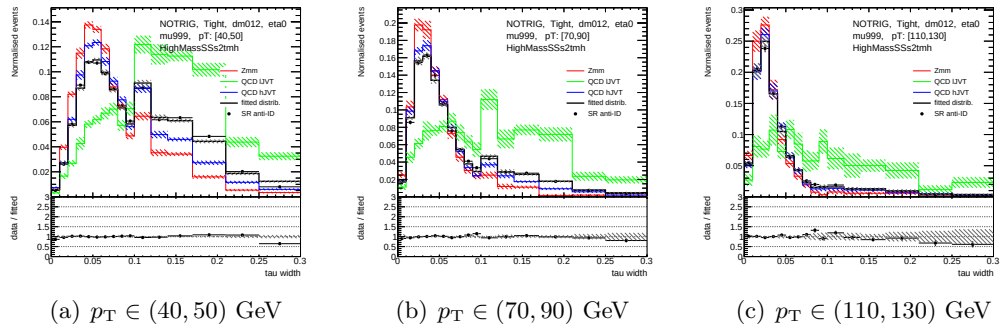


Figure 3.18. Comparison of data and the post-fit combined template in the High Mass Drell-Yan analysis VR anti-ID, for the μ -had channel. The distributions refer to fits in different p_T bins for $|\eta| \in [0, 1]$ and 1-prong decays. The primitive templates are also displayed.

considering the usual three components: uncertainty on the anti-ID data templates, uncertainty on the primitive templates, uncertainty on the primitive FFs.

A selection of templates involved in the fit for FFs determination is shown in Figures 3.17 and 3.18, reporting anti-ID SR data, combined and primitive templates for the e-had and μ -had channels respectively. In both cases, distributions are shown in some bins of tau p_T , for the particular choice of 1-prong decays and $|\eta| \in [0, 1]$.

Results

In the semi-leptonic channel one of the two final state taus decays into an electron or a muon before interacting with the detector. Hence, the di-tau final state is effectively reconstructed by the ATLAS detector as a $e + \tau$ or a $\mu + \tau$ final state, for the e-had and μ -had channels respectively. For this reason, in the semi-leptonic channel it is not necessary to use the combinatorial expression in Eq. 3.12, but it is enough to apply the simple extrapolation reported in Eq. 3.5 where the anti-ID requirement refers to the only available hadronic tau. The uncertainty on the extrapolated background is evaluated, similarly as for the fully hadronic channel, as the combination of the statistical uncertainty associated to the yields in the pass-ID region and the uncertainty on the FFs.

Data versus total predicted background comparisons are provided in Figures 3.19 and 3.20 for the e-had and μ -had channels respectively. It can be noticed that a very good agreement is achieved in the μ -had channel, showing excellent compatibility between data and the total background in both $m_{\mu\tau}$ and tau η distributions. Instead, a $\sim 10\%$ discrepancy is present in the e-had channel, which is almost flat in $m_{e\tau}$ and tau η distributions. However, we notice that the total predicted background yields in the e-had channel in Figure 3.19 show a fair agreement with the data within the total uncertainty band (which is inclusive also of all the experimental uncertainties of the HMDY analysis), hence we can consider acceptable the fakes background estimate also in this channel. We report for completeness in the next section a proposal of procedure, going beyond the validation results presented in this chapter and the FF method implementation adopted in the analysis presented in Chapter 4, which can potentially solve the observed discrepancy.

A potential improvement: extending the FF method to sources of electrons generating tau fakes

The discrepancy between data and the total predicted background shown in the e-had channel in distributions in Figure 3.19 is most likely resulting from a non negligible portion of electrons generating fake taus. As already mentioned in Section 3.2.1, the current implementation of the FF method does not take into account of fake taus originating from electrons or muons. This typology of fake taus are cancelled from the fakes background yields via the *truth subtraction*, and their contribution is added in the total background prediction via the MC simulation (in particular via the Z +jets events). The discrepancy shown in the e-had channel can therefore be attributed to a mismodelling introduced by the MC simulation in representing this portion of events.

To solve this discrepancy, one possibility is to extend the FF method to treat

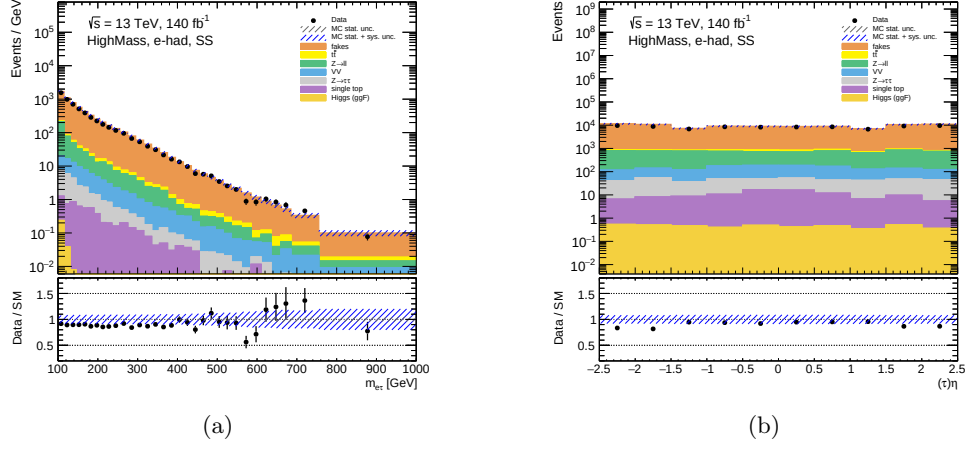


Figure 3.19. Comparison of data with the total predicted background in the High Mass Drell-Yan analysis VR, for the e-had channel: (a) $m_{e\tau}$, (b) leading tau η .

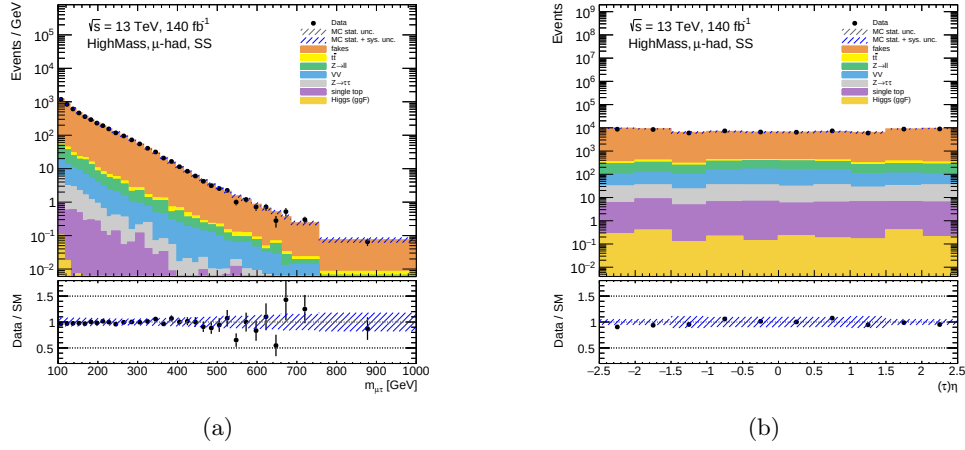


Figure 3.20. Comparison of data with the total predicted background in the High Mass Drell-Yan analysis VR, for the μ -had channel: (a) $m_{\mu\tau}$, (b) leading tau η .

also electrons as a source a fake taus. We report here, as a proposal, the action items that should be taken to implement this extension:

- define a new measurement region, the *electron region*, enriched in electrons generating fake hadronic taus, and measure primitive FFs and primitive templates in such region. Templates measured in the electron region, should be included in the template fits, and the relative FFs should be involved in the calculation of the combined FFs;
- remove electrons from the truth-matching condition of hadronic taus: taus should be considered truth-matched if matched either with a true tau or with a muon. In this way, the events with fake taus generated by electrons will be effectively considered in the FF method;
- remove events with electrons generating fake taus from the MC simulation. This can be implemented by discarding from MC yields all the events in which a reconstructed hadronic tau is matched with a true-electron.

This extension can be taken into consideration to solve the $\sim 10\%$ discrepancy shown in previous distributions and for future developments of the FF method.

Chapter 4

Search for leptoquark particles in di-tau Drell-Yan final states

This chapter describes the physics analysis I have worked on as main topic of this thesis. I have been actively part of the analysis team from the very beginning (even in preliminary discussions before the kick-off meeting) to the very end. I have been involved in all aspects of the analysis, namely: the definition of the analysis strategy, the study of the Monte Carlo simulated and data-driven backgrounds, the experimental and modelling systematics assessment, the statistical interpretation of results and their comparison with theory expectations. My main contributions (i.e. the parts of the analysis almost completely done by me) are the fake taus background estimate and the study of the modelling systematics, although I had a prominent role also in the other mentioned tasks.

4.1 Introduction and physics motivations

The study of the flavour sector of the Standard Model constitutes one of the most considerable parts of the LHC physics program, and has been conducted through several precision measurements and searches for new phenomena. The investigation of flavour physics processes has gained even more importance in recent years, since several anomalous measurements have been obtained in the context of the B -mesons decays (the *flavour anomalies*) [24], which constitute a promising and alternative way to search for new physics. The flavour anomalies, consisting in branching fractions or ratios of branching fractions in B -mesons decays, have mainly been measured by the LHCb experiment at the LHC (see details in Section 1.3.2) and collectively hint for the presence of new physics more strongly coupled to the third family of leptons and quarks [42], motivating the study of the Standard Model flavour sector via final states involving τ -leptons and b -jets.

Among the various new physics scenarios proposed as possible extensions of the Standard Model, leptoquark (LQ) models have gained considerable attention, since they could provide a valuable explanation of the flavour anomalies [41]. Leptoquarks are hypothetical particles coupling to both leptons and quarks in the same interaction

vertex. Such particles have been hypothesized in the '70s by Pati and Salam [47], in models assuming the $SU(4)$ group as a fundamental symmetry of Nature, which have recently been reconsidered and extended. If existing, leptoquarks would be involved in diagrams producing di-tau final states, generating excesses of events and interference with the Standard Model Drell-Yan process with tau leptons $pp \rightarrow \tau\tau$, and could therefore be observed as anomalies in the precision measurement of the Drell-Yan process, mainly located in the range of high invariant mass of the di-lepton system.

I report in this chapter the results of a search for leptoquark particles, conducted by the ATLAS Collaboration at the LHC, exploiting di-tau final states in association with b -jets radiated from the initial state. The Run 2 dataset is exploited, recorded by ATLAS in the years 2015-2018 and containing pp interactions at the centre-of-mass energy of $\sqrt{s} = 13$ TeV. ATLAS has already performed a series of measurements and searches with $\tau^+\tau^-$ final states, including measurements of the $Z \rightarrow \tau\tau$ cross section and its properties [143, 144, 113], the observation of the $H \rightarrow \tau\tau$ decay mode and subsequent study of its properties [115, 145, 146, 147], as well as the search for heavy resonances decays to $\tau^+\tau^-$ pairs [118]. Measurements have been performed also for high-mass e^+e^- and $\mu^+\mu^-$ production [148, 149], as well as searches for new phenomena in the high-mass range [150, 151], however no measurement is currently available in the high-mass range with third family leptons.

The study presented in this chapter, focusing on final states with τ -leptons, in some sense completes an important part of the picture of high-mass di-lepton production at the LHC, constituting one of the first studies conducted by ATLAS with third family leptons in the high-mass kinematic regime. Among the various channels used in the analysis, the fully hadronic channel is utilised, profiting of the high statistics available due to the high decay branching fraction of the tau into hadrons and taking advantage of the developments achieved in the ATLAS experiment on the reconstruction and characterisation of hadronic tau decays.

This chapter is organised as follows. A general overview of the entire analysis strategy is outlined in Section 4.2, while a summary of the utilised data and simulated samples is provided in Section 4.3. The objects and events trigger pre-selection are outlined in Section 4.4. Section 4.5 describes the event selection and categorisation across all the analysis channels, while Section 4.6 reports details on the data-driven estimate of the background of fake taus, which is peculiar of this analysis. The experimental and modelling uncertainties are described in Sections 4.7 and 4.8 respectively, while the statistical interpretation of results is outlined in Section 4.9. Final results are delivered in Section 4.10.

4.2 Analysis overview

The analysis hereby presented is focused on the search for leptoquark particles through the precision study of the Drell-Yan process with tau leptons, shown in Figure 4.1. The U_1 vector leptoquark model is assumed, as developed by Cornella, Isidori et al. in Ref. [41] and briefly summarised in the introductory chapter of this thesis in Section 1.4.1. Within this model several beyond-SM diagrams involving leptoquarks are possible, which modify the yields of the Standard Model Drell-Yan

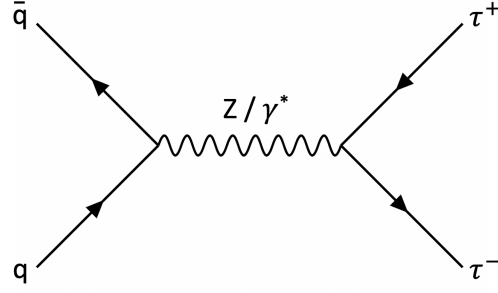


Figure 4.1. Feynman diagram of the Drell-Yan process with tau leptons in the final state.

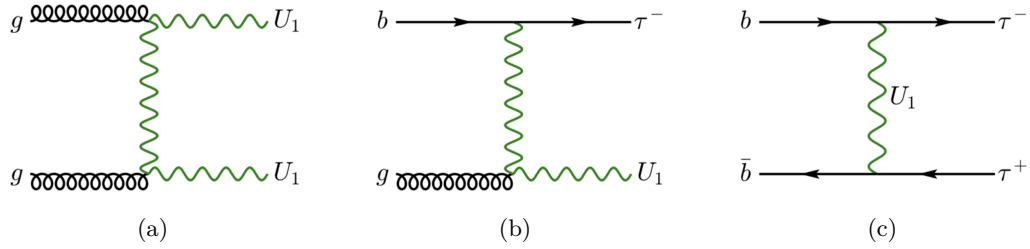


Figure 4.2. Representative Feynman diagrams for leptoquark production, yielding di-tau final states in association with b -jets: (a) pair production, (b) single production, (c) t -channel exchange.

production with di-tau final states. A selection of diagrams is shown in Figure 4.2. Diagrams in Figures 4.2(a) and 4.2(b) generate di-tau final states via the decay of the singly- or doubly-produced leptoquarks, $U_1 \rightarrow b\tau$, yielding additional beyond SM events which sum to the Drell-Yan di-tau events. The diagram in Figure 4.2(c), instead, generates a pure di-tau final state via the t -channel leptoquark exchange, together with additional b -jets radiated from gluon splitting in the initial state, and interferes destructively with the pure SM Drell-Yan diagram. Notice explicitly that the first two diagrams cannot interfere with the SM Drell-Yan diagram, since additional b -jets are part of the final state, but yield additive contribution in an analysis inclusive in an arbitrary number of b -jets, as it is the one presented in this chapter. Instead, the third diagram produces interference with the Drell-Yan process, having exactly two taus in the final state. The interfering diagram yields the dominant contribution for di-tau masses around $m_{\ell\ell} \simeq 200$ GeV (see Figure 4.3) while the non-interfering diagrams dominate for higher masses. In the presence of the exotic signal we therefore expect a distortion of the di-tau mass distribution, with a decrease of the event yields, followed by an increase in the very high mass range.

The analysis exploits both the semi-leptonic channel, in which one tau decays leptonically into an electron or a muon, and the fully hadronic channel, in which both taus decay hadronically. The usage of the hadronic channel is challenging, due to the difficulties related to the identification and reconstruction of tau hadronic decays, but enables to exploit the huge amount of statistics determined by the dominant decay branching fraction of the tau into hadrons. A *signal region* (SR) is

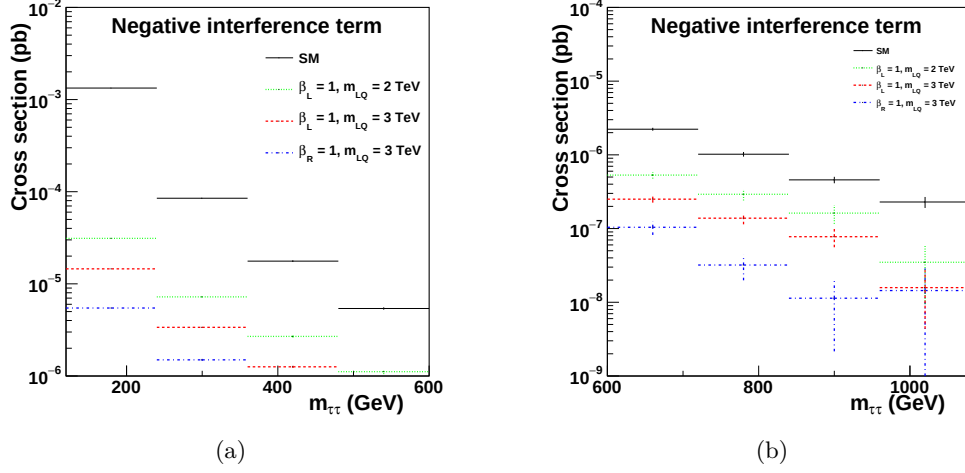


Figure 4.3. Predicted particle level differential cross sections for the pure SM Drell-Yan as well as the expected interference with the LQ diagrams for (a) $100 < m_{\tau\tau}/\text{GeV} < 600$, (b) $600 < m_{\tau\tau}/\text{GeV} < 1000$. Different LQ masses and $\beta_{L/R}$ couplings are shown (see Section 1.4.1 for details).

defined and optimised to maximise the sensitivity to the LQ signal, while *control regions* (CRs) and *validation regions* (VRs) are respectively used to constrain and cross-check the leading background processes estimates. The invariant mass of the di-tau system $m_{\tau\tau}$ is chosen as discriminating variable to perform a *binned likelihood fit* of the $m_{\tau\tau}$ distributions. The *signal strength*, defined as the ratio of the measured LQ signal cross section divided by its prediction is extracted and, in the absence of an observed signal, a 95% CLs limit is set on the leptoquark coupling strength $\lambda = g_U/\sqrt{2}$ (see the LQ lagrangian in Eq. (1.39) for details). Several hypotheses on the U_1 leptoquark mass have been scrutinised in the range from 1 to 3 TeV yielding an exclusion contour in the $m_{U_1} - \lambda$ plane, similar to the one obtained by the CMS collaboration and shown in Figure 1.21.

It is worth mentioning that the analysis here presented is the only one performed up to now in the ATLAS Collaboration exploiting the t -channel signal diagram. It is therefore expected to provide peculiar results, complementary to the ones of other analyses not sensible to the non-resonant leptoquark process.

4.3 Data and simulated samples

4.3.1 Data

The analysis utilises the Run 2 dataset, collected in the years 2015-2018 by the ATLAS experiment at the LHC, recording pp collisions at a centre-of-mass energy of $\sqrt{s} = 13 \text{ TeV}$. Data are required to be part of the Run 2 Good Run List (GRL). This ensures that data are of good quality and recorded while all the relevant ATLAS sub-detectors were in operation. The total luminosity utilised is 140.1 fb^{-1} , measured with an uncertainty of 1.2 fb^{-1} [82].

Table 4.1. Details on MC generators used in the analysis. The acronyms ME and PS stand for matrix element and parton shower respectively. The cross-section order stands for the order of cross-section calculation in QCD, with ((next-to-)next-to-)leading order ((N)N)LO and ((nex-to-)next-to-)leading-logarithm ((N)N)LL, respectively.

Process	ME generator	ME PDF	PS and hadronis.	Tune	Cross-section
LQ signal	MadGraph5 + aMc@NLO2.2.2	NNPDF3.0NLO	Pythia 8.186	A14	NLO
V+jets	Sherpa 2.2.11	NNPDF3.0NNLO	Sherpa 2.2.11	Default	NNLO
ttbar	PowhegBox v2	NNPDF3.0NLO	Pythia 8.230	A14	NNLO, NNLL
single top s	PowhegBox v2	NNPDF3.0NLO	Pythia 8.230	A14	NLO
single top t	PowhegBox v2	NNPDF3.0NLO	Pythia 8.230	A14	NLO
single top Wt	PowhegBox v2	NNPDF3.0NLO	Pythia 8.230	A14	NLO, NNLL
Multi-boson	Sherpa 2.2.11	NNPDF3.0NNLO	Sherpa 2.2.11	Default	NNLO

4.3.2 Simulated samples

The signal and background processes are modelled via Monte Carlo (MC) simulation, except for the background of hadronic jets misidentified as hadronic taus, which is estimated through a data-driven technique. The generated events are interfaced with a detailed simulation of the ATLAS detector, based on GEANT4 [84], used to model the detector’s response to particles. The MC events are reweighted to correctly represent the pile-up distribution observed in data in Run 2. Details on the generators used for the matrix element calculation, the parton shower, the set of PDFs and tunes, and the cross-section order can be found for each process in Table 4.1. A more detailed description is provided in the following sections.

Signal

The signal searched in this analysis comprises diagrams with leptoquarks coupled to third generation of leptons and quarks, hence yielding tau leptons and b -jets in the final state. Two separate signal generations are performed: one to model signal diagrams non-interfering with the di-tau Drell-Yan process (as for example the ones in Figure 4.2(a) and 4.2(b)), and another to model the leptoquark-mediated Drell-Yan diagram (represented in Figure 4.2(c)), which interferes with the SM Drell-Yan. The signal generation also includes events contributions from processes mediated by a heavy Z' boson.

The signal events are generated via a MC simulation based on MADGRAPH5 AMC@NLO 2.2.2 [141], using LO-accurate matrix elements (ME) with up to two final-state partons. The ME calculation employed the NNPDF3.0NLO [131] set of PDFs. Events were interfaced with PYTHIA 8.186 [122] for the modelling of the parton shower, hadronisation and the underlying event, and the A14 [140] tune has been used. The overlap between the matrix element and the parton shower emission was removed using the CKKW-L merging procedure [152, 153]. The decays of the bottom and charm hadrons were performed via EVTGEN 1.2.0 [139].

Since in the off-shell regime the kinematics of b -jets are similar between the beyond-SM and SM Drell-Yan amplitudes, the signal samples have been generated

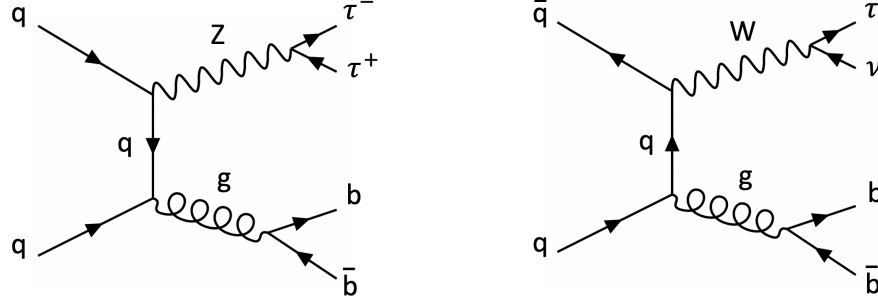


Figure 4.4. Lowest order Feynman diagrams for the quark induced V +jets processes with Z boson (left) and W boson (right).

reweighing the pure SM amplitude to the predictions of the leptoquark models. Only events with di-tau invariant mass higher than 120 GeV have been considered in the reweighing procedure. Signals have been generated independently for several hypotheses on the leptoquark mass in the range 1-3 TeV and for several values of the couplings $\beta_{L/R}$ (see the U_1 vector leptoquark model description in Section 1.4.1 for the details).

V +jets background

The V +jets background includes all the processes in which a vector boson (either a Z or a W) is produced in association with jets. Example diagrams are shown in Figure 4.4. The Z +jets process in which the Z boson decays into two taus constitutes a major background for all the channels of the analysis, while the same process in which the Z decays into light leptons is relevant in the semi-leptonic channel only. The W +jets process, instead, is a sub-leading process in both the analysis channels.

The V +jets events are simulated via the SHERPA 2.2.11 [125] generator, using the next-to-leading-order (NLO) matrix elements (ME) for up to two partons and leading-order (LO) matrix element for up to five partons calculated with the COMIX [154] and the OPENLOOPS [155] libraries. The hadronisation shower is simulated via SHERPA parton shower [126] using the default set of tuned parameters developed by the authors. The NNPDF3.0NNLO set of PDFs [131] was used.

In order to model with significant statistics the phase space regions corresponding to different values of the vector boson transverse momentum p_T^V , events are split into slices. More precisely, the slices are generated at intervals of $\max(p_T^V, H_T)$, where H_T is the scalar p_T sum of all parton-level jets with $p_T > 20$ GeV. To ensure that the MC statistics is high in the phase-space regions where heavy flavour jets are generated, filters are applied to the MC generator to select the flavour composition of the jets produced in association with the vector boson and combine equal statistics filtered slices. The flavour filters used are:

- *BFilter*: at least one b -hadron with $|\eta| < 4$ is required;
- *CFilterBVeto*: at least one c -hadron with $p_T > 4$ GeV and $|\eta| < 3$ is required, and no overlap with the BFilter sample;
- *CVetoBVeto*: events which pass the previous two filters are rejected.

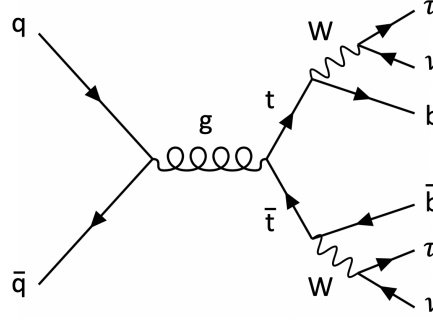


Figure 4.5. Lowest order Feynman diagram for the $t\bar{t}$ process.

The *BFilter* is particularly relevant to guarantee high statistics of events with b -jets, which are included in the final state targeted by this analysis.

In order to extend the statistical power of the V +jets predictions in the region of high di-tau invariant mass $m_{\tau\tau}$, dedicated high-statistics SHERPA samples are considered, modelling events with $m_{\tau\tau} > 120$ GeV and using otherwise identical settings to the inclusive samples described above. The inclusive samples are therefore restricted exclusively for the $m_{\tau\tau} < 120$ GeV prediction.

Top-quark pair background

The top-quark pair production is one of the most relevant backgrounds in the analysis, and yields leading contributions both in the semi-leptonic and in the fully hadronic channel. The lowest order Feynman diagram for the $t\bar{t}$ production is shown in Figure 4.5. The top-quark pair originates from gluon splitting yielding a couple top quarks, subsequently decaying into b -quarks with the emission of two W bosons. The two W bosons can decay leptonically either both into taus, yielding background events in all the analysis channels (depending on the type of decay of the taus), or one into a light lepton and the other into a tau, yielding background events into the semi-leptonic channel. Two b -jets are typically present in these background events, originating from the decay of the two b -hadrons; however also events with one or no b -jets are possible due to the inefficiencies of the b -tagging algorithm.

Events are modelled using the POWHEGBOX v2 [134, 135, 136, 133] generator at NLO, with the NNPDF3.0NLO set of PDFs [131] and the h_{damp} parameter set to $1.5 m_{\text{top}}$ [137]. The events are interfaced with PYTHIA 8.230 [138] to model the parton shower, hadronisation and underlying event, with parameters set to the A14 tune [140]. The decays of bottom and charm hadrons were performed by the EVTGEN 1.6.0 [139].

Filters are available to require particular decays of the W bosons into leptons or hadrons. In this analysis samples are used with the di-lepton filter, which selects events in which both the W bosons decay leptonically. Since the $t\bar{t}$ events constitute a relevant fraction of the background events entering the analysis signal region, modelling systematics are used to assess uncertainty in the matrix element and the parton shower simulation. Further details are given in Section 4.8.

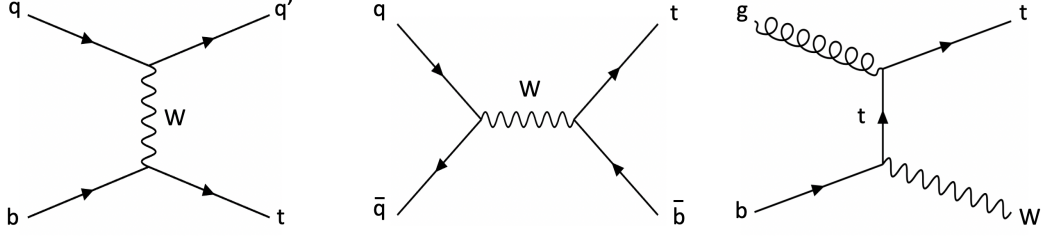


Figure 4.6. Lowest order Feynman diagrams for the three channels of the single top production: t -channel (left), s -channel (centre), Wt -channel (right).

Single top background

The single top production is a sub-leading background process in this analysis, yielding a minor contribution of events in all the analysis channels. Single top production happens via three diagrams, displayed in Figure 4.6: the t -channel, the s -channel and the Wt -channel. The Wt -channel generates the majority of this background events: two W bosons are present (one directly produced and the other generated in the t -quark decay) which can decay producing tau pairs or a tau and a light lepton.

Events are simulated with the POWHEGBOX v2 [134, 135, 136] generator at NLO in QCD, using the NNPDF3.0NLO set of PDFs [131]. The events are interfaced with the PYTHIA 8.230 [138] generator to model the parton shower, using the A14 [140] tune.

Top and anti-top filters are considered in the analysis for the s -channel and t -channel processes, while the di-lepton filter is used for the Wt -channel process, selecting only the events in which the W -bosons are forced to decay leptonically. The overlap between the Wt diagrams at NLO in QCD with LO $t\bar{t}$ diagrams is taken into account and eliminated applying the *diagram removal* (DR) scheme. The uncertainty associated to such procedure is considered among the modelling uncertainties and estimated by comparing the DR scheme with the alternative *diagram subtraction* (DS) scheme.

Multi-boson

The multi-boson processes generate a small background component in the analysis signal region. These processes involve diagrams in which two or more vector bosons are generated in the final state, subsequently decaying either leptonically or hadronically. Examples of lowest order Feynman diagrams for the multi-boson production are provided in Figure 4.7. The majority of the background events is generated by the di-boson process, yielding two vector bosons in the final state (either W or Z bosons). Di-boson background events in this analysis are typically induced by the production of two W -bosons, decaying leptonically into a tau pair or in a tau and a light lepton. Other possibilities involve the production of a Z decaying into a tau pair, accompanied by the production of a W or a Z boson decaying into hadrons. All processes generating more than two vector bosons in the final state yield negligible background events.

The di-boson samples are simulated with the SHERPA 2.2.11 [125] generator,

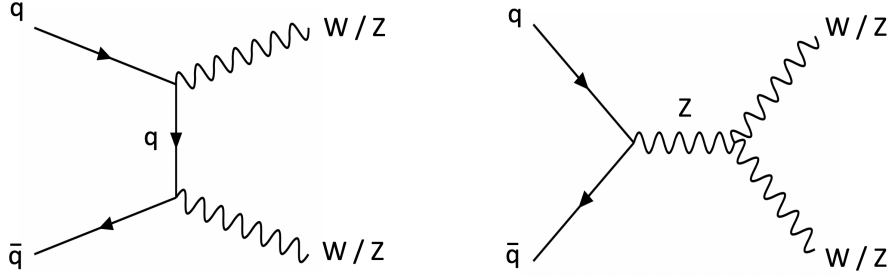


Figure 4.7. Lowest order Feynman diagrams for the di-boson production process.

using matrix elements at NLO accuracy in QCD for up to one additional parton and at LO accuracy for up to three additional parton emissions. Samples for the loop-induced processes $gg \rightarrow VV$ were generated using LO-accurate matrix elements for up to one additional parton emission. The matrix elements were matched and merged with the SHERPA parton shower based on the Catani-Seymour dipole factorisation [154, 126], using the MEPS@NLO prescription [127, 128, 129, 130]. The virtual QCD corrections were provided by the OPENLOOPS library [155, 156, 157]. The NNPDF3.0NNLO set of PDFs [131] was used, along with the default set of tuned parameters developed by the SHERPA authors.

Several filters are available for di-boson samples, selecting events with assigned lepton multiplicity in the final state. In this analysis all samples yielding at least two leptons in the final state are included.

4.3.3 Event weights

Monte Carlo generated events have to be multiplied by weights and *scale factors* in order to correctly represent the data. Such rescaling happens in several steps and accounts for multiplicative factors, summarised in what follows.

Monte Carlo samples normalisation

The yield of each event i simulated by the matrix element (ME) generator and matched with the parton shower (PS) generator has to be scaled by a weight w_i . This weight is necessary to achieve the correct cross-section distribution once a sufficient number of events is simulated and also takes into account of the Sudakov form factors associated with the QCD emissions in the parton shower development. Negative weights are possible, and are used to reproduce the cancellations which arise in the ME calculation. Each event is also divided by the sum of weights $\sum_i w_i$ of all the events present in a given Monte Carlo dataset (identified with a given dataset-ID within the ATLAS Physics Modelling Group database). Events are also multiplied by the filter efficiency ϵ_f , representing the efficiency of the filter which has been applied in the Monte Carlo generation to select events yielding a particular required final state. This is necessary since events have been originally generated (and therefore the w_i weights have originally been tuned) referring to a statistics a factor $1/\epsilon_f$ higher.

Each Monte Carlo event yield has also to be scaled by the cross-section σ of the relative physics process, and by an additional factor, called k -factor. The cross section values as well as the k -factors are made available to the analysers by the ATLAS Physics Modelling Group and are evaluated to the highest order achievable. Finally, to obtain Monte Carlo predictions matching the luminosity observed in data, the event yields need to be multiplied by the total integrated luminosity $\mathcal{L}$ corresponding to the analysed data (e.g. for a full Run 2 analysis $\mathcal{L} = 140 \text{ fb}^{-1}$).

Considering all the aforementioned multiplicative factors, the scaling factor to be applied to each Monte Carlo event yield to obtain normalised distributions is

$$w_{\text{tot}}^i = \frac{w_i \epsilon_f k \sigma}{\sum_i w_i} \times \mathcal{L} , \quad (4.1)$$

where each symbol has the meaning specified in the text above.

Scale factors

The reconstruction of physics objects performance is subject to imprecision which has to be corrected with further multiplicative factors applied to Monte Carlo events yields, called *scale factors* (SF). The SF corrects the efficiencies predicted by the Monte Carlo simulation and associated with the performance algorithms to match the values observed in data. For example, the triggers used for the events pre-selection have an turn-on curve (due to the finite resolution on the variable on which the trigger cut is applied) which is imprecisely predicted by the Monte Carlo simulation. This generates a discrepancy between the predicted distributions and the data, which is corrected by the trigger scale factor. Other scale factors are considered, associated to the reconstruction, identification, isolation and tagging algorithms used in the analysis. The Monte Carlo event yield is therefore multiplied by

$$\text{SF}_{\text{tot}} = \prod_j \text{SF}_j , \quad (4.2)$$

where j index runs over all the object performance algorithms used in the analysis.

4.4 Objects and events pre-selection

Preliminary requirements are applied both at object- and event-level, previous to the proper events selection and categorisation.

4.4.1 Objects selection

This analysis makes use of reconstructed tau leptons, muons, electrons, hadronic jets and b -jets. The objects are built using the standard ATLAS reconstruction and identification algorithms, which are described in Section 2.3 of this thesis. To be considered in the analysis, the reconstructed objects need to verify additional requirements, as detailed in the following sections.

Primary vertices

Events that enter the analysis are required to have at least one reconstructed primary vertex, based on the primary vertex reconstruction using tracks in the ID [85]. The hard scatter is defined as the primary vertex with the highest sum of the square of the transverse momenta of the associated tracks.

Hadronically decaying taus

Tau leptons are the main objects targeted by this analysis. Hadronically decaying tau leptons (τ_{had}) are reconstructed starting from seed jets built from locally calibrated topological clusters [105]. The anti- k_T algorithm [93] is used, with a radius parameter $R = 0.4$. Tau candidates are required to have rapidity $|\eta| < 2.47$ and transverse momentum $p_T > 20$ GeV after applying the energy calibration. Tau identification is done via the RNN neural-network algorithm, described in Section 2.3.7, which is trained on a wide set of simulated tau leptons, originated from pure γ^* Drell-Yan production. The “Tight” operating working point is chosen for the tau identification.

Fake hadronic taus can be simulated from electrons and muons. To limit the amount of electrons misidentified as fake hadronic taus, a specialised BDT is used (the eBDT), which is also described in Section 2.3.7. The “Loose” eBDT working point is chosen, except for the semi-leptonic channel $\tau_e \tau_{\text{had}}$, in which the “Medium” working point is adopted, to compensate the higher amount of electrons involved in that channel. Calorimeter tagged muons in the central $|\eta|$ region have a high probability to induce the reconstruction of fake hadronic taus, due to the poor coverage of the ATLAS muon system. Hence, for this region, τ_{had} candidates within $\Delta R < 0.1$ of a calorimeter tagged muon are removed. Differences between data and simulation are assessed for tau leptons from the Z boson decays, for the RNN identification and the eBDT selection, and corrected via dedicated scale factors.

Electrons

Electrons are generated either by tau leptonic decays or promptly in the hard scatter, and are included among the objects targeted by this analysis. Electrons can constitute final state objects for the searched signal, originating from tau leptons decays in the electronic channel. Electrons are reconstructed from ID tracks matched with energy clusters in the electromagnetic calorimeter [88, 89]. All electrons must have $p_T > 7$ GeV and must fall within the rapidity range $|\eta| < 2.47$. The transverse momentum threshold is relatively low since electrons generated from tau leptons decays carry a rather small fraction of the original leptons momentum, due to the emission of neutrinos. The *Medium* operating working point is chosen for the identification algorithm, and the *FCHighPtCaloOnly* isolation working point is adopted [88]. Differences in reconstruction and identification efficiencies between simulated events and data are accounted for by scale factors, derived in the Z and J/ψ mass peaks. The momentum scale is similarly calibrated using $Z \rightarrow \ell\ell$ decays ($\ell = e, \mu$).

Muons

Muons are generated by tau leptonic decays or promptly, similarly to the case of electrons, and can be included as final state objects in the signal targeted by this analysis. Muons are reconstructed from tracks in the ID, matched with the corresponding tracks in the muon spectrometer [90, 91]. Muon candidates must have $p_T > 7$ GeV and $|\eta| < 2.5$. Similarly to the case of electrons, the momentum threshold is low to include muons generated in tau leptonic decays. The *Medium* identification working point is chosen, and the *FCLoose* isolation working point is required [90]. Scale factors are derived from studies on the Z and J/ψ peaks to account for discrepancies between data and simulation in the reconstruction and identification efficiencies.

Jets

The analysis signal region is constructed to target final states inclusive in one or more b -tagged jets, which are therefore playing a prominent role in the analysis. Jets are built from Particle Flow objects using the anti- k_T algorithm [93] with a radius parameter $R = 0.4$.

Jets are classified as *central*, if they have $|\eta| < 2.5$ or *forward* if they have rapidity in the range $2.5 < |\eta| < 4.5$. The resulting jets transverse momenta are corrected to the corresponding particle-level jet p_T using simulation. After these calibrations, jets are required to have transverse momentum $p_T > 25$ GeV. The JVT multi-variate discriminant [95] is used to remove jets with $p_T < 60$ GeV and $|\eta| < 2.4$ that have large estimated energy fractions from pileup collision vertices; above this p_T scale this correction becomes unnecessary.

To identify hadronic jets originating from b -hadrons, the DL1r b -tagging algorithm [102] is used, with the 77% b -jet identification efficiency operating point. Further details on this b -tagging algorithm as well as the tagging efficiency measurement are provided in Section 2.3.5. Jets are corrected for their JVT efficiencies and p_T scale and resolution using *in-situ* measurements of these quantities in multijet, γ +jets, Z +jets data [92]. Simulated tagging rates are also corrected via proper scale-factors to cover discrepancies between the tagging efficiencies in simulated events and in data.

Missing transverse momentum

Neutrinos originating in tau leptons decays generate missing transverse momentum in the final states targeted by this analysis. However, this object is not considered in the events selection, and is not playing any particular role in the analysis strategy. The missing transverse momentum E_T^{miss} is reconstructed as the negative vectorial sum of the transverse momenta of all physics objects measured by ATLAS and the *soft term* [103]. Performance on E_T^{miss} reconstruction is evaluated in $Z \rightarrow \ell\ell$ events, in which E_T^{miss} has a null expected value, or in W or top-quark decays, in which a non-null E_T^{miss} is expected from the neutrino in the decay products.

Table 4.2. Criteria used in the overlap removal between reconstructed objects, listed in the order of their application.

Object to remove	Object to keep	Criteria
Tau	Electron	The tau is removed if $\Delta R_y < 0.2$
Tau	Muon	The tau is removed if $\Delta R_\eta < 0.2$
Electron	Muon	The electron is removed if a track is present in the muon chambers. Otherwise the muon is removed.
Jet	Electron	The jet is removed if $\Delta R_y < 0.2$
Jet	Muon	The jet is removed if $\Delta R_y < 0.2$
Electron	Jet	The electron is removed if $0.2 < \Delta R_y < 0.4$
Muon	Jet	The muon is removed if $0.2 < \Delta R_y < 0.4$
Jet	Tau	The jet is removed if $\Delta R_y < 0.2$

Overlap removal

It may occur that the same set of tracks and energy deposits are associated with more than one reconstructed object. An overlap removal algorithm (OLR) is therefore applied in order to avoid double counting of objects associated with the same detector signals. The selection criteria are based on the angular separation between the two objects, evaluated as $\Delta R_y = \sqrt{(\Delta y)^2 + (\Delta \phi)^2}$. Only the tau-muon overlap is evaluated using the pseudo-rapidity coordinate, instead of the rapidity: $\Delta R_\eta = \sqrt{(\Delta \eta)^2 + (\Delta \phi)^2}$. Criteria are listed in Table 4.2 in the exact order of application, and are summarised as follows:

- tau - electron (muon): the tau is removed if $\Delta R_{y,(\eta)} < 0.2$, as the electron (muon) reconstruction is considered more stable;
- electron - muon: if the two objects share the same track in the ID, the electron is removed if the track is matched with a segment in the muon spectrometer. If no matched signal is present in the muon chambers, the muon is discarded and the electron is kept;
- jet - electron (muon): the electron (muon) is kept and the jet discarded if the two objects overlap within $\Delta R_y < 0.2$. If, instead, the overlap is in the angular region $0.2 < \Delta R_y < 0.4$, the jet is kept and the electron (muon) removed, since most likely the light lepton has been originated in the displaced decay of a hadron in the jet;
- tau - jet: the jet is removed if the angular distance $\Delta R_y < 0.2$. In fact in this case, it is likely that the jet is actually the seed required to start the tau reconstruction chain.

4.4.2 Triggers pre-selection

Events are pre-selected making use of trigger chains, accepting only events which present the final state objects relevant for this analysis. The unprescaled triggers with loosest selection criteria are used for different years and periods of the data-taking.

Table 4.3. Triggers list for the di-tau semi-leptonic channels. EH (MH) refers to the channel in which the leptonically decaying tau generates an electron (muon). The triggers the same period of data-taking are applied in logical OR.

Year	Period	Trigger name (EH channel)	Trigger name (MH channel)
2015	All	HLT_e24_lhmedium_L1EM20VH	HLT_mu20_iloose_L1MU15
		HLT_e60_lhmedium	HLT_mu40
		HLT_e120_lhloose	
2016	A-D3	HLT_e26_lhtight_nod0_ivarloose	HLT_mu24_ivarmedium
		HLT_e60_lhmedium_nod0	HLT_mu50
		HLT_e140_lhloose_nod0	
	D4-end	HLT_e26_lhtight_nod0_ivarloose	HLT_mu26_ivarmedium
		HLT_e60_lhmedium_nod0	HLT_mu50
		HLT_e140_lhloose_nod0	
2017	All	HLT_e26_lhtight_nod0_ivarloose	HLT_mu26_ivarmedium
		HLT_e60_lhmedium_nod0	HLT_mu50
		HLT_e140_lhloose_nod0	
2018	All	HLT_e26_lhtight_nod0_ivarloose	HLT_mu26_ivarmedium
		HLT_e60_lhmedium_nod0	HLT_mu50
		HLT_e140_lhloose_nod0	

The trigger requirements are increasingly selective along the years and periods, to cope with the evolving rate of events in Run 2. Typically, several triggers are associated with each period, and are put in logical OR.

In the semi-leptonic channel, the single-electron and single-muon triggers are used to trigger on the final state light-lepton. The possibility of adding in logical OR single tau triggers, to recover events corresponding to single electron and single muon triggers inefficiencies has been investigated, and finally not adopted since it over-complicates the scale factors evaluation. Table 4.3 reports the triggers used in the semi-leptonic channel. The trigger thresholds are expressed in GeV in the trigger names (e.g.: “e24” and “mu20” indicate an electron with $p_T > 24$ GeV and a muon with $p_T > 20$ GeV respectively). The keyword “lhloose” denotes that the lepton is required to verify the *Loose* identification criterion (the same applies for *Medium* and *Tight*). Moreover, the “iloose” and “ivarmedium” keywords indicate that the light lepton satisfies the *Loose* and *Medium* isolation requirements respectively. The suffix “nod0”, instead, indicates that no requirement is set on the d_0 parameter, while the additional keywords “L1EM20VH” and “L1MU15” denote requirements assigned on the energy and momentum reconstructed at the first trigger level (L1).

In the fully hadronic channel, single-tau and di-tau triggers are used in logical OR. The single tau triggers yield high events selection efficiency in the high p_T range, but have high thresholds. Efficiency at low p_T is therefore recovered by di-tau triggers. Table 4.4 reports the full list of triggers utilised. The trigger threshold is expressed in GeV in the trigger name (e.g. “tau80” indicates that a tau lepton is required with $p_T > 80$ GeV). The keyword “L1TAU60” and similar indicate the p_T requirement to be satisfied by the tau lepton at L1 trigger level.

Table 4.4. Trigger list for the fully hadronic channel. The triggers the same period of data-taking are applied in logical OR.

Year	Period	Trigger name
2015	All	HLT_tau80_medium1_tracktwo_L1TAU60
		HLT_tau35_medium1_tracktwo_tau25_medium1_tracktwo_L1TAU20IM_2TAU12IM
2016	A	HLT_tau80_medium1_tracktwo_L1TAU60
		HLT_tau80_medium1_tracktwo_L1TAU60_tau50_medium1_tracktwo_L1TAU12
	B-D3	HLT_tau125_medium1_tracktwo
		HLT_tau80_medium1_tracktwo_L1TAU60_tau50_medium1_tracktwo_L1TAU12
	D4-end	HLT_tau160_medium1_tracktwo
		HLT_tau80_medium1_tracktwo_L1TAU60_tau50_medium1_tracktwo_L1TAU12
2017	B1-B7	HLT_tau160_medium1_tracktwo
		HLT_tau80_medium1_tracktwo_L1TAU60_tau50_medium1_tracktwo_L1TAU12
	B8-end	HLT_tau160_medium1_tracktwo_L1TAU100
		HLT_tau80_medium1_tracktwo_L1TAU60_tau60_medium1_tracktwo_L1TAU40
2018	B-J	HLT_tau160_medium1_tracktwoEF_L1TAU100
		HLT_tau80_medium1_tracktwoEF_L1TAU60_tau60_medium1_tracktwoEF_L1TAU40
	K-end	HLT_tau160_medium1_tracktwoEF_L1TAU100
		HLT_tau160_mediumRNN_tracktwoMVA_L1TAU100
		HLT_tau80_medium1_tracktwoEF_L1TAU60_tau60_medium1_tracktwoEF_L1TAU40
		HLT_tau80_mediumRNN_tracktwoMVA_L1TAU60_tau60_mediumRNN_tracktwoMVA_L1TAU40

opposite sign				same sign		
	0b	1b	2b+	0b	1b	2b+
had had	SR		CR	VR (fake taus)		
e had						
mu had						
e e	VR (Monte Carlo)					
mu mu						
e mu						

Figure 4.8. Graphical representation of the analysis strategy. The analysis channels are displayed, each one divided into b -jets multiplicity categories. One signal region (SR), one control region (CR) and two validation regions (VR) are defined.

The *trigger matching* is applied in the analysis. Therefore, for single lepton triggers, at least one lepton of the corresponding flavour is required to closely overlap with the trigger object. Similarly, for di-tau triggers, two taus are required to be reconstructed near the triggering candidates. In simulated events, a trigger efficiency scale factor is applied to account for the differences between the predicted and observed trigger efficiencies.

4.5 Events selection and categorisation

This analysis targets the detection of a beyond SM leptoquark signal, in di-tau Drell-Yan final states in the high invariant mass range. The high mass requirement enables to cut the major backgrounds of light leptons Drell-Yan production, which are located in the invariant mass range around the Z boson peak ($m_{\ell\ell} \simeq 90$ GeV). The exotic leptoquark signal is searched as an anomaly in the precision measurement of the Standard Model di-lepton mass spectrum. For this reason, the analysis cuts are kept as minimal as possible, to enlarge the fiducial phase space region in which the precision measurement is performed.

The analysis selection strategy is summarised in Figure 4.8. Two analysis channels are jointly used: the fully hadronic channel, and the semi-leptonic channel, the latest being further divided in the electronic and muonic sub-channels, depending on the flavour of the tau leptonic decay product. Events are classified in b -jets categories, depending on the multiplicity of the b -jets present in the final state.

A *signal region* (SR) is defined, collecting the majority of the expected signal events, together with a *control region* (CR), used to constrain the dominant top background in the SR. Both the SR and the CR collect several channels and b -jets categories combinations. Two *validation regions* (VR) are also exploited. A first VR collects events in the light leptons channels (ee , $\mu\mu$, $e\mu$), and is used to check the

closure between data and the MC predictions for the major background estimated via simulation. A second VR collects events with same charge sign leptons in the $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_e\tau_{\text{had}}$, $\tau_\mu\tau_{\text{had}}$ channels and is used to check the data driven estimate of the background of fake taus.

4.5.1 Analysis channels selection

The selections for all the analysis channels are summarised in Table 4.5. In the fully hadronic channel ($\tau_{\text{had}}\tau_{\text{had}}$) two final state hadronic taus are required, while in the semi-leptonic channels ($\tau_e\tau_{\text{had}}$, $\tau_\mu\tau_{\text{had}}$) one light lepton and one hadronic tau are required. The light lepton is generated in the leptonic decay of a tau lepton, but it is reconstructed exactly as a prompt light lepton, as there is currently no strategy in ATLAS to distinguish between these two cases. Further details on the analysis selections are given in the next sections.

The fully hadronic channel $\tau_{\text{had}}\tau_{\text{had}}$

Events are selected in the fully hadronic channel using the single- and di-tau triggers, collecting events in which one or two hadronic taus are present. The di-tau triggers are efficient in all the di-tau invariant mass range probed by the analysis, while the single-tau triggers are efficient at high mass only, and are mostly used to compensate the di-tau trigger inefficiencies.

Exactly two hadronic taus must be present in the final state. An additional veto on light leptons is added, to discard events in which an electron or a muon is present. The leading tau is required to have transverse momentum $p_T > 90$ GeV, while the sub-leading tau must verify $p_T > 60$ GeV. These two thresholds have been set to be fairly on the trigger efficiency plateau, to limit mis-modellings generated by discrepancies between data and simulation in the trigger turn-on curves. The eBDT discriminant variable is used with the *Loose* identification working point, since a small quantity of electrons misidentified as fake hadronic taus is expected in this channel. Requirements in the di-lepton system are also set. The di-tau invariant mass needs to verify $m_{\tau\tau} > 100$ GeV, and the two leptons are required to have opposite electric charge sign. The selection is inclusive in the presence of b -jets radiated from the initial state, and events are further categorised according to the b -jets multiplicity, as will be further detailed in a following section.

Figure 4.9 shows the distributions of some kinematical variables, measured in data and compared to the backgrounds prediction, drawn separately in the different b -jets categories. A fair agreement is observed between data and predictions in most of the kinematical distributions, except for a mis-modelling in the high- p_T tail of the leading tau- p_T distribution in the 0 b -jets category (see Figure 4.9(b)). This should be caused by a limitedness of the fake taus background estimate, since FFs are calculated in thin bins of tau p_T only up to 110 GeV, while only a single inclusive bin is used to evaluate a FF for higher values of tau p_T , as will be further detailed in Section 4.6.1.

Table 4.5. Summary of the selection requirements for the main analysis channels and regions.

Hadronic channel ($\tau_{\text{had}}\tau_{\text{had}}$)	
Trigger	Single- and di-tau triggers
Tau	exactly two τ_{had} Leading $\tau_{\text{had}} p_T > 90$ GeV Subleading $\tau_{\text{had}} p_T > 60$ GeV eBDT <i>Loose</i> working point
Di-lepton	$m_{\tau\tau} > 100$ GeV opposite charge sign
Veto	veto events with light leptons (e, μ)
Semi-leptonic channel ($\tau_e\tau_{\text{had}}$)	
Trigger	Single electron triggers
Tau	one τ_{had} with $p_T > 25$ GeV eBDT <i>Medium</i> working point
Electron	one e with $p_T > 27$ GeV
Di-lepton	$m_{e\tau} > 100$ GeV opposite charge sign
Veto	veto events with > 2 leptons
Semi-leptonic channel ($\tau_\mu\tau_{\text{had}}$)	
Trigger	Single muon triggers
Tau	one τ_{had} with $p_T > 25$ GeV eBDT <i>Loose</i> working point
Muon	one μ with $p_T > 27$ GeV
Di-lepton	$m_{\mu\tau} > 100$ GeV opposite charge sign
Veto	veto events with > 2 leptons
Light leptons regions ($ee, \mu\mu, e\mu$)	
Trigger	Single electron and single muon triggers
Leptons	exactly $2e/2\mu/1e1\mu$ in $ee/\mu\mu/e\mu$ channels respectively Leading lepton $p_T > 27$ GeV Subleading lepton $p_T > 27$ GeV
Di-lepton	$m_{\ell\ell} > 100$ GeV opposite charge sign
Veto	veto events with hadronic taus
Same sign regions ($\tau_{\text{had}}\tau_{\text{had}}, \tau_e\tau_{\text{had}}, \tau_\mu\tau_{\text{had}}$)	
Same selection as for the respective channels, but requiring two leptons with same charge sign	

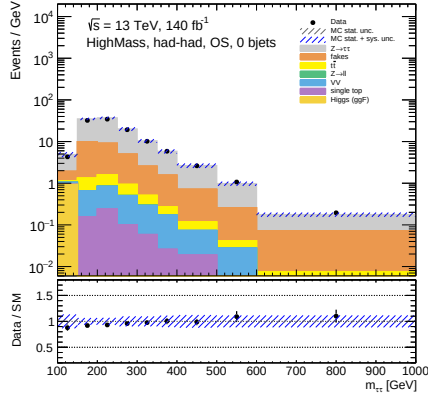
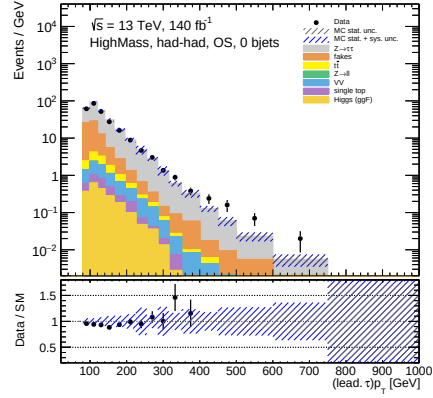
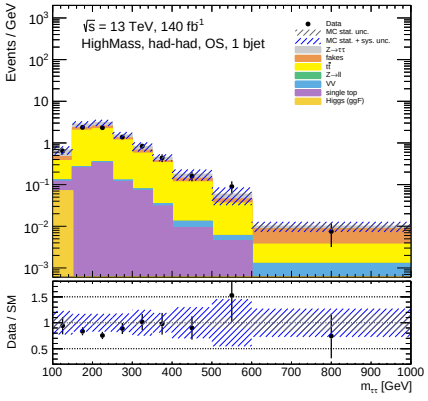
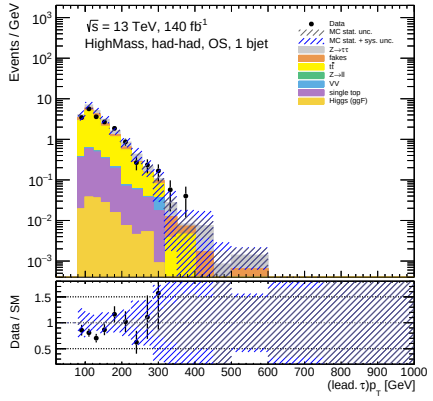
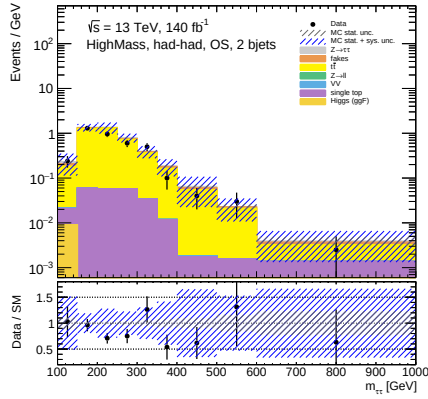
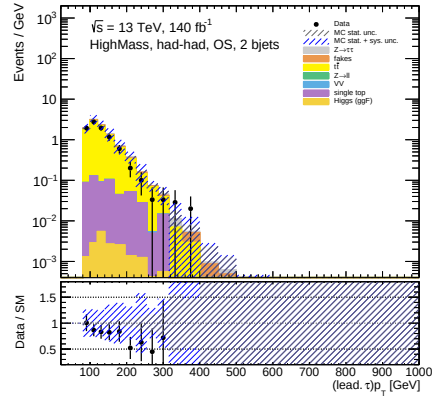
(a) $m_{\tau\tau}$, 0 b -jets(b) Leading tau p_T , 0 b -jets(c) $m_{\tau\tau}$, 1 b -jets(d) Leading tau p_T , 1 b -jets(e) $m_{\tau\tau}$, 2 b -jets(f) Leading tau p_T , 2 b -jets

Figure 4.9. Distributions in the fully hadronic channel $\tau_{\text{had}}\tau_{\text{had}}$ for the di-tau visible invariant mass $m_{\tau\tau}$ and the leading tau p_T , drawn separately for events in different b -jets multiplicity categories.

The semi-leptonic channel $\tau_e\tau_{\text{had}}$

Events are selected in the semi-leptonic channel $\tau_e\tau_{\text{had}}$ using the single electron triggers. These triggers are preferred to the single-tau ones since they have lower thresholds and enable to efficiently select events in the phase space region probed by this analysis.

Exactly one hadronic tau and one electron are required in the final state. The required electron is generated from the leptonic decay of a tau lepton in the electronic channel, however it is reconstructed exactly as a prompt lepton, as in ATLAS these two cases are currently indistinguishable. A veto is also applied on events presenting more than two leptons, to prevent the selection of final states containing muons. The tau lepton is required to have $p_T > 25$ GeV, while the electron needs to verify $p_T > 27$ GeV. The eBDT discriminant variable is used, to reject electrons misidentified as fake hadronic taus. The *Medium* working point is chosen in this channel, as an enhanced quantity of these objects is expected. A cut in the di-lepton invariant mass is applied, $m_{e\tau} > 100$ GeV, to select events in the high mass range, and the two final state leptons are required to have opposite electric charge sign. As in the hadronic channel, the selection is inclusive in the presence of b -jets, and events are categorised according to b -jets multiplicity, as further detailed in a following section. Figure 4.10 shows the distributions of the di-lepton invariant $m_{e\tau}$ and of the tau lepton p_T , drawn separately in the different b -jets categories.

The semi-leptonic channel $\tau_\mu\tau_{\text{had}}$

The selection in the semi-leptonic channel $\tau_\mu\tau_{\text{had}}$ is triggered by the single-muon triggers. As in the $\tau_e\tau_{\text{had}}$ channel these triggers are used, instead of the single-tau triggers, as they yield a better selection efficiency in the analysis phase space.

Exactly one hadronic tau and one muon are required in the final state. The muon originates from a tau decay, but is reconstructed exactly as a prompt muon, as in ATLAS is not possible to distinguish between these two cases. A veto is added to discard events with more than two leptons, in order to avoid contamination from final states containing electrons. The final state hadronic tau must verify $p_T > 25$ GeV, and the final state muon should have $p_T > 27$ GeV. The eBDT discriminant variable is used to reject electrons misidentified as fake hadronic taus. The *Loose* working point is selected in this channel as, similarly to the hadronic channel, electrons are not part of this channel selection. A cut on the di-lepton invariant mass is applied, $m_{\mu\tau} > 100$ GeV and the two leptons are required to have opposite charge sign. The selection is inclusive in the presence of b -jets in the final state, and events are divided in categories according to b -jets multiplicities, as detailed in a following section. Figure 4.11 shows the distributions for the di-lepton invariant mass $m_{\mu\tau}$ and for the tau lepton p_T , drawn separately in the different b -jets categories.

Events categorisation in b -jets multiplicity

As mentioned in the previous sections, events selected in the analysis channels are further classified according to the multiplicity of b -jets present in the final state. Three categories are defined, listed in the following:

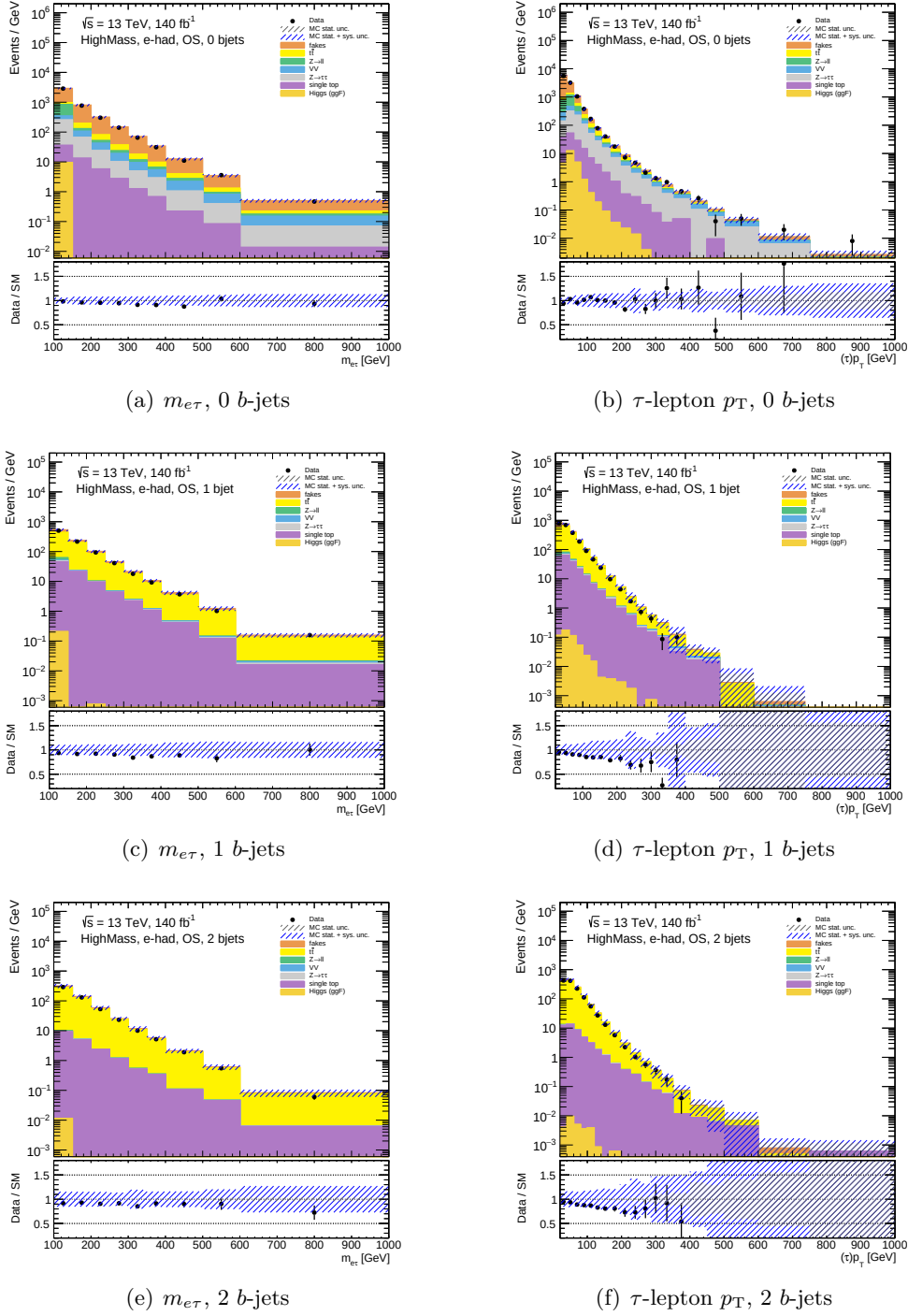


Figure 4.10. Distributions in the semi-leptonic channel $\tau_e\tau_{\text{had}}$ for the di-tau visible invariant mass $m_{e\tau}$ and the leading tau p_T , drawn separately for events in different b -jets multiplicity categories.

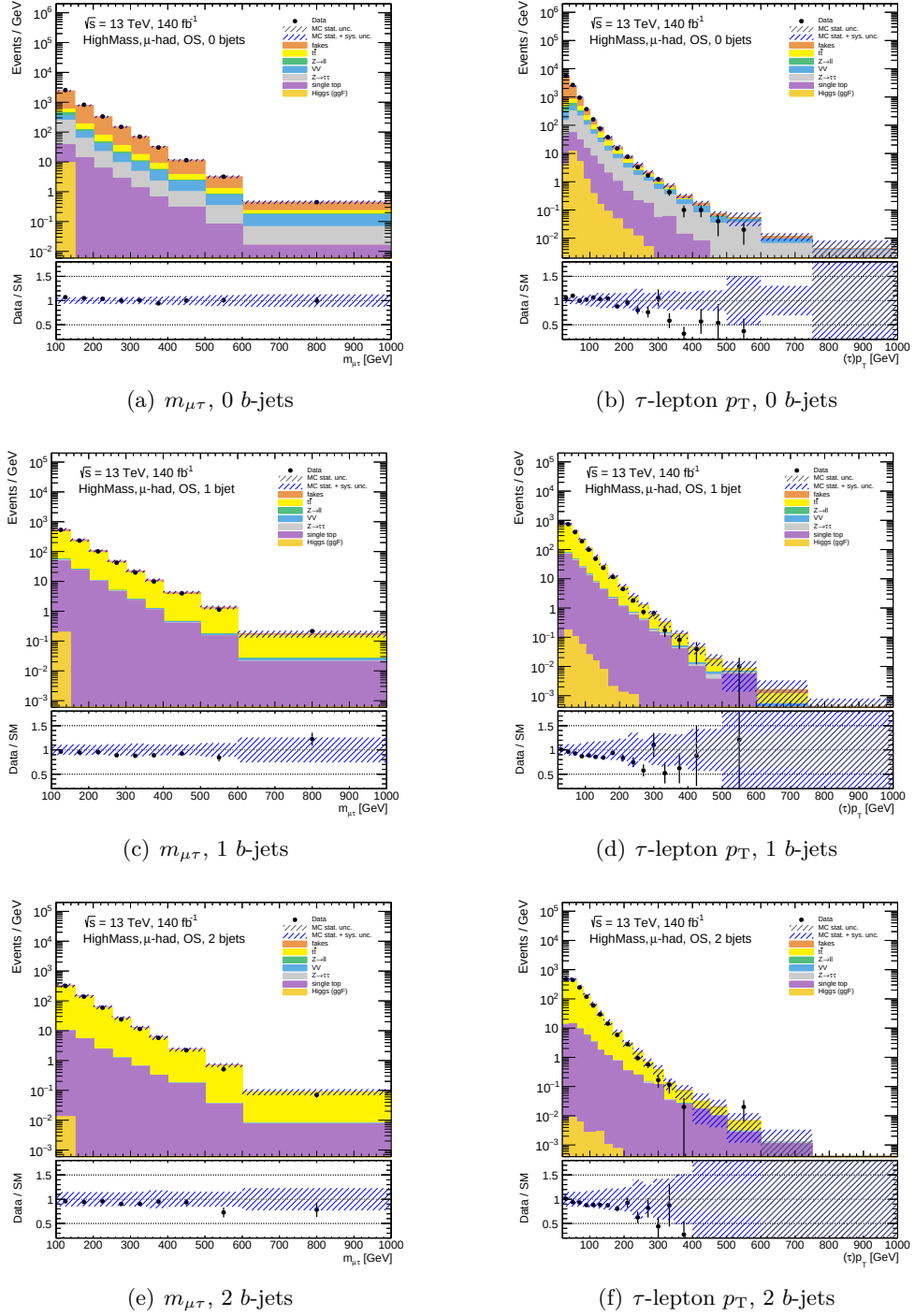


Figure 4.11. Distributions in the semi-leptonic channel $\tau_\mu\tau_{\text{had}}$ for the di-tau visible invariant mass $m_{\mu\tau}$ and the leading tau p_T , drawn separately for events in different b -jets multiplicity categories.

- **0b**: the final state includes no b -jets;
- **1b**: the final state includes one b -jet, radiated from the initial state;
- **2b+**: the final state includes two or more b -jets radiated from the initial state.

The events multiplicity varies across the three categories, the first being by far the most populated, the last being the least populated of the three.

Signal region

The analysis signal region (SR) is defined to include the phase space region in which the largest amount of signal events is located. It is defined as a joint combination of several analysis channels and b -jets event categories. The leptoquark signal process produces final states with two taus, eventually accompanied by the emission of up to one b -jet, radiated from the initial state. The signal region is therefore defined to include events falling in the three analysis channels, $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_e\tau_{\text{had}}$, $\tau_\mu\tau_{\text{had}}$, and in the 0b or 1b categories, as also shown graphically in Figure 4.8.

Top control region

The top background, constituted of single top and $t\bar{t}$ events, is one of the major backgrounds of the analysis. It yields relevant contributions in the fully hadronic channel and is the dominant background in both the semi-leptonic channels, $\tau_e\tau_{\text{had}}$ and $\tau_\mu\tau_{\text{had}}$. Top background events in the SR are mainly located in the 1b category, since b -jets are present, generated by the top-quark decays. The Monte Carlo simulation has a finite precision in modelling this background, hence the top control region (CR) is defined to constraint this background and improve its MC estimate in the SR. The top CR includes events falling in the three analysis channels, $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_e\tau_{\text{had}}$, $\tau_\mu\tau_{\text{had}}$ in the 2b+ region. No leptoquark signal events are expected in this region, which is enriched in single top and $t\bar{t}$ events, as also confirmed in the kinematical distributions in Figures 4.9, 4.10, 4.11. A joint SR plus CR likelihood fit is performed, as will be detailed in Section 4.9, fitting Monte Carlo yields to data in the top CR and determining a fine tuning of the top background in the SR.

4.5.2 The light leptons validation region

The light leptons validation region (VR) is used in the analysis strategy to check the agreement between data and the background predictions obtained via the Monte Carlo simulation. This validation region is spread across three light leptons channels ee , $\mu\mu$, $e\mu$, collecting di-electron, di-muon and electron-muon final states respectively.

Distributions of the di-lepton invariant mass and the leading lepton p_T are shown in Figure 4.12. The same-flavour ee and $\mu\mu$ channels are enriched in events generated from the $Z \rightarrow \ell\ell$ Drell-Yan production, $\ell = e, \mu$ being the lepton of the proper flavour. A minor component of di-boson events is also present, generated by Z decays into lepton pairs, accompanied by the hadronic decay of another W or Z boson, or by W -boson pairs, decaying into leptons of the same flavour. The different flavour $e\mu$ channel is, instead, mainly enriched in $t\bar{t}$ and di-boson events. In both cases different flavour leptons are generated in the final state by the decay of a pair

of W -bosons, either originating from the top-quark pair decay or directly from the di-boson production.

Events are selected in the light lepton channels using single-electron or single-muon triggers, or combinations of both. Exactly two light leptons are required in the final state, either two e , or two μ , or one e and one μ , depending on the considered channel. A veto on hadronic taus is applied, to avoid contamination of events falling in the analysis channels $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_e\tau_{\text{had}}$, $\tau_\mu\tau_{\text{had}}$. The leading and the sub-leading light leptons are both required to have minimum transverse momentum $p_T > 27$ GeV, and should have an opposite electric charge sign. Moreover, the di-lepton system is required to have high invariant mass $m_{\ell\ell} > 100$ GeV. As for the analysis channels, this VR is inclusive in the presence of b -jets, and final states with zero, one, two or more b -jets are accepted in the selection.

The validation region is not included in the SR + CR likelihood fit of the analysis (see Section 4.9), hence it does not contribute to the fine-tuning of the backgrounds in the SR, but is only used to check the consistency between data and the MC prediction within its uncertainty.

4.5.3 The same sign validation region

A second validation region (VR), called same sign VR, is included in the analysis strategy, as also shown in Figure 4.8. This VR is used to test the accuracy of the data-driven estimate of the events containing hadronic jets misidentified as fake hadronic taus, which is done via the Fake Factors method. Events selected in this region verify exactly the same requirements used for the analysis SR and CR, with the exception that the final state leptons are required to have the same sign of the electric charge, instead of the opposite one. This ensures that at least one tau is a fake lepton, since real taus, originated from the decay of a neutral Z boson, must necessarily have opposite electric charge. The region is extended across the analysis channels, $\tau_{\text{had}}\tau_{\text{had}}$, $\tau_e\tau_{\text{had}}$, $\tau_\mu\tau_{\text{had}}$, and is divided into categories with different b -jets multiplicity, according to whether the number of b -jets is zero, one, two or more. More details on the data-driven estimate of the fake taus background can be found in Section 4.6.

4.6 Data-driven estimate of the fake taus background

One of the most relevant backgrounds of this analysis is the tau fakes background, constituted of all the di-tau events, in which at least one of the two taus is originating from an hadronic jet misidentified as a fake hadronic tau. This background cannot be estimated via the Monte Carlo simulation, since the current precision of the multijet events modelling is not sufficient to have a reliable prediction. Therefore, a data-driven technique has been utilised, called the *Fake Factors method*, which is described in detail in Chapter 3 of this thesis, since the author has participated in the validation of the method with di-tau final states.

As described in Section 3.2.1, the Fake Factors method is based on the separation of the analysis SR phase space into two sub-regions, the SR ID and the SR anti-ID. Events are included in the ID or anti-ID sub-region according to whether the final state taus verify or not the tau identification requirement. Fake Factors (FF) are

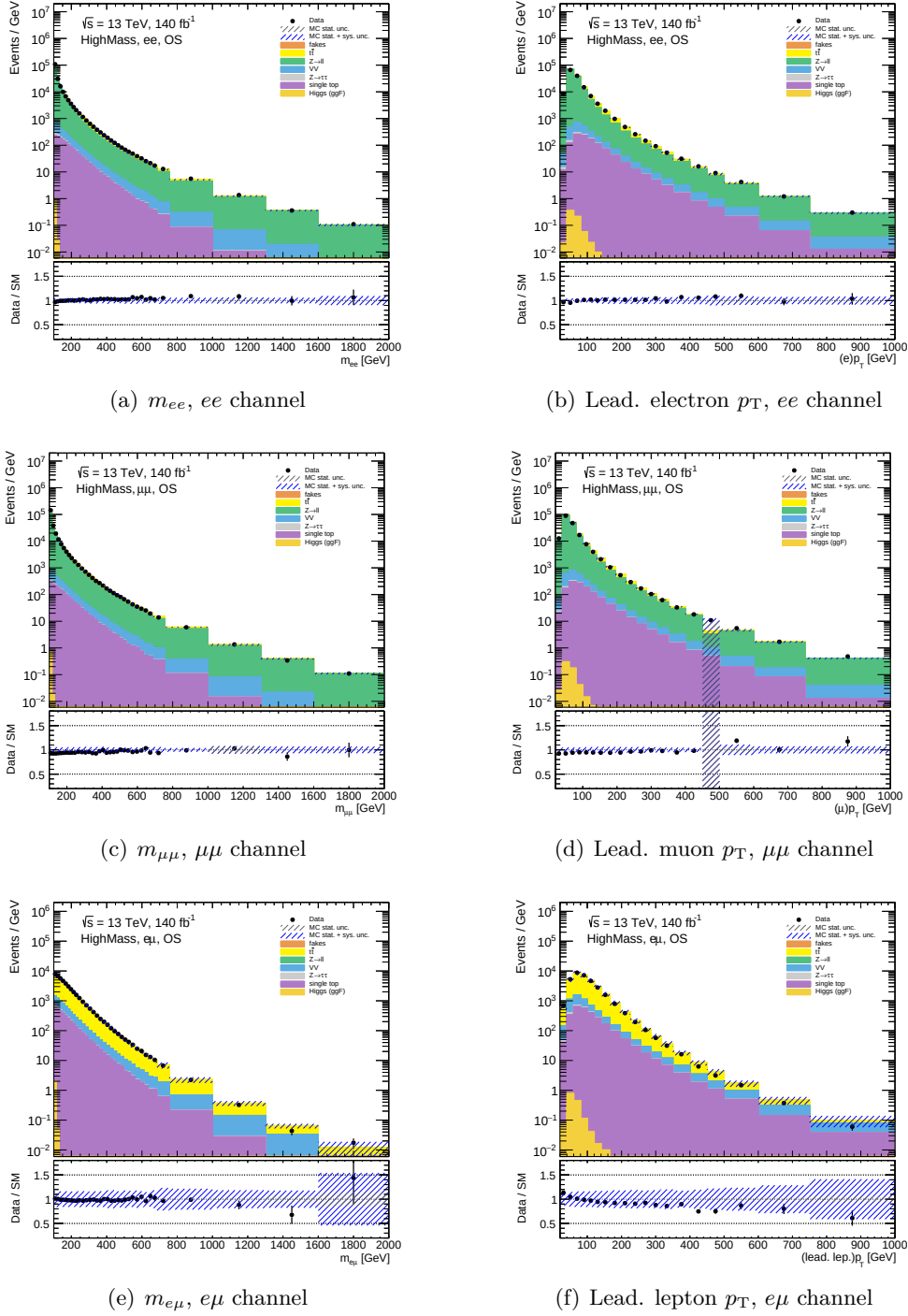


Figure 4.12. Distributions of the di-lepton invariant mass and leading lepton p_T in the light lepton channels. The distributions shown are inclusive across the b -jets categories.

evaluated and used to extrapolate the background in the SR ID, from the measured data yields in the SR anti-ID (i.e. they are *transfer factors* from the SR anti-ID to the SR ID).

In this implementation of the FF method, the *Tight* working point of the tau RNN identification algorithm (see Section 2.3.7) is adopted to classify events as ID or anti-ID.

4.6.1 Combined fake factors evaluation

As mentioned in detail in Section 3.2.2, several sources of fake taus exist, each one originating objects characterised by a different probability of inducing the reconstruction of a fake tau. For this reason, the FFs cannot be calculated directly in a suitable control region, but are obtained as combination of primitive FFs, measured in regions enriched in a single source of fake taus. In this analysis we consider the following possible sources of fake taus:

- hadronic jets originating from a quark (*quark jets*);
- hadronic jets originating from a hard scatter gluon (*gluon jets*);
- hadronic jets originating from pile-up activity (*pile-up jets*).

We mention that the source of b -jets misidentified as fake taus should have been in principle also considered, since the analysis is inclusive in such type of jets and the top and $t\bar{t}$ processes are the most relevant ones among the backgrounds, but this has not been possible since the primitive templates and fake factors for this source have been released only when the analysis was already in an advanced state of progress. Following the description detailed in Section 3.2.2, the combined FFs will be obtained as:

$$\text{FF}_{\text{comb}} = \mu_Z \text{FF}_Z + \mu_{\text{MJh}} \text{FF}_{\text{MJh}} + \mu_{\text{MJl}} \text{FF}_{\text{MJl}} , \quad (4.3)$$

where FF_Z , FF_{MJh} , FF_{MJl} are the primitive FFs measured in the regions enriched in quark-/gluon-/pile-up jets respectively and the μ_Z , μ_{MJh} , μ_{MJl} are the fractions representing the relative abundance of the fake taus sources in the analysis SR.

The primitive FFs measurement is described in Section 3.3 of this thesis, and their values are graphically displayed in Figure 3.4. The μ_x fractions, instead, are evaluated from a fit, performed on templates of the jet-width variable, defined as the p_T -weighted average of the angular separation between the jet constituents and the jet axis:

$$j = \frac{\sum_i p_T^i \Delta R^i}{\sum_i p_T^i} . \quad (4.4)$$

The fractions are obtained as the values that best represent the template for the analysis data in the SR anti-ID as a linear combination of the primitive templates, measured jointly with the primitive FFs in the respective regions.

Fake factors are measured in multi-dimensional bins of the phase-space, and a different fake factor is derived for each different bin. Hence, the linear combination in Eq. (4.3) and the template fit procedure is iterated several times, once for each bin. Figure 4.13 shows an example of primitive and fitted template distributions, for one particular exemplary bin.

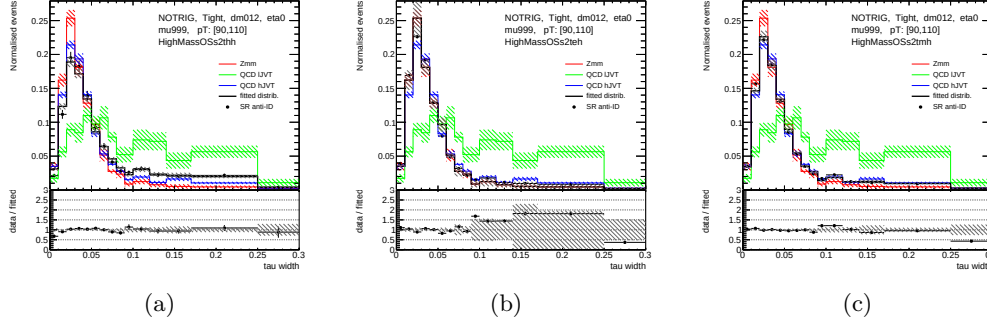


Figure 4.13. Primitive and fitted template distributions in one exemplary bin: 1-prong, $p_T \in (90, 110)$, $\eta \in [0, 1]$, NOTRIG, opposite sign. Templates are displayed for: (a) $\tau_{\text{had}}\tau_{\text{had}}$ channel, (b) $\tau_e\tau_{\text{had}}$ channel, (c) $\tau_\mu\tau_{\text{had}}$ channel.

Table 4.6. Binning used for the evaluation of the combined FFs in the High Mass Drell-Yan analysis. The same binning is used in all the analysis channels.

Variable	Bin edges	Comment
τ_{had} decay mode	1-prong, 3-prong	—
τ_{had} p_T [GeV]	20, 30, 40, 50, 70, 90, 110, 13000	FF = 0 if $p_T < 50$ GeV in $\tau_{\text{had}}\tau_{\text{had}}$ channel
τ_{had} $ \eta $	0., 1., 1.37, 1.52, 2.50	FF = 0 for $ \eta \in [1.37, 1.52]$
Trigger condition	TRIG, NOTRIG	TRIG only in $\tau_{\text{had}}\tau_{\text{had}}$ channel
Di-tau sign condition	same sign, opposite sign	—

Choice of the binning for the Fake Factors evaluation

The FFs are evaluated in multi-dimensional bins, which are portions of the phase-space restricted to some intervals of the tau kinematic variables and characteristics. The FFs are calculated independently and are assumed constant within each of these bins. Hence, the binning has to be sufficiently thin to make the constant FF assumption acceptable. At the same time the binning has to be sufficiently large to limit the statistical fluctuations in the primitive FFs and templates, which increase with decreasing dimension of the bins.

Table 4.6 shows the binning strategy adopted for the fake taus background estimate in the High Mass Drell-Yan analysis. FFs are evaluated separately for 1-prong and 3-prong tau decays, while no distinction is made on the number of neutrals emitted in association with the charged decay products. Seven bins in tau p_T and three bins in tau η are utilised to segment the tau kinematical phase space. In the fully hadronic channel, the FFs are set to zero for taus with $p_T < 50$ GeV, since only taus with higher transverse momentum can exist due to the analysis selections. Similarly, the FFs are assumed null for taus falling in the rapidity range corresponding to the transition region between barrel and end-cap, $\eta \in [1.37, 1.52]$, as no fake tau can be measured in such non-instrumented region of the detector. In the hadronic channel FFs are further differentiated according to whether the tau trigger condition is satisfied (TRIG) or not (NOTRIG). This distinction is not possible in

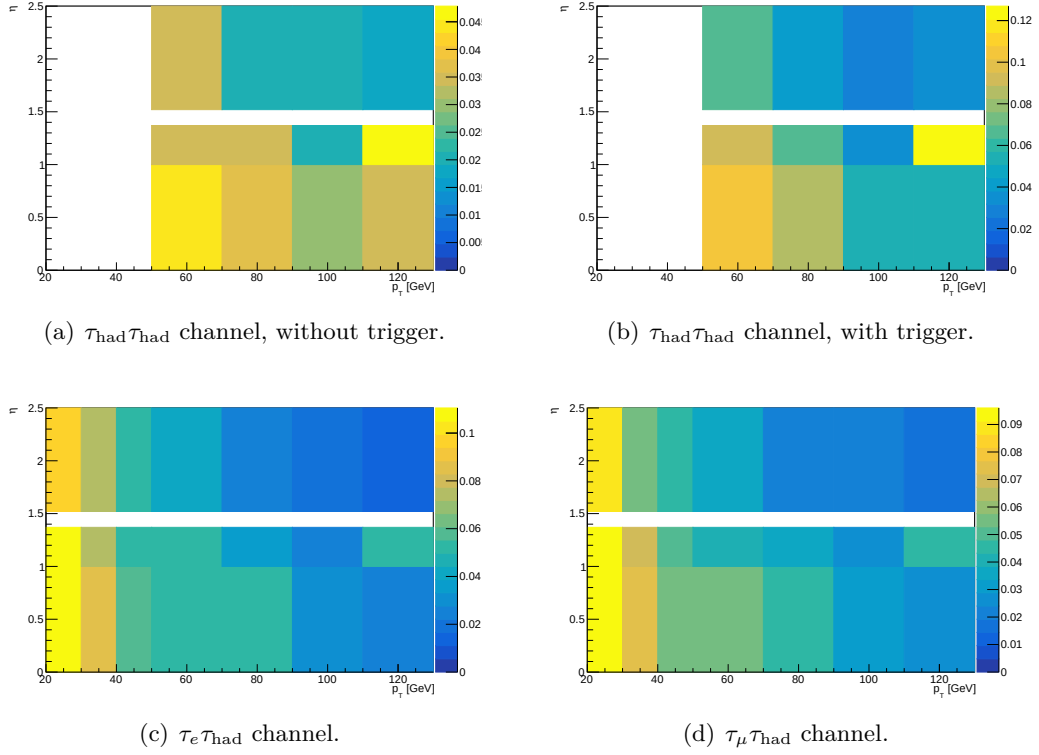


Figure 4.14. Combined FF maps evaluated for the High Mass Drell-Yan analysis. Maps are drawn in the (p_T, η) space for the opposite sign region, in the 1-prong bin, for all the analysis channels. For the $\tau_{\text{had}}\tau_{\text{had}}$ channel, maps are drawn separately in the NOTRIG and TRIG bins.

the semi-leptonic channel, since tau triggers are not used and events are pre-selected via the light leptons triggers. Finally, a further distinction is made according to the di-tau charge product sign. Different FFs are derived for the opposite sign region (OS), where the analysis background is extrapolated, and the same sign region (SS), where the fake background estimate is validated.

Estimated fake factor maps

The FFs have been evaluated, using the fit model reported in Eq. 4.3. The resulting FFs are on average of the order of 5 – 10%, as shown in the example maps reported for all the analysis channels in Figure 4.14.

An uncertainty has been associated to each FF central value, following the guidelines reported in this thesis in Section 3.4. The systematic uncertainty associated with the variability of the FFs due to their neglected dependence on variables other than the ones considered is neglected in this analysis. Moreover, the modelling uncertainty, associated with the choice of the Monte Carlo generator to simulate the truth component events is negligible, as it is further detailed in Section 4.6.3.

The following statistical uncertainty sources have instead been considered:

- uncertainty due to limited statistics of the fitted data template;

- uncertainty due to the limited statistics of the primitive templates;
- uncertainty associated to the primitive FFs.

These three uncertainties have been estimated using the alternative procedure based on variance sampling, proposed by the author as an alternative strategy to the traditional uncertainty propagation, and described in detail in Section 3.4.1. Multiple fits are iterated, considering the data and primitive templates varied according to the statistical uncertainty of each bin-content, and bands have been derived from the standard deviation of the series of fit results. The reader is referred to Section 3.4.1 for every detail on this procedure. On average, the uncertainty band associated with the FFs ranges from 5% to 25% of the central central value.

4.6.2 Background extrapolation

Given the combined FFs, the fake taus background is extrapolated in the SR ID (i.e. the analysis SR) starting from the measured data yields in the SR anti-ID. The extrapolation is different between the fully hadronic channel and the semi-leptonic channel: in the first case the final state includes two hadronic taus, while in the second case only one hadronic tau is present in the final state, since the electrons and muons originated in the tau leptonic decay are reconstructed exactly as prompt light leptons. In both cases, the *truth subtraction* is done, to remove from the extrapolated background any contribution of event yields associated with contamination of true taus or light leptons originating fake taus, as referred more in detail in Section 3.2.1.

Extrapolation in the fully hadronic channel

In the fully hadronic channel, the final state includes two hadronic taus, hence the background extrapolation has to account for all the possible types of fake events, generated by the presence of one or both fake taus. The correct background yield is described by the combinatorial formula in Eq. (3.12) of Section 3.2.3.

Operatively, events are classified according to the following categories:

- $N_{\text{antiID1,passID2}}$: the leading tau fails the identification requirement (anti-ID) and the sub-leading passes it (pass-ID);
- $N_{\text{passID1,antiID2}}$: the leading tau passes the identification requirement and the sub-leading fails it;
- $N_{\text{antiID1,antiID2}}$: both taus fail the identification requirement.

These three yields are evaluated both in data and in all Monte Carlo simulated events and subtracted, after having being combined with the FFs, (see Eq. (3.12)), to obtain the fake taus background estimate.

The background extrapolation in the analysis SR is validated in the same-sign validation region (VR). This VR, enriched in fake taus, has the same selection as the SR except for the reversed requirement on the final state leptons charge product. The extrapolated background in the VR, for the fully hadronic channel, is shown in Figure 4.15, separated in categories of b -jets (refer to Section 3.6.1 for distributions of additional variables). An excellent closure between data and the background

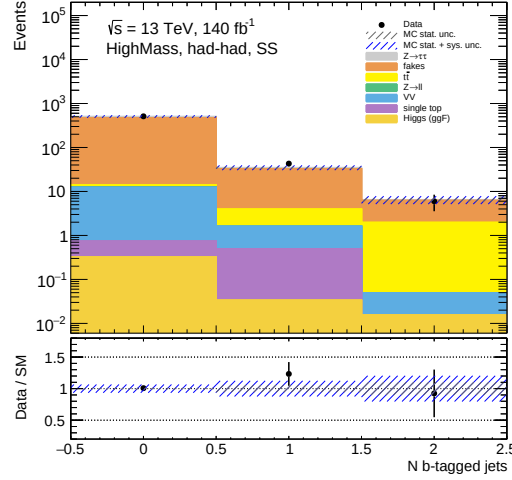


Figure 4.15. Comparison between data and background events in the same sign (SS) validation region in the fully hadronic channel, including the data-driven estimated background of tau fakes.

predictions is shown in the 0 and 2 b -jets categories, while a 20% under-fluctuation of the background is observed in the 1 b -jets category. Possible improvements on the fake taus estimate which could cover this mis-modelling would be either evaluating separately the FFs in bins referred to the different b -jets multiplicities, or, most importantly, introducing a fourth primitive FF in the combination in Eq. (4.3), measured in a region enriched in b -jets, as the $t\bar{t}$ region described in Section 3.3.3 of Chapter 3. Such additional primitive FF has not been considered in this analysis, since the $t\bar{t}$ measurement region has only recently been defined and made available by the ATLAS Tau Combined Performance group. However, since the discrepancy in the 1 b -jet category is fairly covered by the estimated uncertainties, it is considered acceptable, and foreseen not to have a critical impact on the results of this analysis.

Extrapolation in the semi-leptonic channel

The background extrapolation is simpler in the semi-leptonic channel, since the final state comprises only one hadronic tau and therefore is not necessary the combinatorial expression adopted for the hadronic channel. The simpler expression in Eq. (3.5) of Section 3.2.1 is utilised: the yields in the anti-ID SR are simply rescaled by the FFs referred to the only available tau in the final state. The event yields are evaluated both on data and on all Monte Carlo simulated events, and subtracted to obtain the final background yield, as reported in Eq. (3.5).

Figure 4.16 shows the background estimate validation in the same-sign region, separated in categories of b -jets (refer to Section 3.6.2 for distributions of additional variables). The agreement between the data and the total background prediction is excellent in the $\tau_\mu\tau_{\text{had}}$ channel for all the b -jets categories, as shown in Figure 4.16(b). A slight background overestimation is shown, instead, in the $\tau_e\tau_{\text{had}}$ channel (see Figure 4.16(a)), which is covered by the estimated uncertainty on the background, and hence is not considered to have a critical impact on the analysis results.

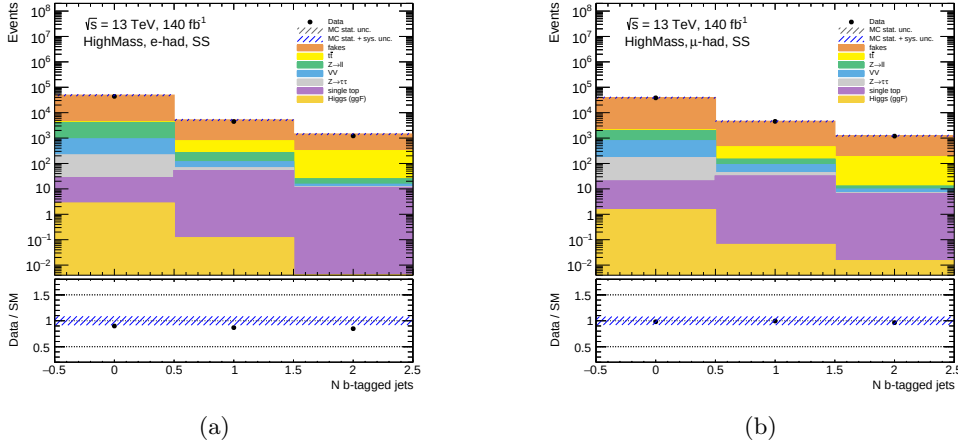


Figure 4.16. Comparison between data and background events in the same sign (SS) validation region for the semi-leptonic channel, including the data-driven estimated background of tau fakes: (a) $\tau_e \tau_{\text{had}}$ channel, (b) $\tau_\mu \tau_{\text{had}}$ channel.

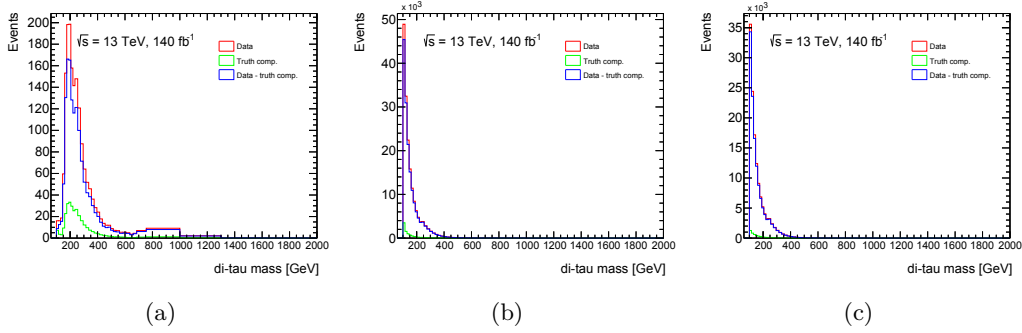


Figure 4.17. Di-lepton invariant mass distribution in the SR ID previous to and after the truth subtraction, and the truth component for: (a) $\tau_{\text{had}} \tau_{\text{had}}$ channel, (b) $\tau_e \tau_{\text{had}}$ channel, (c) $\tau_\mu \tau_{\text{had}}$ channel.

4.6.3 Impact of the truth component subtraction

The FF method is currently formulated to estimate the background of fake taus originating only from hadronic jets. Therefore, every contamination of events containing true taus in the final state, or fake taus originating from sources other than hadronic jets (e.g. light leptons) has to be removed. This is done via the *truth subtraction* procedure, as described in detail in Section 3.2.1 and mentioned before.

The impact of the truth subtraction has been evaluated a posteriori, and is shown in Figure 4.17, reporting the di-lepton invariant mass distribution previous to and after the truth subtraction, as well as the truth component distribution, for all the analysis channels. The truth component is negligible in the $\tau_e \tau_{\text{had}}$ and $\tau_\mu \tau_{\text{had}}$ channels, while is small but non-negligible in the $\tau_{\text{had}} \tau_{\text{had}}$ channel.

The subtraction of the truth component can constitute an additional source of uncertainty, since this component is evaluated via the Monte Carlo simulation and is therefore affected by the modelling uncertainty associated to the chosen generator.

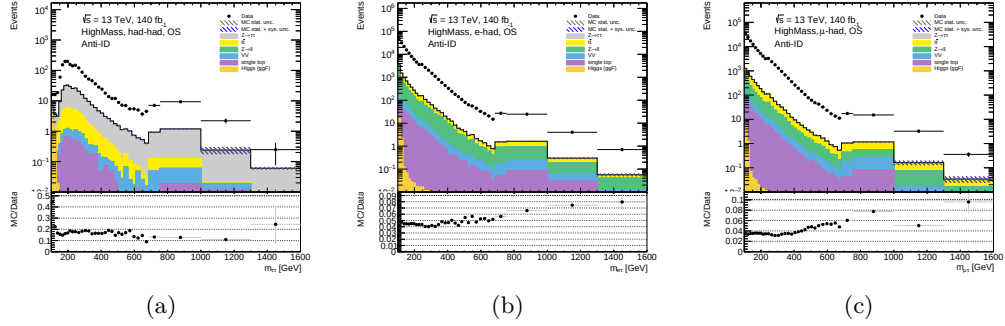


Figure 4.18. Di-lepton invariant mass distribution in the SR anti-ID for data and the truth component for: (a) $\tau_{\text{had}}\tau_{\text{had}}$ channel, (b) $\tau_e\tau_{\text{had}}$ channel, (c) $\tau_\mu\tau_{\text{had}}$ channel.

This uncertainty component is however expected to have a very small impact, since, as shown in the distributions in Figure 4.18, the truth component in the SR anti-ID is very small (one or two orders of magnitude less) than the data yields. We therefore neglect this uncertainty in all what follows.

4.7 Experimental systematic uncertainties

The experimental systematic uncertainties represent the imprecision associated to the ATLAS detector. They originate from our imperfect knowledge of the experimental apparatus and affect the reconstruction of the physics objects involved in the analysis final state. Analysis independent sets of these uncertainties are derived within the ATLAS Combined Performance groups, and associated with each reconstructed object in the ATLAS experiment. Only subsets of these uncertainties have been considered this analysis, selected as the ones that have the largest effect on the di-lepton invariant mass distribution used for the statistical analysis.

4.7.1 Overview of the experimental uncertainties

The experimental systematic uncertainties considered in the analysis are reported in Table 4.7 for the triggers and leptons, and in Table 4.8 for the jets and flavour tagging. These tables include only the selected systematics, according to the criteria further reported in Section 4.7.2. More details on each uncertainty source is given in what follows.

Luminosity uncertainty

The Run 2 integrated luminosity has been measured combining the information from several ATLAS sub-detectors and is affected by uncertainty. The uncertainty on the Run 2 luminosity has been found to be of the order of 1%, as outlined in Ref. [82].

Pile-up uncertainty

An uncertainty on the pile-up distribution in simulated events is also assessed. In Monte Carlo simulated events, only the best-guess of the data pile-up conditions are

Table 4.7. Summary of the experimental systematic uncertainties related to triggers, taus and light leptons.

Systematic uncertainty	Description
Tau triggers	
TAUS_TRUEHADTAU_EFF_TRIGGER_STATDATA[16,17,18]	Tau trigger SFs uncertainty: statistics in data
TAUS_TRUEHADTAU_EFF_TRIGGER_STATMC[16,17,18]	Tau trigger SFs uncertainty: statistics in MC
TAUS_TRUEHADTAU_EFF_TRIGGER_SYST[16,17,18]	Tau trigger SFs systematic uncertainty
Hadronic taus	
TAUS_TRUEHADTAU_SME_TES_DETECTOR	Tau energy scale uncertainty: detector to single particle response
TAUS_TRUEHADTAU_SME_TES_INSITUEXP	Tau energy scale uncertainty: <i>in-situ</i> from experimental measurement
TAUS_TRUEHADTAU_SME_TES_INSITUFIT	Tau energy scale uncertainty: <i>in-situ</i> from fit
TAUS_TRUEHADTAU_SME_TES_MODEL_CLOSURE	Tau energy scale uncertainty: modelling
TAUS_TRUEHADTAU_SME_TES_PHYSICSLIST	Tau energy scale uncertainty: physics list
TAUS_TRUEHADTAU_EFF_RECO_TOTAL	τ_{had} reconstruction efficiency uncertainty
TAUS_TRUEHADTAU_EFF_RNNID_1PRONGSTATSYSTPTGE40	τ_{had} identification efficiency uncertainty for 1-prong decays and $p_T \geq 40$ GeV
TAUS_TRUEHADTAU_EFF_RNNID_3PRONGSTATSYSTPTGE40	τ_{had} identification efficiency uncertainty for 3-prong decays and $p_T \geq 40$ GeV
TAUS_TRUEHADTAU_EFF_RNNID_HIGHPT	τ_{had} identification efficiency uncertainty for $p_T > 100$ GeV
TAUS_TRUEHADTAU_EFF_RNNID_SYST	τ_{had} identification efficiency systematic unc.
TAUS_TRUEELECTRON_EFF_ELEBDT_STAT	eBDT efficiency uncertainty
TAUS_TRUEHADTAU_EFF_ELEOLR_TOTAL	Overlap removal τ_{had} - e efficiency uncertainty
Electrons	
EG_SCALE_ALL	Energy scale total uncertainty
EL_EFF_Reco_SIMPLIFIED_UncorrUncertaintyNP8	Electrons reconstruction efficiency unc.
EL_EFF_Iso_SIMPLIFIED_UncorrUncertaintyNP[8,17]	Electrons isolation efficiency uncertainties
Muons	
MUON_ID	p_T resolution uncertainty: inner detector
MUON_MS	p_T resolution uncertainty: muon system
MUON_SAGITTA_RESBIAS	Momentum scale uncertainty covering local mis-alignment effects
MUON_SCALE	Momentum scale uncertainty
MUON_EFF_RECO_STAT	Muon reconstruction efficiency statistical uncertainty (for $p_T > 15$ GeV)
MUON_EFF_RECO_SYS	Muon reconstruction efficiency systematic uncertainty (for $p_T > 15$ GeV)
MUON_EFF_ISO_SYS	Muon isolation efficiency systematic unc.
MUON_EFF_TTVA_STAT	Muon track-to-vertex association efficiency: statistical uncertainty
MUON_EFF_TTVA_SYS	Muon track-to-vertex association efficiency: systematic uncertainty

Table 4.8. Summary of the experimental systematic uncertainties related to jets and flavour tagging.

Systematic uncertainty	Description
Jets	
JET_EffectiveNP_Mixed2	JES <i>in-situ</i> analysis uncertainty
JET_EffectiveNP_Modelling[1,2,3]	JES <i>in-situ</i> analysis uncertainty
JET_EffectiveNP_Statistical2	JES <i>in-situ</i> analysis uncertainty
JET_EtaIntercalibration_Modelling	Jet energy calibration unc.: η -intercalibration
JET_EtaIntercalibration_NonClosure_2018data	Jet energy calibration unc.: η -intercalibration
JET_EtaIntercalibration_TotalStat	Jet energy calibration unc.: η -intercalibration
JET_Pileup_OffsetMu	Pile-up uncertainty
JET_Pileup_OffsetNPV	Pile-up uncertainty
JET_Pileup_RhoTopology	Pile-up uncertainty
JET_JER_DataVsMC_MC16	Jet energy resolution total uncertainty
JET_JER_EffectiveNP_[1-11,12restTerm]	Jet energy resolution total uncertainty
JET_Flavor_Composition	q-/g-jets composition uncertainty
JET_Flavor_Response	q-/g-jets composition uncertainty
Flavour tagging	
FT_EFF_Eigen_B_[1,2,3]	<i>b</i> -jet flavour tagging efficiency uncertainty
FT_EFF_Eigen_C_0	<i>c</i> -jets flavour tagging efficiency uncertainty
FT_EFF_Eigen_Light_[0,1,2]	Light-jets flavour tagging efficiency uncertainty
FT_EFF_extrapolation	Flavour tagging efficiency uncertainty extrapolated on high p_T -jets
FT_EFF_extrapolation_from_charm	τ -jets tagging uncertainty extrapolated from <i>c</i> -jets

considered. The simulated pile-up conditions are corrected to match the conditions observed in data via a procedure called *pile-up reweighting*, which is subject to uncertainty. A systematic uncertainty, as large as the rescaling, is assigned to the estimated pile-up distribution, resulting of the order of 2-3%.

Triggers uncertainties

Single- and di-tau triggers are used to pre-select events in the fully hadronic channel. Systematic uncertainties are assessed to quantify imprecision in the trigger scale factors (SFs) evaluation. Two systematic uncertainties are assigned to cover the statistical fluctuation in the measurement of the trigger efficiencies in data and simulated events, from whose ratio the SFs are derived. A third systematic uncertainty is used to cover the uncertainty associated to the measurement procedure (e.g the fact that SFs are measured in regions different from the analysis SR). In the semi-leptonic channel, events are pre-selected via the single-electron and single-muon triggers, and similar uncertainties are available for light-leptons triggers. However, these systematic uncertainties are neglected, since they have a small impact in the analysis.

Hadronic taus uncertainties

Hadronic taus are complex objects to measure and are relevant for this analysis as they are included both in the fully hadronic and semi-leptonic channel final states.

Several systematic uncertainties are introduced to represent indetermination in the calibration of the tau energy scale (TES). More in detail, one systematic represents uncertainties in the detector response to the single particles included in the tau-jet, two systematics represent uncertainties on the *in-situ* energy calibration, and two additional systematics are used to represent modelling uncertainties. Inaccuracy in the tau reconstruction is also considered, with one dedicated systematic uncertainty. Four additional systematics are introduced to represent inaccuracies in the estimate of the RNN tau identification algorithm efficiency. Some of these uncertainties are separately referred to effects related to 1-prong or 3-prong decaying taus, or to taus with high transverse momentum. Finally, additional sources of uncertainty are introduced to represent imprecision in the efficiency estimate of the eBDT algorithm, used to reject electrons originating fake hadronic taus, and of the overlap-removal algorithm between electron and hadronic taus.

Electrons uncertainties

Systematic uncertainties related to electrons have been scrutinised, since these leptons are included in the analysis final state in the semi-leptonic channel $\tau_e \tau_{\text{had}}$. The electron reconstruction and identification efficiencies, and the associated systematic uncertainties, are derived by comparing data and simulated samples in $Z \rightarrow e^+e^-$, $W \rightarrow e\nu$ and $J/\psi \rightarrow e^+e^-$ events, and are provided in bins of p_T and $|\eta|$. Uncertainties related to the energy calibration and to the isolation efficiency are provided too. For the reconstruction and isolation uncertainties, more than 60 correlated systematics are considered and a simplified scheme is adopted, considering only the main uncorrelated uncertainty components. Only three systematic uncertainties on

electrons are finally included in the analysis among the several available: one for the energy scale calibration, one for the reconstruction efficiency and one for the isolation efficiency.

Muons uncertainties

Muons systematic uncertainties have been also scrutinised, as these leptons are present in final states in the semi-leptonic channel $\tau_\mu\tau_{\text{had}}$. The muon scale-factors are calibrated in the $Z \rightarrow \mu^+\mu^-$ and $J/\psi \rightarrow \mu^+\mu^-$ events. For low- p_T muons the J/ψ measurement is more relevant, while for high- p_T muons the measurement at the Z peak plays the leading role. Several uncertainties have been selected to be included in this analysis. Two systematic uncertainties represent the finite p_T resolution, separately in the inner detector (ID) and in the muon system (MS). Two additional uncertainties, represent the inaccuracies in the muon momentum scale measurement, one being particularly referred to effects due to eventual muon chambers mis-alignments. Three additional uncertainties account for imprecision in the reconstruction and isolation efficiencies determination. Inaccuracies in the track-to-vertex association have also been considered, and are represented by two dedicated systematic uncertainties.

Jets uncertainties

Systematic uncertainties on jets are considered in this analysis, as the final state is inclusive in the presence of one or more b -jets. In the jet reconstruction and calibration procedure a full set of around 50 systematics is derived, and several of these are selected to be considered in this analysis. The most relevant uncertainties represent the inaccuracy in the measurement of the jet energy scale (JES) and the finite jet energy resolution (JER). JES and JER uncertainties are parameterised using only a subset of effective nuisance parameters, which is derived by performing a principal component analysis and combining the resulting variations into a minimal set. Three additional systematic uncertainties have been considered to represent specific effects in the η -intercalibration procedure (see Section 2.3.4 for details), while other three uncertainties are used to account for pile-up effects in the jet reconstruction. Some inaccuracy is present also due to the finite precision with which the Monte Carlo simulation is able to predict the quark-/gluon-jets composition and response observed in data, and is accounted for by two additional systematic uncertainties.

Flavour tagging uncertainties

Flavour tagging is used in the analysis to tag the final state jets as originating from a b -quark. The relative uncertainties are therefore included among the ones considered in this analysis. The calibration of flavour tagging scale factors originates approximately 20 different systematic uncertainties related to the tagging of all jet flavours. A principal component analysis is performed to reduce the number of systematic uncertainties to a minimal set. In this analysis, three systematic uncertainties are used to account for inaccuracies in the tagging efficiency of b -jets, c -jets and light-jets respectively. Two additional extrapolation uncertainties are

added: one for b -jets and c -jets with high p_T , and another for the tagging efficiency of tau-jets, extrapolated from the one relative to c -jets.

4.7.2 Uncertainties pruning and smoothing

Pruning criterion

The number of systematics provided by the ATLAS Combined Performance groups to represent the uncertainties related to the physics objects involved in this analysis is about 260. However, many of these uncertainties have sub-percent impact on the di-lepton invariant mass $m_{\ell\ell}$ distribution used to perform the statistical analysis. Such small uncertainties have no power at all in the fit, nor are able to impact the analysis final results. On the other hand, the presence of a high number of nuisance parameters in the fit, associated to the systematic uncertainties, could generate numerical instabilities in its convergence, leading to biased results.

For this reason a *pruning* criterion is adopted to cancel the systematic uncertainties which have a negligible impact in the analysis. The pruning criterion adopted is the following: for each experimental systematic uncertainty, varied at $\pm 1\sigma$, the relative variation with respect to the nominal value is computed in each bin of the $m_{\ell\ell}$ distribution. For each bin the relative statistical uncertainty on the expected number of events is also computed. The experimental uncertainty under examination is neglected if its relative variation is smaller than 10% of the relative statistical uncertainty in every bin of the $m_{\ell\ell}$ distribution. This pruning criterion reduces the initial set of experimental systematic uncertainties, to the sub-set shown in Tables 4.7 and 4.8, and discussed in the previous sections.

Figure 4.19 shows the relative variation of the pre-fit di-lepton invariant mass, in the analysis channels and the 0 b -jets and 1 b -jets categories. As can be seen, hadronic taus uncertainties yield the leading uncertainty component in the had-had channel 0 b -jets, while the uncertainty on fakes is leading in the lep-had channels with 0 b -jets. For the 1 b -jets categories, modelling and statistical uncertainties dominate the experimental ones in all channels.

Gaussian smoothing

The systematic-varied distributions can show large non-physical fluctuations in the content of adjacent bins, caused by the limited statistics of the Monte Carlo simulation. These fluctuations can damage the statistical analysis, since they can generate numerical instabilities in the minimisation procedure of the likelihood fit. For these reason, a *smoothing* procedure is adopted, to reduce the fluctuations in the bin contents of the pre-fit $m_{\ell\ell}$ distribution. In this analysis a Gaussian smoothing is used, with variance parameter set to $\sigma = 2$.

4.8 Modelling uncertainties

The Monte Carlo simulation has a finite precision and is therefore subject to a certain degree of uncertainty. For this reason, modelling systematic uncertainties are introduced in the analysis to represent the limited precision with which the theory

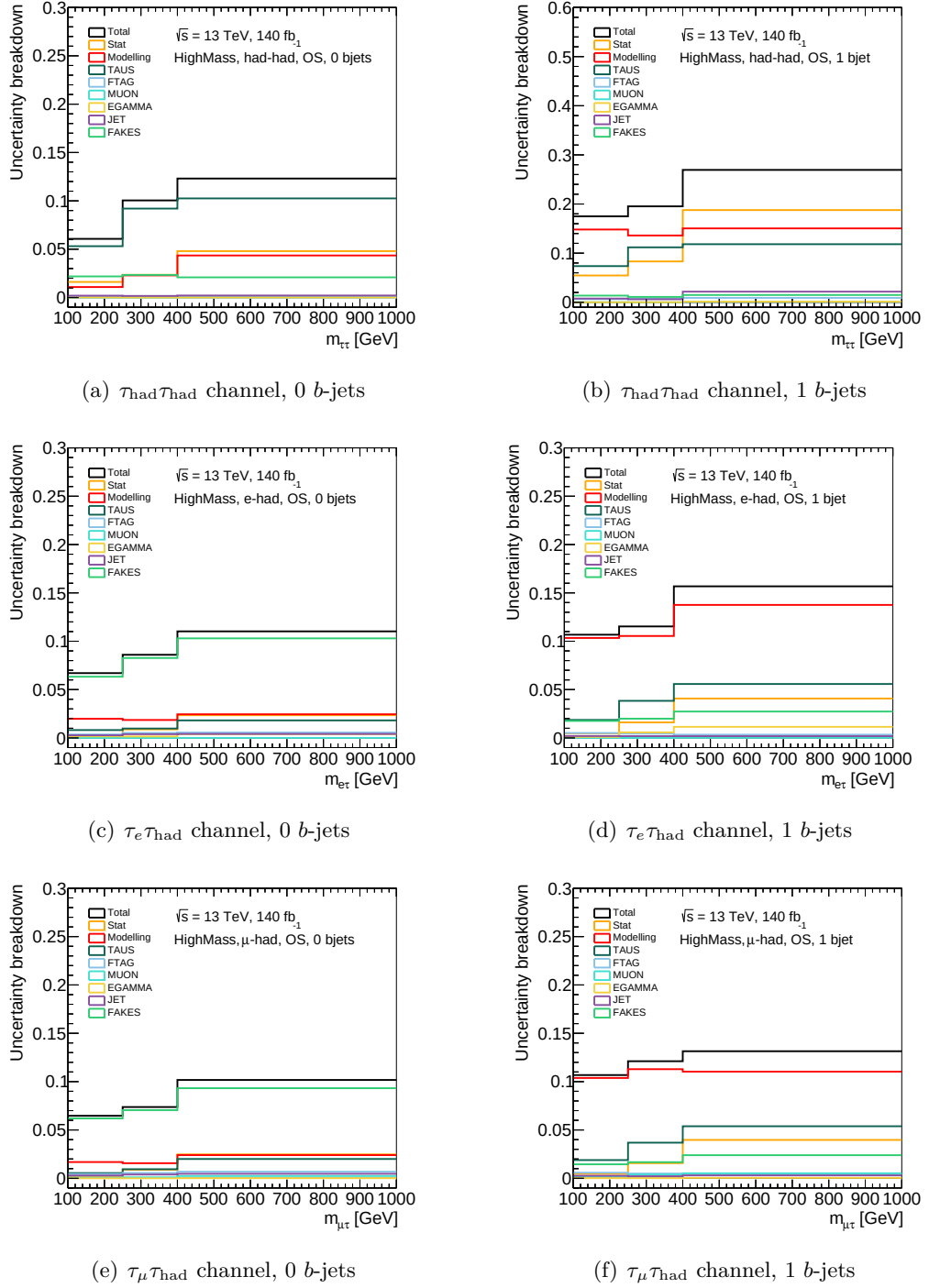


Figure 4.19. Uncertainties breakdown on the pre-fit $m_{\ell\ell}$ distribution in the analysis channels, for the 0 b -jets and 1 b -jets categories. Experimental uncertainties are combined in objects categories and statistical and modelling uncertainties are additionally shown.

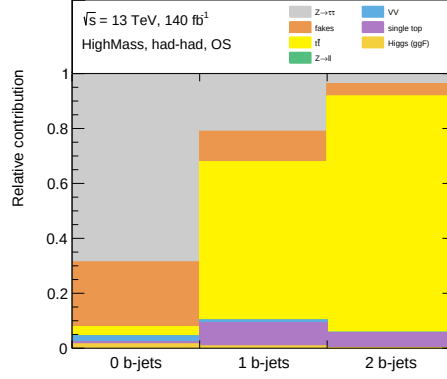


Figure 4.20. Backgrounds composition in the fully hadronic channel, in the different b -jets regions.

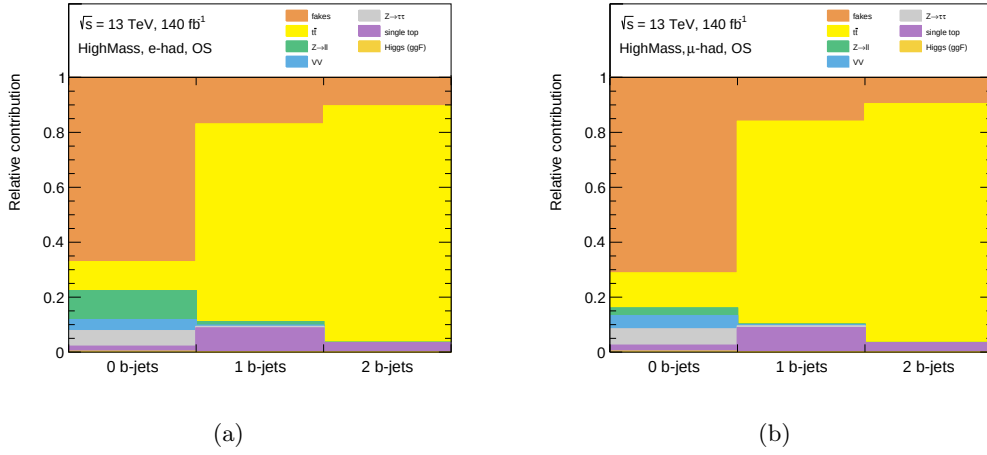


Figure 4.21. Backgrounds composition in the semi-leptonic channel, in the different b -jets regions: (a) $\tau_e \tau_{\text{had}}$ channel (b) $\tau_\mu \tau_{\text{had}}$ channel.

background predictions are obtained. Each Monte Carlo sample, representing a particular physics process, is subject to a set of modelling uncertainties. However, only the modelling uncertainties associated with the dominant backgrounds in the analysis have a relevant impact on the final results. For this reason, before assessing the sub-set of modelling uncertainties relevant for this analysis it is necessary to examine the background composition the different channels.

4.8.1 Background composition in the different channels

The backgrounds composition in the analysis channels is shown in Figure 4.20 and 4.21 for the fully hadronic and the semi-leptonic channels respectively. Further details are added in what follows.

Fully hadronic channel. The backgrounds layout varies considerably across the separate b -jets multiplicity categories. The 0b category, collecting events with no

b -tagged jets, is enriched in di-tau Drell-Yan events and fake taus events. Both these two types of events, in fact, yield real or fake taus in the final state without being associated b -jets. The 1b and 2b+ categories, containing respectively events with one and two or more b -jets, are enriched in single-top and top-quark pair productions, since both these two processes yield b -jets in the final state, originating from the top-quark decay. A minor contribution of di-boson background is also present, mainly located on the 0b category. Di-tau final states can be, in fact, generated either from WW leptonic decays, or from WZ and ZZ decays, in which one Z boson decays into taus and the other vector boson decays hadronically.

Semi-leptonic channel. Similarly to the fully hadronic channel, the background layout varies across the b -jets multiplicity categories, but is substantially the same between the $\tau_e\tau_{\text{had}}$ and $\tau_\mu\tau_{\text{had}}$ sub-channels. The 0b category is dominated by di-tau Drell-Yan events, fake taus events, and a large component of di-lepton Drell-Yan events (here lepton refers to light-leptons). The 1b and 2b+ categories, instead, are enriched in single-top and top-quark pair productions, as in the hadronic channel. A minor contribution of di-boson events is also present, including WW , WZ , ZZ pairs.

4.8.2 Modelling uncertainties assessment

The modelling uncertainties, associated to each sample representing a physical process, can be estimated according to two major strategies. A first strategy is based on the comparison between the predictions obtained with a *nominal* Monte Carlo generator and the ones obtained with an *alternative* generator. This type of modelling uncertainties are called *two-point* and are the most common ones. Another strategy is based instead on the comparison between the predictions of the nominal generator and the ones of the nominal generator but varying the internal weights used to rescale the simulated events. This strategy, called *weight variations based*, is adopted to model the uncertainties associated with the finite order of expansion in α_s in the QCD processes, as well as the uncertainty introduced by the choice of the renormalisation and factorisation scales μ_R and μ_F .

The Monte Carlo generation of events is generally factorised in two steps. A first generator is used to model the matrix element, and hence to evaluate the amplitude of the physical process under study. A second generator is then used to model the induced parton shower, and is connected to the first generator through a matching and merging scheme. Several two-point modelling systematics can therefore be obtained by changing the matrix element generation, the parton shower generation or both at the same time.

Table 4.9 shows the list of the modelling uncertainties utilised in this analysis, comprehensive of both two-point and weight variations based systematics. In addition to the uncertainties listed in the table, parton distribution functions (PDFs) uncertainties are also assessed for the processes. An uncertainty band is derived for each systematic from the difference between the nominal $m_{\ell\ell}$ distribution and the varied one, considering jointly the normalisation and shape differences. All systematics are considered independent and the relative bands are summed in quadrature.

Table 4.9. Summary of the two-point modelling systematics used in the analysis. The abbreviations ME and PS stand for matrix element and parton shower respectively.

Sample	Nominal generator	Alternative generator	Effect described
ttbar	Powheg + Pythia 8	Powheg + Pythia 8 ($p_T^{\text{hard}} = 1$)	Matching and merging
ttbar	Powheg + Pythia 8	Powheg + Herwig 7	PS
ttbar	Powheg + Pythia 8	Powheg + Pythia 8 ($h_{\text{damp}} = 517.5$)	Scale variations
single top	Powheg + Pythia 8 (DR)	Powheg + Pythia 8 (DS)	Interference scheme
single top	Powheg + Pythia 8	Powheg + Herwig 7	PS
Drell-Yan di-tau	Sherpa 2.2.11	Powheg + Pythia 8	ME and PS
Drell-Yan di-lepton	Sherpa 2.2.11	Powheg + Pythia 8	ME and PS
Drell-Yan di-lepton	Sherpa 2.2.11	Sherpa 2.2.11 (varied μ_R and μ_F)	Scale variations

Top-quark pair modelling

The top-quark pair production is simulated via the POWHEGBOX v2 generator for the matrix element calculation and PYTHIA 8 for the parton shower modelling. Uncertainties on the parton shower modelling are assessed by comparing the nominal set-up with the one based on POWHEGBOX v2 for the matrix element and HERWIG 7 for the parton shower. A modelling systematic is also assessed to describe uncertainties arising from the choice of the h_{damp} parameter, which controls the initial state radiation (ISR) recoiling against the $t\bar{t}$ system. Alternative POWHEGBOX v2 + PYTHIA 8 samples are used, with the h_{damp} parameter varied from the nominal value $1.5 \cdot m_{\text{top}}$ to $3 \cdot m_{\text{top}} = 517.5$ GeV. An additional modelling systematic is also introduced to represent the uncertainty associated with the choice of the matching and merging scheme. This uncertainty is assessed by comparing the predictions of the nominal setup, with the ones obtained using POWHEGBOX v2 + PYTHIA 8 generators with parameter $p_T^{\text{hard}} = 1$. Figure 4.22 shows the nominal and varied dilepton mass distributions of $t\bar{t}$ simulated events, with variations evaluated according to each of the assessed modelling systematics.

Single top modelling

Single top quark production is modelled via the POWHEGBOX v2 + PYTHIA 8 generators for the matrix element calculation and parton shower modelling respectively. The uncertainty on the parton shower modelling is assessed, similarly to the top-quark pair production, comparing the nominal predictions to the ones obtained with the alternative POWHEGBOX v2 + HERWIG 7 generators. In the single top production, some diagrams relative to the Wt mode overlap with the ones relative to the top-quark pair production. A removal scheme is therefore needed to avoid double counting of the events associated with the overlap. The diagram removal (DR) scheme [158] is utilised in the nominal Monte Carlo generator, to cancel the overlap at the cross section level, while keeping in the prediction the event counts associated to the interference between Wt and $t\bar{t}$ diagrams, which can yield non negligible contributions in some regions of the phase space. An uncertainty is attributed to the DR scheme, which is assessed comparing the nominal predictions with the ones obtained using another Monte Carlo sample based on the alternative

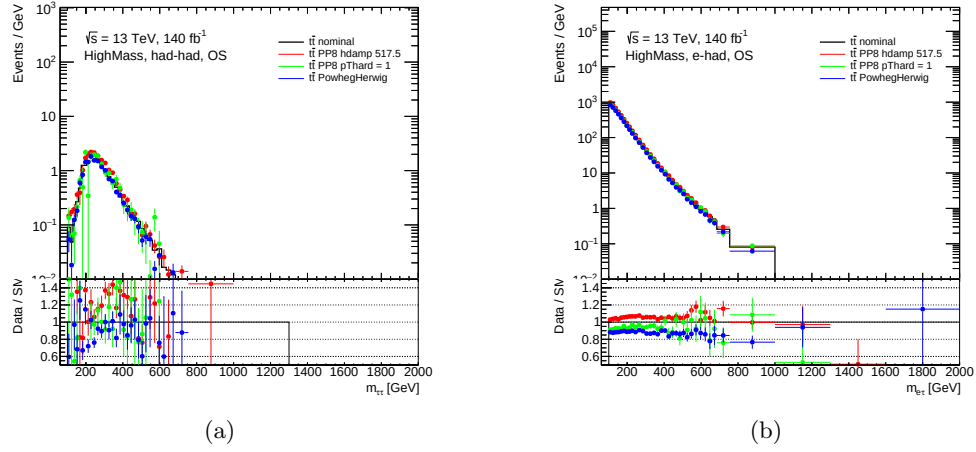


Figure 4.22. Nominal and varied $m_{\ell\ell}$ distributions, according to the considered $t\bar{t}$ modelling systematics, for the (a) $\tau_{\text{had}}\tau_{\text{had}}$ and (b) $\tau_e\tau_{\text{had}}$ channels. The distributions in the $\tau_\mu\tau_{\text{had}}$ are similar to the ones in the $\tau_e\tau_{\text{had}}$ channel.

diagram subtraction (DS) scheme [137, 158]. The nominal and varied di-lepton mass distributions corresponding to each assessed systematic uncertainty are displayed for single top events in Figure 4.23.

Drell-Yan di-tau modelling

The di-tau Drell-Yan process is dominant in all the three channels, since its producing the same final state as the signal process and its diagram is interfering with the signal. The process is modelled with a nominal Monte Carlo simulation based on SHERPA 2.2.11. A modelling uncertainty on the matrix element generator and the parton shower modelling is assessed by comparing the nominal predictions with the ones obtained from the POWHEGBOX v2 + PYTHIA 8 generators. Notice that, since the SHERPA Monte Carlo generator calculates both the matrix element and parton shower development, the modelling uncertainties on these two separate effects have to be evaluated jointly. Figure 4.24 displays the nominal and varied distributions, according to all the assessed modelling systematics, for the di-tau Drell-Yan events.

Drell-Yan di-lepton modelling

Similarly to the di-tau Drell-Yan, the di-electron and di-muon Drell-Yan events are nominally simulated via the SHERPA 2.2.11 generator, accounting for both the matrix element calculation and the parton shower development. A joint modelling systematic on these two effects is assessed by comparing the nominal prediction with the one obtained via the POWHEGBOX v2 + PYTHIA 8 generators. An additional modelling systematic is considered to represent uncertainties associated with the choice of the renormalisation and factorisation scales, μ_R , μ_F . These scales are varied by a factor 0.5 and 2, one at a time and simultaneously, and a band is extracted from the varied distributions envelop using the 7-points scheme. The modelling uncertainty is estimated as half of the envelope band.

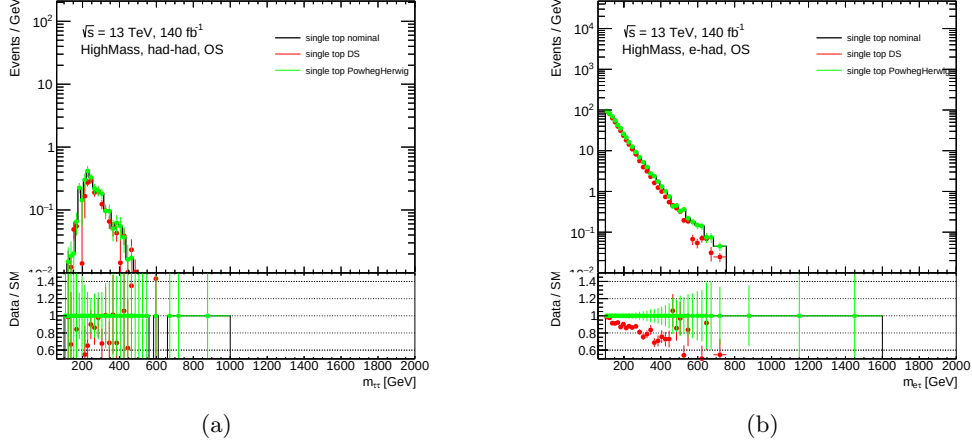


Figure 4.23. Nominal and varied $m_{\ell\ell}$ distributions, according to the considered single-top modelling systematics, for the (a) $\tau_{\text{had}}\tau_{\text{had}}$ and (b) $\tau_e\tau_{\text{had}}$ channels. The distributions in the $\tau_{\mu}\tau_{\text{had}}$ are similar to the ones in the $\tau_e\tau_{\text{had}}$ channel.

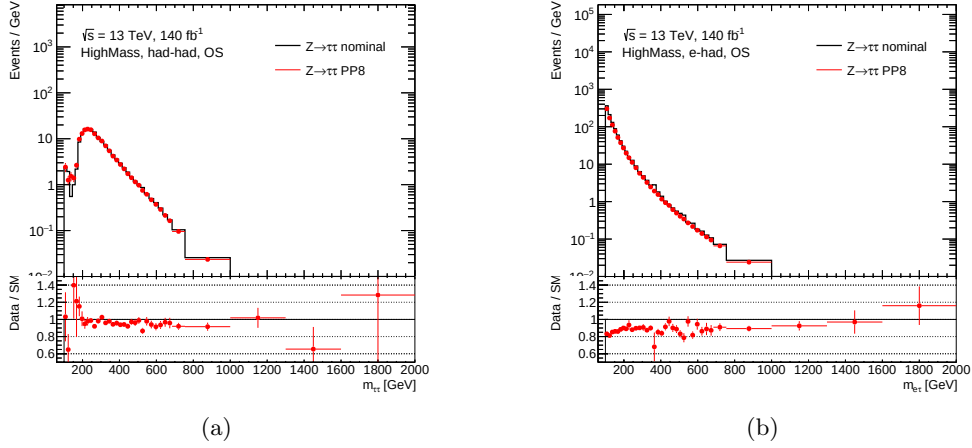


Figure 4.24. Nominal and varied $m_{\ell\ell}$ distributions, according to the considered di-tau Drell-Yan modelling systematics, for the (a) $\tau_{\text{had}}\tau_{\text{had}}$ and (b) $\tau_e\tau_{\text{had}}$ channels. The distributions in the $\tau_{\mu}\tau_{\text{had}}$ are similar to the ones in the $\tau_e\tau_{\text{had}}$ channel.

Parton distribution functions variations

Parton distribution functions (PDFs) enable to access the parton-level kinematics in pp collisions. In this analysis either NNPDF3.0NNLO or NNPDF3.0NLO distributions are used, depending on the considered sample, as detailed in Table 4.1 of Section 4.3.2. A modelling systematic is considered, to describe the uncertainty in the PDFs determination for the Z +jets, $t\bar{t}$ and single top productions. The uncertainty is assessed following the standard PDF4LHC [159] prescriptions, evaluating a band from variations obtained from several replicas of the PDFs included in the set.

4.9 Statistical analysis

The statistical treatment in this analysis consists in the implementation of a likelihood fit of the predicted yields to the observed data and, in the absence of an observed signal, to the setting of an upper limit on the leptoquark models under investigation. The upper limit is set according to the CL_s method, which is the standard procedure for the LHC experiments [160, 161].

4.9.1 Generalities on the statistical treatment

We discuss the generalities of the likelihood model for this analysis, and how it is used to build the test statistics utilised for the CL_s limit setting.

Definition of the likelihood function

The fit is performed by maximising a likelihood function, evaluated in the predicted yields and the observed data, taken as a function of the signal strength and of the nuisance parameters. The *signal strength* μ is the parameter of interest, and is defined as the ratio between the measured signal cross section, and the one predicted by the theory under investigation. The nuisance parameters, instead, are the additional parameters used to represent the systematic and statistical uncertainties, as well as background components normalisations.

We discuss the construction of the likelihood in several steps. The first part of the likelihood function consists of Poissonian probability terms, based on the expected signal and background yields in each bin:

$$\mathcal{L}_b(\mu, \underline{k}) = \prod_{i \in \text{bins}} \text{Pois}(N_i | \mu s_i + b_i(\underline{k})) = \prod_{i \in \text{bins}} \frac{(\mu s_i + b_i(\underline{k}))^{N_i}}{N_i!} e^{-(\mu s_i + b_i(\underline{k}))}, \quad (4.5)$$

where μ is the signal strength, N_i are the counts observed in data in bin i , while s_i and b_i are the signal and background yields predicted in the same bin, the latter depending on the background components normalisations $\underline{k}$.

To account for the systematic uncertainties affecting the measurement, a set of nuisance parameters $\underline{\theta}$ is introduced, which modifies the signal and background predicted yields: $\{s_i, b_i(\underline{k})\} \rightarrow \{s_i(\underline{\theta}), b_i(\underline{k}, \underline{\theta})\}$. The chosen functional dependence is such that the choice $\underline{\theta} = 0$ returns the nominal values of s_i and b_i . Each systematic

uncertainty is described by a variance $\Delta\theta$, characterizing the size of the systematic fluctuation. A set of Gaussian penalty terms are added to the likelihood

$$\mathcal{L}_{\text{syst}}(\underline{\theta}) = \prod_{\theta \in \underline{\theta}} \text{Gaus}(\theta|0, \Delta\theta) = \prod_{\theta \in \underline{\theta}} \frac{1}{\sqrt{2\pi\Delta\theta^2}} e^{-\frac{\theta^2}{2\Delta\theta^2}} . \quad (4.6)$$

The effect of these gaussian penalty terms is to drive the convergence of the likelihood maximisation to final values $\hat{\theta}_i$ fluctuating around zero within the variance $\Delta\theta_i$. The $\underline{\theta}$ nuisance parameters represents all the analysis systematic uncertainties, including both the modelling and the experimental ones. The only parameters which are not subject to a penalty term in the likelihood model are the background components normalisations $\underline{k}$, which are determined purely from data and are therefore called *free-floating* normalisations.

An additional set of nuisance parameters is finally introduced, to account for the fact that the predicted background yields are subject to fluctuations due to the limited statistics of the simulated samples. One γ -parameter is introduced in each analysis bin, modifying the expected background yield: $b_i(\underline{k}, \underline{\theta}) \rightarrow \gamma_i b_i(\underline{k}, \underline{\theta})$. Correspondingly, penalty terms are added in the likelihood model, to drive the fit convergence around unitary values of the γ -parameters. The penalty terms consists of gamma distribution functions¹

$$\mathcal{L}_{\text{stat}}(\underline{\gamma}) = \prod_{i \in \text{bins}} \text{Gamma}(\gamma_i|0, \sigma_{\text{rel}}^i) , \quad (4.7)$$

with width proportional to the relative statistical uncertainty in the bin i , $\sigma_{\text{rel}}^i \simeq 1/\sqrt{b_i}$.

The full likelihood model is the product of all the aforementioned terms

$$\mathcal{L}(\mu, \underline{k}, \underline{\theta}, \underline{\gamma}) = \mathcal{L}_{\text{b}}(\mu, \underline{k}) \times \mathcal{L}_{\text{syst}}(\underline{\theta}) \times \mathcal{L}_{\text{stat}}(\underline{\gamma}) , \quad (4.8)$$

and is a function of the signal strength μ , the background components normalisations $\underline{k}$ and of the nuisance parameters $\underline{\theta}$ and $\underline{\gamma}$.

The CL_s limit setting

Starting from the likelihood in Eq. (4.8), a test statistics can be constructed as follows

$$q_\mu = -2 \ln \frac{\mathcal{L}(\mu, \hat{\hat{\alpha}})}{\mathcal{L}(\hat{\mu}, \hat{\hat{\alpha}})} . \quad (4.9)$$

In this notation $\underline{\alpha} = (\underline{k}, \underline{\theta}, \underline{\gamma})$ is a vector collecting all the likelihood nuisance parameters; $(\hat{\mu}, \hat{\hat{\alpha}})$ are the values which maximise the likelihood globally, while $\hat{\hat{\alpha}}$ are the nuisance parameters values maximising the likelihood at μ fixed. Notice

¹The “gamma” distribution (also called log-normal) is:

$$\text{Gamma}(x|\mu, \sigma) = \frac{1}{x\sigma\sqrt{2\pi}} \exp \left[-\frac{(\log x - \mu)^2}{2\sigma^2} \right] .$$

For the particular choice of the parameters $\mu = 0$, $\sigma = \sigma_{\text{rel}}^i = 1/\sqrt{b_i} \ll 1$, the distribution is peaked at one and has a width as tiny as higher is the number of event counts b_i .

that the test statistics definition depends on the signal strength, hence an optimised variable is used for each signal strength hypothesis.

From Monte Carlo toys, the probability distribution functions of the test statistics under the hypothesis of a given signal strength $f(q_\mu|\mu)$ and under the hypothesis of background only $f(q_\mu|0)$ can be evaluated. Once the observed value of the test statistics q_μ^{obs} is obtained evaluating q_μ in the data, the following p -values can be defined:

$$CL_{s+b}^{(\mu)} = \int_{q_\mu^{\text{obs}}}^{\infty} f(q_\mu|\mu) dq_\mu \quad (4.10)$$

$$CL_b^{(\mu)} = \int_{q_\mu^{\text{obs}}}^{\infty} f(q_\mu|0) dq_\mu \quad (4.11)$$

$$CL_s^{(\mu)} = \frac{CL_{s+b}^{(\mu)}}{CL_b^{(\mu)}}. \quad (4.12)$$

To reject the signal hypothesis with signal strength μ , a low $CL_s^{(\mu)}$ value is required². More in detail we say that the value of μ^* for which the $CL_s^{(\mu)}$ is equal to $1 - \alpha$ is the *observed* upper limit for the signal strength with confidence level α . This limit can be interpreted as the signal strength value such that the probability of observing a dataset with a μ value above the determined limit is $1 - \alpha$. In the LHC community, the value of $\alpha = 0.95$ corresponds to a standard choice.

The *expected* upper limit, representing the predicted sensitivity of the analysis to the searched signal, is obtained following exactly the same procedure, but substituting q_μ^{obs} with $\tilde{q}_\mu$, defined as the median of the background only pdf $f(q_\mu|0)$.

4.9.2 Fit implementation

The technical implementation of the fit is done via the `cabinetry` [162] framework. This framework is based on the `pyhf` [163] environment, building upon `HistFactory` [164], `RooFit` [165] and `RooStats` [166], which are the standard tools used for the statistical analysis in the LHC experiments.

Definition of the binning and fit parameters

The fit is implemented exploiting the distributions of di-lepton invariant mass $m_{\ell\ell}$ in the signal and control regions. Only the fully hadronic channel and the events in 0b and 1b categories are exploited in the implementation described here.

The $m_{\ell\ell}$ distributions are re-binned properly, before being processed by the fitting framework. The binning is chosen such to be sufficiently thin to ensure high statistical sensitivity, and at the same time sufficiently wide to limit fluctuations of the bin contents. Dedicated studies have shown that an optimal configuration is obtained re-binning the events in three bins with edges at 100, 250, 400, 1000 GeV.

²Notice that the CL_s is actually the p -value in the signal hypothesis, normalised to the one in the background only hypothesis. A low CL_s value implies that the observed value of the test statistics is incompatible with the signal hypothesis pdf and simultaneously compatible with the background hypothesis pdf. The CL_s procedure follows therefore a “conservative” approach.

The likelihood model described in Eq. (4.8) is used for the fit implementation. The parameters involved in the fit, whose values are determined from the likelihood maximisation, are the following:

- the signal strength μ of the LQ signal, which is set as the parameter of interest. The LQ signal enters in the analysis via both the pure-BSM diagram and the interference between the BSM and the di-tau Drell-Yan diagram. The first component is scaled by μ^2 , while the second is scaled by μ ;
- the background components normalisations $\underline{k}$. More specifically, one single independent free-floating normalisation is set for each of the following background components: $Z \rightarrow \ell\ell$, $Z \rightarrow \tau\tau$, fake taus, higgs, VV , single top, $t\bar{t}$;
- the systematic uncertainties nuisance parameters $\underline{\theta}$. One independent gaussian-constrained nuisance parameter is attributed to each experimental uncertainty described in Section 4.7 and to each modelling uncertainty described in Section 4.8;
- the statistical uncertainty nuisance parameters $\underline{\gamma}$. For each bin of the fitted distribution an independent parameter is adopted, constrained in the likelihood with a γ -function.

Pre-fit yields evaluation

The pre-fit yields in the $m_{\ell\ell}$ distributions for all of the signal and background components and the data are shown numerically in Table 4.10 and graphically in Figure 4.25. The backgrounds layout is different across the different event categories and varies along the bins of the distributions, providing significance to fit. At the same time, a sufficient number of counts is collected in each bin, limiting the statistical fluctuations. A slight disagreement between the data and the total Monte Carlo predictions is observed, which is corrected through the fitting procedure.

Post-fit yields evaluation

The fit procedure adjusts the likelihood parameters to improve the agreement between the Monte Carlo predicted yields and the data. The post-fit yields for all of the signal and background components as well as the data are shown in Table 4.11 and represented graphically in the distributions in Figure 4.26. The fit primarily adjusts the $Z \rightarrow \tau\tau$ and the $t\bar{t}$ backgrounds, which were overestimated in the pre-fit yields and are decreased post-fit of respectively $\simeq 13\%$ and $\simeq 16\%$. Slight variations are obtained also for the VV and single top backgrounds which are increased by approximately 6%. The post-fit total uncertainties are lower than the corresponding pre-fit ones, due to the constraint imposed by the fit model.

4.9.3 Tools for the validation of the fit

The validation of the fit results is an important task to perform after the execution of the fit, to verify that the post-fit values of the nuisance parameters are consistent with the expectations and to check that the chosen likelihood model is suitable to

Table 4.10. Signal and background pre-fit yields compared with data yields in all of the analysis channels and events categories considered in the fit.

	$\tau_{\text{had}}\tau_{\text{had}}, 0b$	$\tau_{\text{had}}\tau_{\text{had}}, 1b$
LQ sgn. (BSM)	31.03 ± 3.19	42.84 ± 5.05
LQ sgn. (interference)	-39.58 ± 0.33	-48.49 ± 0.40
$Z \rightarrow \ell\ell$	1.93 ± 0.07	0.15 ± 0.02
$Z \rightarrow \tau\tau$	4462.02 ± 363.43	97.11 ± 10.62
fake taus	1326.39 ± 135.36	56.42 ± 6.77
higgs	46.67 ± 1.18	3.53 ± 0.11
VV	109.13 ± 8.77	3.95 ± 0.38
single top	26.59 ± 2.45	40.96 ± 3.92
$t\bar{t}$	118.87 ± 11.67	293.24 ± 27.18
data	5759	427
total bkg	6083.04 ± 408.74	489.71 ± 42.20
data/bkg	0.946	0.872

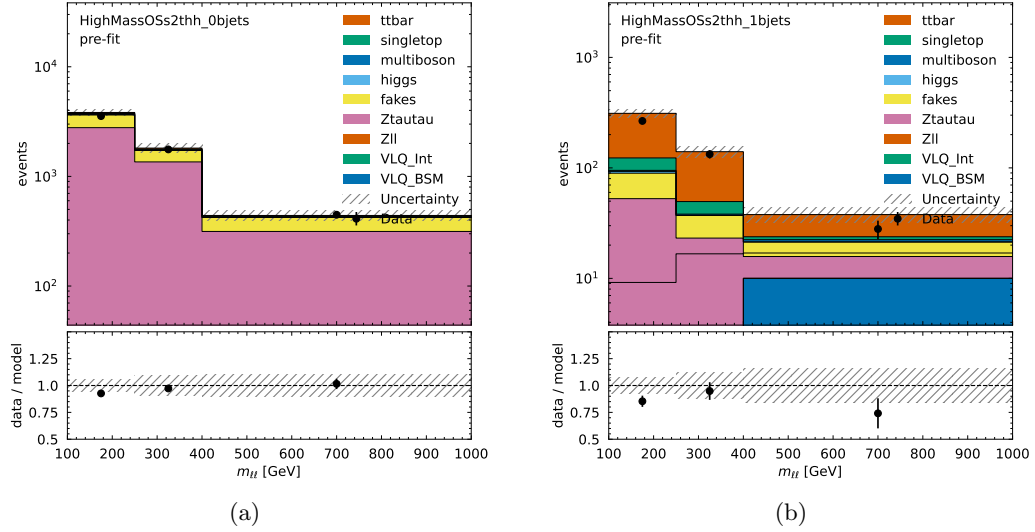
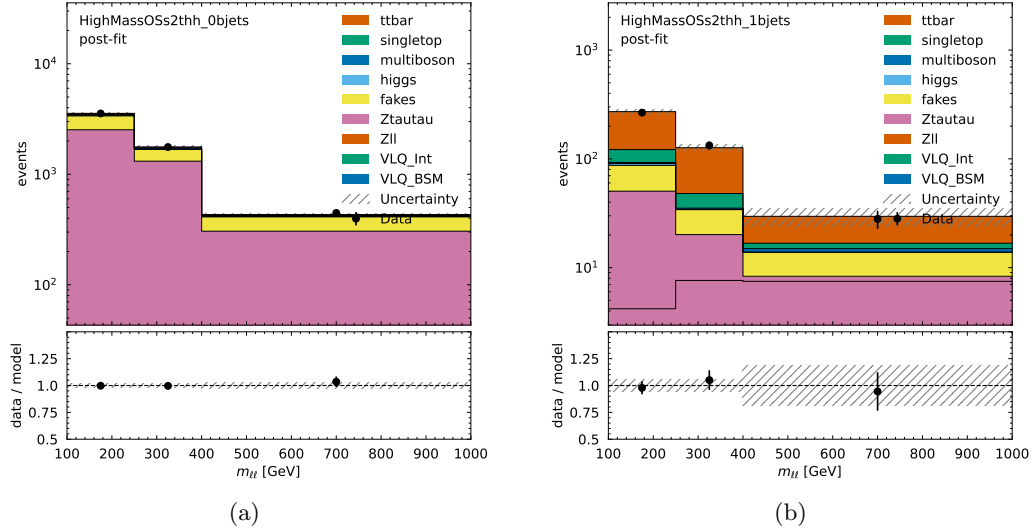
**Figure 4.25.** Pre-fit $m_{\ell\ell}$ distributions in the $\tau_{\text{had}}\tau_{\text{had}}$ channel for the (a) 0b and (b) 1b event categories.

Table 4.11. Signal and background post-fit yields compared with data yields in all of the analysis channels and events categories considered in the fit.

	$\tau_{\text{had}}\tau_{\text{had}}, 0\text{b}$	$\tau_{\text{had}}\tau_{\text{had}}, 1\text{b}$
LQ sgn. (BSM)	14.21 ± 18.29	19.30 ± 23.78
LQ sgn. (interference)	-26.72 ± 17.07	-32.73 ± 20.91
$Z \rightarrow \ell\ell$	1.69 ± 0.12	0.13 ± 0.02
$Z \rightarrow \tau\tau$	4156.44 ± 135.02	92.23 ± 5.56
fake taus	1322.82 ± 107.22	56.18 ± 5.36
higgs	46.63 ± 1.17	3.51 ± 0.11
VV	115.69 ± 6.58	4.20 ± 0.29
single top	28.28 ± 1.80	43.63 ± 2.75
$t\bar{t}$	98.71 ± 10.17	241.63 ± 22.08
data	5759	427
total bkg	5757.74 ± 76.03	428.08 ± 20.63
data/bkg	1.00	0.997

**Figure 4.26.** Post-fit $m_{\ell\ell}$ distributions in the $\tau_{\text{had}}\tau_{\text{had}}$ channel for the (a) 0b and (b) 1b event categories.

represent all the systematic effects involved in the analysis. A series of tools is used to this purpose, which include pulls and ranking plots for the nuisance parameters, as well as the study of the correlation among them.

As a further tool the fit procedure validation, the *Asimov dataset* is introduced. This dataset is obtained from the Monte Carlo simulation, and is defined as the fictitious data sample showing total yields exactly equal to the sum of the simulated background yields. The dataset is used to validate the fitting code self-consistency before unblinding the analysis dataset.

Pull plot

The pull plot is used to check the post-fit values of the nuisance parameters and to verify that they are consistent with a good behaviour of the fit. The pull of a systematic nuisance parameter θ , subject to a pre-fit constraint with mean θ_0 and standard deviation $\Delta\theta$ is

$$pull(\theta) = \frac{\hat{\theta} - \theta_0}{\Delta\theta}, \quad (4.13)$$

where θ_0 is set to zero in the standard gaussian constraint. The pull is therefore quantifying the distance of the post-fit value from the pre-fit expectation in number of pre-fit standard deviations. In a well behaved fit all the pulls are expected to be almost zero, so any large pull has to be investigated in detail.

The fit procedure associates to every nuisance parameter a post-fit uncertainty $\Delta\hat{\theta}$. This uncertainty is normalised with respect to the pre-fit one, $\Delta\hat{\theta}/\Delta\theta$, and is drawn in the pull plot on top of the central values. Normally, each systematic nuisance parameter is expected to show a post-fit uncertainty slightly lower than the pre-fit one, $\Delta\hat{\theta}/\Delta\theta \lesssim 1$, and we say that it is *constrained* by the fit. This happens because the level of uncertainty of each single point is decreased by the information emerging from the correlation with the other points through chosen likelihood model. If a nuisance parameter shows a post-fit uncertainty much smaller than the pre-fit one, $\Delta\hat{\theta}/\Delta\theta \ll 1$, we say that the parameter has been *over-constrained* by the fit. This typically is a sign that the nuisance parameters scheme chosen in the likelihood model is not properly describing the data and requires some modification. This case can arise, for example, when the systematic effect described by the over-constrained parameter has different sizes in different regions of the phase space, and the analysis works in a very restricted region compared to the one the uncertainty has been evaluated in. In this case, the over-constraint is solved by decoupling the nuisance parameter in two or more parameters, each of them referred to a phase space region in which systematic uncertainty has a constant size. We say that we *decorrelate* the nuisance parameter into several ones. A similar scenario is obtained when a single nuisance parameter is jointly representing several physical effects with different sizes, inducing an over-constraint. Also in this case the over-constraint is solved by introducing more parameters in the fit to represent separately all the effects. Conversely, it can also happen that a nuisance parameter is *under-constrained*, i.e. $\Delta\hat{\theta} \gtrsim \Delta\theta$. This is also typically caused by the nuisance parameter representing more effects jointly, in an analysis restricted only to the phase space region dominated by the systematic effect with larger size, and is solved by decorrelating the parameter into several ones.

On the same pull plot also the post-fit values of the statistical nuisance parameters $\underline{\gamma}$ and the normalisation factors $\underline{k}$ are displayed with their absolute uncertainty. For these parameters no particular check is done for their over- or under-constraint, but they are expected to assume a post-fit value near unity and to have small post-fit uncertainty much less than unity.

The pull plot for the analysis described in this chapter is shown in Figure 4.27. As can be seen by direct inspection, almost all the systematic nuisance parameters are showing good behaviour, meaning that the set of uncertainties considered in the likelihood model is correctly describing the dataset. The only nuisance parameter which is significantly pulled and is showing an over-constraint is the `TAUS_TRUEHADTAU_SME_TES_DETECTOR_Barrel_LowPt`, which needs to be investigated in more detail. A minor pull is also observed for the `TAUS_TRUEHADTAU_SME_TES_PHYSICSLIST` parameter, while a minor over-constraint is obtained for the `FAKES_ErrorTotal`, meaning that such uncertainty could have been estimated too conservatively in the Fake Factors method.

The pull plot has also been evaluated using the Asimov dataset instead of the unblinded dataset. No particular issues have been identified, except for the few under-constraints and pulls already mentioned in the discussion of the unblinded plot.

Correlation matrix

The correlation matrix is another relevant tool for the validation of the fit results. It can be directly derived normalising the covariance matrix of the nuisance parameters, as follows

$$\text{corr}[\alpha_i, \alpha_j] = \frac{\text{cov}[\alpha_i, \alpha_j]}{\sqrt{\text{var}[\alpha_i] \cdot \text{var}[\alpha_j]}}, \quad (4.14)$$

where we indicate with $\underline{\alpha} = (\underline{k}, \underline{\theta}, \underline{\gamma})$ the comprehensive set of nuisance parameters and $\text{var}[\alpha_i] = \text{cov}[\alpha_i, \alpha_i]$.

In the large sample limit, the covariance matrix can be evaluated as the inverse of the second derivative matrix of the log-likelihood function

$$\text{cov}[\alpha_i, \alpha_j] = \left[-\frac{\partial^2 \ln \mathcal{L}(\mu, \underline{\alpha})}{\partial \alpha_i \partial \alpha_j} \right]_{\hat{\mu}, \hat{\underline{\alpha}}}^{-1}, \quad (4.15)$$

where the derivatives are evaluated at the parameters values $(\hat{\mu}, \hat{\underline{\alpha}})$ maximising the likelihood.

The correlation values range in the interval $[-1, +1]$ and can help in the fit validation process to identify potential problems at the origin of over- or under-constraints. In general, low correlation values are expected between the systematic uncertainties nuisance parameters. If a very high correlation is observed between two parameters of this group, it means that they can be merged into a single one. A higher correlation, instead, is normally observed between the background normalisation parameters, since their values are correlated through the data: the increase of one background implies the decrease of the others to accommodate the same data yields.

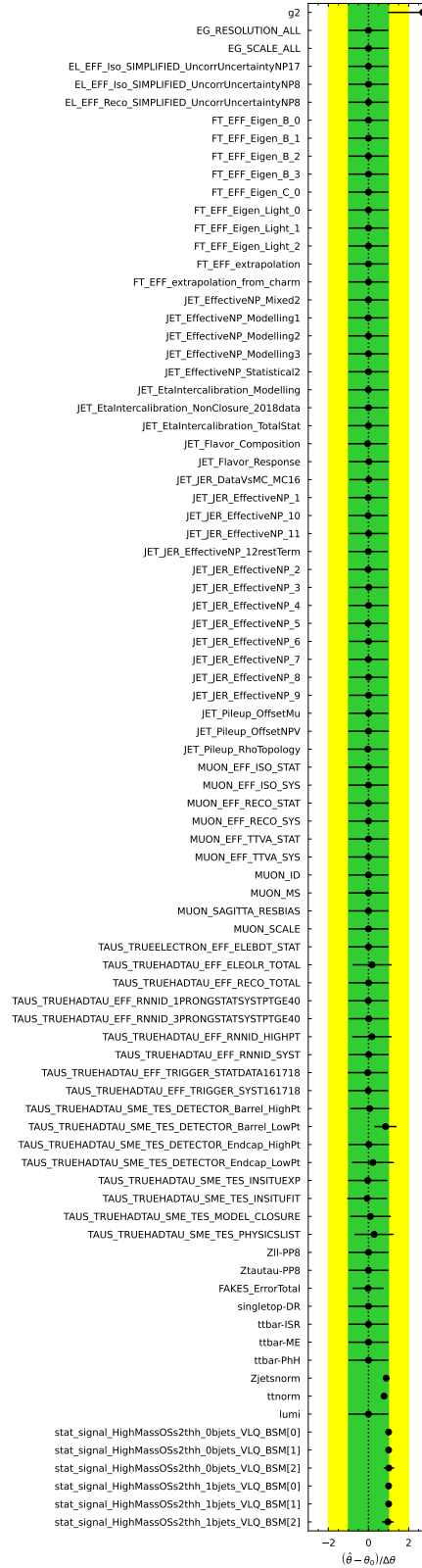


Figure 4.27. Pull plot for the systematic uncertainty nuisance parameters. The pulls are also shown for the statistical uncertainty parameters and for the background normalisations. Refer to Tables 4.7 and 4.8 for the systematics naming meaning.

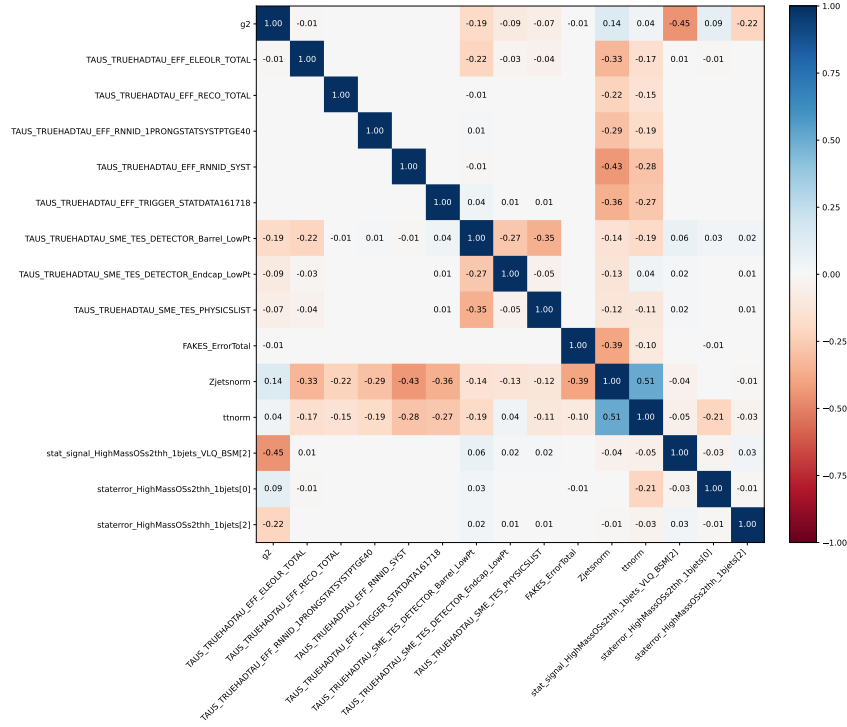


Figure 4.28. Correlation matrix of the nuisance parameters. Only the parameters with at least one correlation higher than 0.2 are shown. Refer to Tables 4.7 and 4.8 for the systematics naming meaning.

Figure 4.28 shows the correlation matrix for the analysis described in this chapter, evaluated on the unblinded data. Only the nuisance parameters with at least one correlation higher than 0.2 are drawn in the matrix. Low correlations are observed between the systematics nuisance parameters, while some higher correlations are present between the systematics parameters and the Z +jets and $t\bar{t}$ normalisations. A high correlation is observed between the `TAUS_TRUEHADTAU_SME_TES_DETECTOR_Barrel_LowPt` and the `TAUS_TRUEHADTAU_SME_TES_PHYSICSLIST` parameters, which is most likely related to the first parameter over-constraint, visible in Figure 4.27. A high correlation is also present between the `TAUS_TRUEHADTAU_SME_TES_DETECTOR_Barrel_LowPt` and the `TAUS_TRUEHADTAU_SME_TES_DETECTOR_Endcap_LowPt` parameters, meaning the these two systematic effects are partially overlapped.

Ranking of the nuisance parameters

The systematic and statistical sources of uncertainty jointly contribute to determine the post-fit values of the signal strength. However, not all the sources of uncertainty are equally important. We say that a source has as higher relevance as the post-fit value of the parameter of interest is varied by changes of the associated nuisance parameter within its post-fit uncertainty.

To quantify this, we define impact of a nuisance parameter α_i the quantity

$$\text{impact} = \hat{\mu} - \mu' \quad (4.16)$$

were $\hat{\mu}$ is the post-fit value of the signal strength, while μ' is the value obtained fitting the likelihood model with α_i parameter fixed to $\alpha_i = \hat{\alpha}_i \pm \Delta\hat{\alpha}_i$. The ranking plot shows the impact on the signal strength, for all the nuisance parameters of the analysis, displayed by decreasing impact. The most critical uncertainties are the most highly ranked ones: for these uncertainties particular attention has to be devoted and it has to be carefully checked that they are not showing over- or under-constraints in the pull plot or anomalous correlation values.

It can happen that, due to an over-constrained nuisance parameter, the associated impact is fictitiously small. In fact, if $\Delta\hat{\alpha}_i \ll 1$ due to the over-constraint, it will results in $\mu' \simeq \mu$, i.e. in an impact illusorily almost null. To spot this kind of situations, the *pre-fit* impact is also drawn in the ranking plot, which has exactly the same definition in Eq. (4.16), except that the μ' value is evaluated by varying the α_i parameter by its pre-fit uncertainty $\alpha_i = \hat{\alpha}_i \pm \Delta\alpha_i$. It is a convection to draw on the ranking plot also the post-fit values of the nuisance parameters and their uncertainty; however this information is already delivered in the pull plot, as discussed in Section 4.9.3

The ranking plot for the analysis described in this chapter, evaluated on the unblinded dataset, is shown in Figure 4.29. The first 30 most highly ranked parameters are displayed, showing values compatible with expectations. The only anomalous parameter is `TAUS_TRUEHADTAU_SME_TES_DETECTOR_Barrel_LowPt`, which shows a difference between pre- and post-fit impacts. This is clearly related to the parameter over-constraint, observed in Figure 4.27.

Breakdown of uncertainties

Similarly to the impact on the central values, is worth assessing also the impact of the individual nuisance parameters on the signal strength post-fit uncertainty.

The impact on the signal strength uncertainty of a nuisance parameter α_i is defined as

$$\text{uncertainty impact} = \sqrt{\Delta\mu^2 - \Delta\mu'^2}, \quad (4.17)$$

where $\Delta\mu$ is the post-fit uncertainty on the signal strength evaluated with the full likelihood model, while $\Delta\mu'$ is the uncertainty evaluated with the likelihood model with α_i parameter fixed to its post-fit value, $\alpha_i = \hat{\alpha}_i$. The value of $\Delta\mu'$ is lower than $\Delta\mu$, since it is obtained with a likelihood with one parameter less, and hence yielding more constraint.

It is possible to calculate the total uncertainty components originating from the statistical and systematic nuisance parameters. The statistical contribution is evaluated as the signal strength post-fit uncertainty obtained from a fit with all the systematic nuisance parameters fixed at their post-fit values. Conversely, the systematic uncertainty is evaluated as the quadrature difference between the total uncertainty and the statistical component³. It is worth noting that it is not possible to interpret the total systematic uncertainty as a quadrature sum the individual systematic components. These components, in fact, are not independent, hence the

³Notice that the quadrature difference rule can be used since statistical and systematic uncertainties are independent sources.

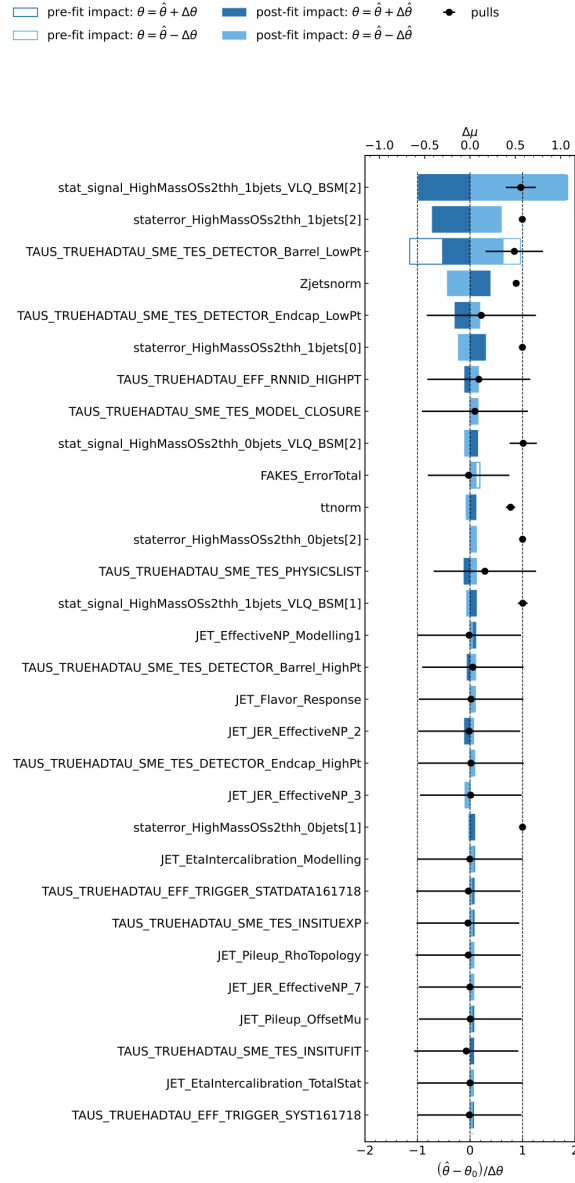


Figure 4.29. Ranking plot of the nuisance parameters. The $\Delta\mu$ notation on the x -axis refers to the impact on the signal strength. Refer to Tables 4.7 and 4.8 for the systematics naming meaning.

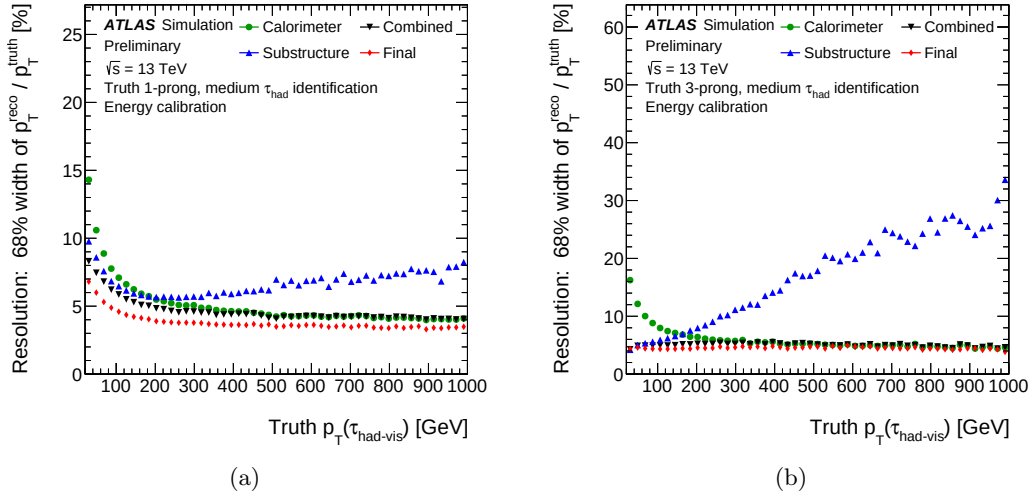


Figure 4.30. Resolution of the hadronic taus energy calibration for the (a) 1-prong (b) 3-prong decays. Figures taken from Ref. [167].

quadrature sum rule does not apply due to the presence of the correlations between the parameters.

4.9.4 How to solve over- and under-constraints? A practical example

The presence of over- or under-constrained nuisance parameters in the statistical model of a physics analysis is quite common. We discuss here an exemplary use case, encountered in the analysis described in this chapter.

As mentioned in Section 4.9.3, over- or under-constrained parameters are typically associated with systematic effects presenting a non-uniform value in the analysis phase space used by the Combined Performance groups to estimate the pre-fit expectations. If the analysis is restricted to a sub-region of the phase space in which a systematic effect has a lower size with respect to the whole phase-space region, its pre-fit expectation results too conservative, and an over-constraint is obtained. If, instead, the sub-region in which the analysis is restricted is characterised by a higher size of the systematic effect, the pre-fit estimate results too small, and the parameter is under-constrained.

We encountered this case in the High Mass Drell-Yan analysis, when dealing with the uncertainty associated with the tau energy resolution. As can be seen in Figure 4.30, the resolution varies across the tau p_T range $[0, 1]$ TeV taken as reference to evaluate the pre-fit uncertainty estimate. More specifically the total uncertainty on the resolution is higher at low momentum ($p_T < 200$ GeV), and is lower at high momentum ($p_T > 200$ GeV). From direct inspection of the kinematic plots in Figures 4.9, 4.10, 4.11 it can be verified the High Mass Drell-Yan analysis is enriched in low- p_T taus, which induces an under-constraint in the nuisance parameter associated with the tau energy resolution. To solve this effect, we split the nuisance parameter into four, `TAUS_TRUEHADTAU_SME_TES_DETECTOR_{Barrel,Endcap}_{Low,High}Pt`,

Table 4.12. Final expected and observed limits on the coupling g_U^2 of the U_1 vector leptoquark model. The pure left-handed scenario is assumed: $|\beta_L| = 1$ and $|\beta_R| = 0$. The limits are adimensional.

LQ mass [TeV]	Expected limit	Observed limit
1.5	5.28	6.49
2.0	9.17	10.50
2.5	14.16	16.48
3.0	20.23	23.38

distinguishing between the case of taus with low/high p_T and falling into the barrel/end-caps. As expected, the nuisance parameters referred to low p_T taus are highly ranked (since the analysis is enriched in such taus), while the parameters referred to high p_T taus have a lower rank, as can be directly verified in Figure 4.29.

4.10 Results

In the absence of an observed signal the likelihood fit model can be used to set an exclusion limit on the searched new physics model, according to the CL_s method as described in Section 4.9.1. The new physics model under investigation in this analysis is the U_1 vector leptoquark model, reported in Section 1.4.1 of the introductory chapter of this thesis. The model is characterised by four parameters: the leptoquark mass M_U , its coupling constant g_U and the parameters β_L and β_R , describing the left- and right-handed couplings of the LQ interactions. We restrict in this analysis to the particular case of a left-handed coupling scenario, $|\beta_L| = 1$, $|\beta_R| = 0$.

A 95% CL_s limit is obtained for several leptoquark masses hypotheses in the range $1.5 < M_U < 3$ TeV on the signal strength μ , which is the parameter of interest in the fit, and translated into a corresponding limit on the coupling g_U^2 . Since the signal events enter the analysis signal region both originating from the pure-beyond-SM diagram (with amplitude scaling as g_U^4), and from the interference contribution between the pure-beyond-SM diagram and the di-tau Drell-Yan diagram (with amplitude scaling as g_U^2), the translation of the limit on μ into a limit on g_U^2 is obtained via a custom modified version of the `cabinetry` [162] fitting framework, using the model $\mu = g_U^2/2 + g_U^4/4$. Table 4.12 reports the obtained results for the expected limits, representing the sensitivity of the analysis on the model exclusion, and the observed limits, representing the real exclusion obtained from the data.

Figure 4.31 shows the exclusion contour displayed in the $M_U - \lambda$ space, where $\lambda = g_U/\sqrt{2}$ is the normalised coupling strength. The $\pm 1\sigma$ and $\pm 2\sigma$ bands for the expected limit contour are also drawn, showing that the observed limit falls within a 1σ fluctuation of the expected one.

The excluded area has to be compared with the phase space region addressed by theorists as the preferred one to build leptoquark models interpreting the B -physics anomalies described in Section 1.3.2 of Chapter 1, which were among the physics motivations of this study. Following the work by Isidori et al. in Ref. [42], the preferred regions at 90% CL based on the B -physics anomalies are:

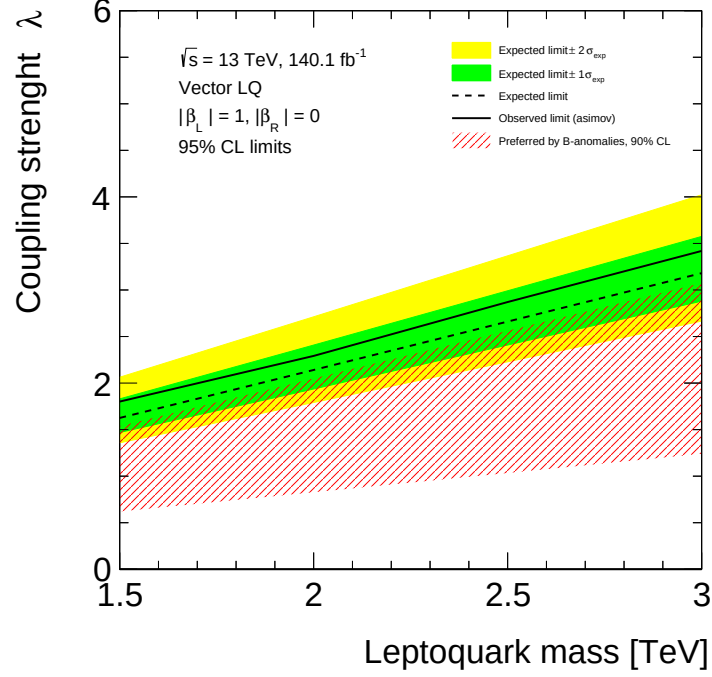


Figure 4.31. Observed and expected exclusion contours in the M_U - λ phase space for the U_1 vector leptoquark model. The preferred region for the B -physics anomalies interpretation is also displayed.

- for $|\beta_R| = 0$ (pure left-handed case): $M_U/g_U \in [0.69 \text{ TeV}, 1.71 \text{ TeV}]$;
- for $|\beta_R| = 1$ (Pati-Salam-like leptoquark): $M_U/g_U \in [0.91 \text{ TeV}, 2.19 \text{ TeV}]$.

The area corresponding to the pure-left handed case is displayed in Figure 4.31, and, as can be seen, the exclusion contour obtained in this search fairly approaches the preferred region of phase space.

The exclusion contour obtained in this analysis has also to be compared with the corresponding one published by the CMS experiment at the LHC in Ref. [62], and reported in Figure 1.21 of Section 1.5.3. As can be verified by the direct inspection of the contour corresponding to the non-resonant leptoquark production mode, the expected exclusion obtained in this analysis is almost identical with respect to the one set by CMS. However, we notice that while CMS observed contour was showing a consistent disagreement with expected contour, the observed contour obtained in this analysis is fairly in agreement with the expected one. This suggests to interpret the CMS excess more as a fluctuation, rather than a real signal of new physics, and strengthens the exclusion of leptoquark models in this region of phase space.

4.10.1 Projections of the exclusion limits at HL-LHC

Around 2028 the LHC complex is expected to be upgraded to start the High-Luminosity LHC (HL-LHC) program. In this program, the machine will be operated at the highest instantaneous luminosity achievable, and will collect an integrated

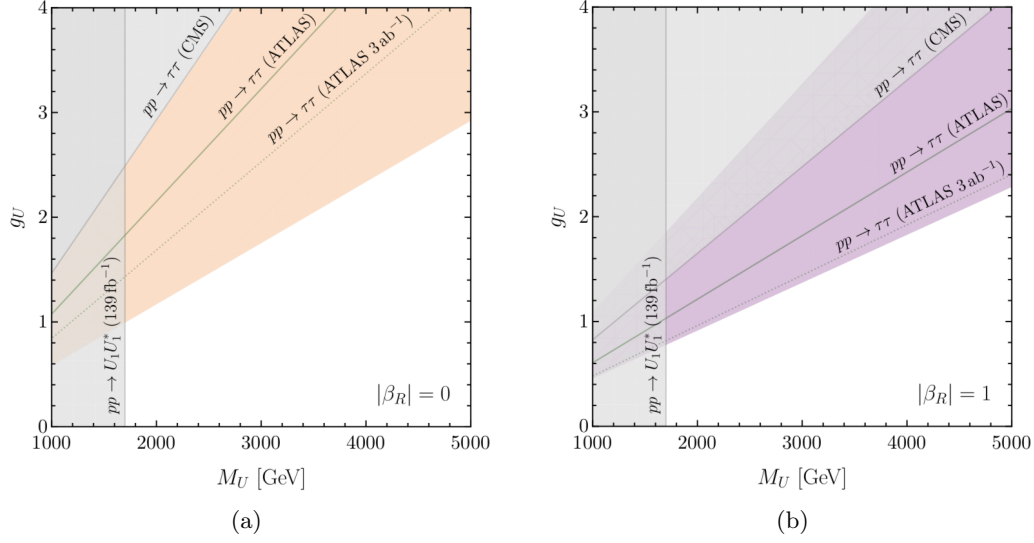


Figure 4.32. Projection of the U_1 leptoquark model exclusion contour to the High-Luminosity LHC dataset with 3000 fb^{-1} data: (a) pure left-handed case, (b) Pati-Salam case. Figures taken from Ref. [42].

luminosity of 3000 fb^{-1} , in pp collisions at the increased centre-of-mass energy of 14 TeV. The study of the flavour sector of the Standard Model and the search for possible lepton universality violation signatures are among the main physics motivations for this program, and the investigations of the B -physics anomalies and their interpretation via leptoquark models play a central role in this context. For this reason, extrapolation studies have been performed to predict the exclusion contour on leptoquark models foreseen with the HL-LHC dataset.

When doing a limit extrapolation to a higher luminosity, one has to take into account of several aspects. In first approximation, the CL_s exclusion limit on the signal strength scales as the ratio between the uncertainty on the background and the signal, $\mu \propto \Delta B/S$. In fact, if the background has an uncertainty similar to the signal, it is difficult to discriminate if a fluctuation in the data is originating from real new physics signal or from a background fluctuation, and the exclusion limit is poor. Instead, if the uncertainty on the background is small, it is easier to attribute an eventual data fluctuation to the presence of a signal and the exclusion limit is stronger. The uncertainty on the background in the future HL-LHC analyses will be decreased for several reasons. First of all, the improved Monte-Carlo samples will provide simulations with an increased precision, which will decrease the statistical component of the background uncertainty, as well as the modelling uncertainties. Moreover, the improvement in the experimental techniques for the objects reconstruction in the detector will decrease the magnitude of all the experimental systematic uncertainties involved in the analysis. Most importantly, the increased integrated luminosity of the dataset from 140 fb^{-1} to 3000 fb^{-1} will largely improve the statistical sensitivity of the analysis. This is by far the element which mostly determines the improvement of the exclusion limit, since an enlarged dataset also enables to set an improved analysis strategy (e.g. with thinner binnings in the pre-fit distribution).

Figure 4.32 reports the results of a projection to 3000 fb^{-1} published by Isidori et al. in Ref. [42], for an exclusion contour for the U_1 vector leptoquark model, obtained with the ATLAS experiment. The projection has been evaluated starting from the 140 fb^{-1} observed contours and considering only the improvement due to the increased data statistics. Contours are drawn both for the pure left-handed ($|\beta_L| = 1, |\beta_R| = 0$) and the Pati-Salam ($|\beta_L| = 1, |\beta_R| = 1$) cases, and are compared to the respective B -physics anomalies preferred regions. As can be seen, while the contour set within the analysis reported in this thesis slightly approaches the B -anomalies preferred region, the contour with the HL-LHC dataset is foreseen to largely cover such region, and hence to substantially contribute to the understanding of the flavour anomalies and their eventual connection with leptoquark particles.

Chapter 5

Readout firmware for the Phase-II L0 Muon barrel trigger

I report in this chapter the original work performed as part of the Phase-II L0Muon trigger upgrade. My personal contribution has been the development of the readout functionality for the barrel Sector Logic sub-system. I designed the readout firmware via VHDL language, I tested it through a Vivado simulation and implemented it into a Xilinx FPGA circuit. I also contributed to the integration of the readout firmware with the logic implementing the other functionalities performed by the Sector Logic, and participated to the preliminary testing campaigns of the board prototype at the CERN Laser Room experimental facility.

The High-Luminosity LHC is the long term program, aiming at operating the Large Hadron Collider at the highest luminosity achievable by the machine. In order to work in such high-intensity environment the electronics of the ATLAS trigger system will be largely redesigned. This chapter presents first results of the ongoing upgrade program for the L0Muon Barrel trigger, with focus on the readout logic of the muon trigger chambers. After a brief overview of the ATLAS trigger system upgrade and the L0Muon barrel sub-system in Section 5.1 and 5.2 respectively, the readout logic firmware is presented in Section 5.3. The new trigger algorithm is described in Section 5.4, and the complete firmware implementation results are delivered in Section 5.5. Finally, preliminary hardware tests performed in the CERN Laser Room experimental facility are reported in Section 5.6, with some information on the future testing campaigns to be performed on the board prototype to finalise its design.

5.1 The trigger upgrade for the High-Luminosity LHC program

5.1.1 LHC roadmap and physics motivations

The High-Luminosity LHC (HL-LHC) program plays a crucial role in the middle-long term development of the LHC. This program, referred to also as LHC Phase-II, aims at pushing the LHC potential to its ultimate limit, operating the accelerator facility

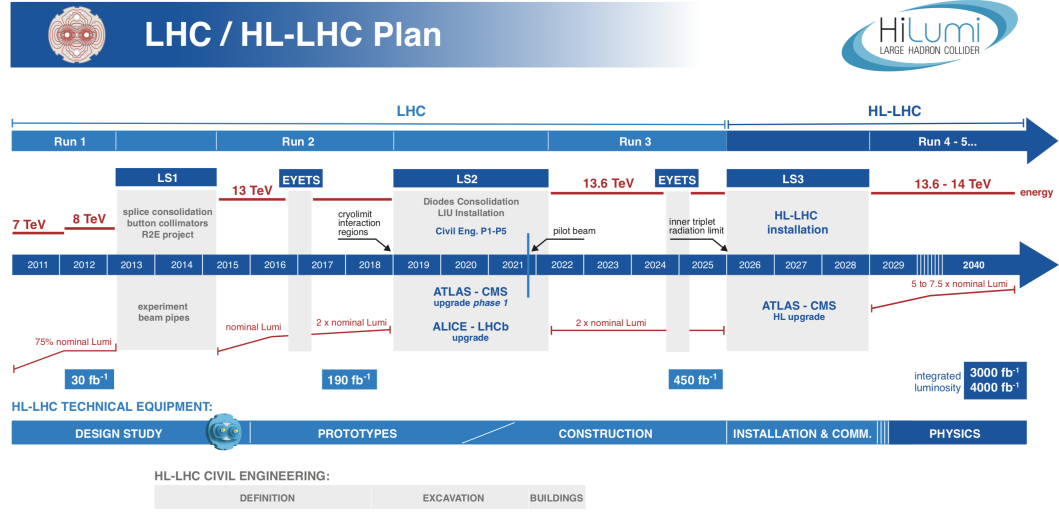


Figure 5.1. The LHC roadmap, showing the major milestones and operational parameters for the Phase-I and Phase-II of LHC operations. Taken from [168].

at the highest instantaneous luminosity achievable.

Figure 5.1 shows the LHC and HL-LHC project schedule. The LHC has been operated in Run 2 in the years 2015-2018 with a centre of mass energy of $\sqrt{s} = 13$ TeV and delivered an instantaneous luminosity up to $\mathcal{L} = 2.0 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ and an average of up to $\langle\mu\rangle \simeq 60$ collisions per bunch crossing. During Run 2 approximately 150 fb^{-1} of pp collisions have been delivered to the ATLAS experiment. In the Long Shutdown 2 ATLAS has been upgraded in preparation for Run 3, which started in 2022. During Run 3 the peak luminosity is kept at $\mathcal{L} = 2.0 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$, delivering approximately 300 fb^{-1} more of collision data to ATLAS. At the end of Run 3 another shut-down period (Long Shutdown 3) will enable an intensive upgrade of both the detector and the accelerators after which the HL-LHC program will start. HL-LHC operations are foreseen to begin in 2029 and to deliver 3000 fb^{-1} of data in the next 10 years. Table 5.1 shows a comparison between LHC and HL-LHC accelerator parameters. The accelerating complex will deliver pp collisions at $\sqrt{s} = 14$ TeV, with an instantaneous luminosity of $\mathcal{L} = 5 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ and $\langle\mu\rangle \simeq 140$. If the performance of the HL-LHC can be pushed further, the ultimate HL-LHC configuration could be realised, delivering to the experiments an instantaneous luminosity $\mathcal{L} = 7.5 \times 10^{34} \text{ cm}^{-2}\text{s}^{-1}$ and $\langle\mu\rangle \simeq 200$ inelastic collisions per bunch crossing. In this ultimate configuration the integrated luminosity delivered at the end of the HL-LHC lifetime would be 4000 fb^{-1} .

The physics drivers motivating the HL-LHC program mainly include a broad set of precision Higgs boson and Standard Model measurements, along with the study of rare processes, the search for beyond the Standard Model signatures and flavour physics. Heavy-ion collisions are also included among the program's goals. The physics requirements on the trigger system consist of a series of p_T thresholds on the relevant objects (e , μ , τ , jet, ...), impacting single lepton, di-lepton, multi-jet and missing transverse energy triggers. Ideal triggers select with the highest possible efficiency events verifying the p_T threshold condition, and discard the others. Trigger

Table 5.1. Comparison of the main LHC and HL-LHC operational parameters, referred respectively to the design report and standard operational configuration. Table adapted from [168].

Parameter	LHC	HL-LHC
Beam energy in collision [TeV]	7	7
Number of protons per bunch [$\times 10^{11}$]	1.15	2.2
Number of bunches	2808	2748
Beam current [A]	0.58	1.09
crossing angle [μrad]	285	590
Transverse emittance β^* [m]	0.55	0.15
Luminosity [$\times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$]	2.0	5.32

thresholds are ideally kept as low as possible, to increase the events acceptance in the physics analyses. In this way, the highest sensitivity is achieved in exotic searches and, most importantly, the largest possible fiducial region is used in Standard Model measurements.

Single-electron and single-muon triggers will be crucial for the selection of $t\bar{t}$ and $W \rightarrow l\nu$ production, as well as the study of the $HH \rightarrow b\bar{b}\tau\tau$ process, in which at least one $\tau \rightarrow e$ or μ . The study of the di-Higgs production will be relevant for the precision measurement of the Higgs boson properties as well as for the search for anomalous Higgs boson self-couplings. Di-lepton triggers will enable to measure the decay branching fraction of the Higgs boson to leptons, mainly exploiting the most favoured channel into third family leptons $H \rightarrow \tau\tau$. Similarly di-tau hadronic triggers will enable the study of the $H \rightarrow \tau\tau$ process in the fully hadronic channel, in which also spin and CP measurements are possible, as well as the study $HH \rightarrow b\bar{b}\tau\tau$ with hadronically decaying taus.

5.1.2 The ATLAS muon system upgrade

The muon spectrometer has been described in its Phase-I configuration in Section 2.2.1. To enable the ATLAS detector to operate in the high intensity environment of the Phase-II HL-LHC, the muon system will be upgraded mainly during LS3, in preparation for Phase-II. Figure 5.2 shows a view of the upgraded system layout, in a small longitudinal sector of the muon spectrometer.

The upgrade comprises the installation of new chambers, the replacement of some existing chambers and the substitution of the majority of the front-end electronics, with the aim of maintaining low trigger thresholds in the harsh high-rate environment of the LHC Phase-II. The electronics chain of the MDT precision chambers will be completely re-designed. This will enable the MDT to transfer to the trigger system information on muons p_T , which will be exploited to confirm RPC and TGC trigger candidates within a higher momentum resolution. Moreover, most of the RPC and TGC trigger electronics will be moved in the off-detector chamber USA15, which will enable to build an enlarged setup to manage more complex trigger decisions.

In the barrel region of the muon spectrometer, a new RPC layer will be introduced, corresponding to the BI MDT chambers. This additional layer will compensate

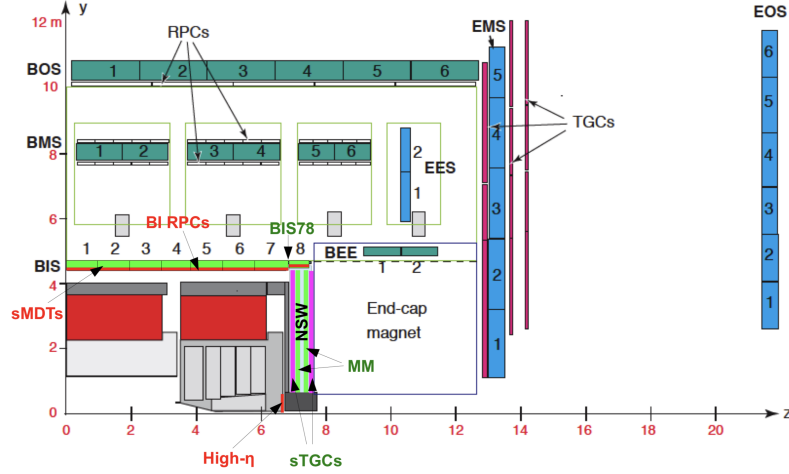


Figure 5.2. Schematic view of the muon system after the Phase-II upgrade. The R - z projection is shown for a small sector. Taken from [169].

the acceptance holes present in RPCs located on the BM MDT chambers in the small sectors, caused by the supporting structures of the toroidal magnet coils. The BI RPCs will also recover the loss of efficiency of RPC chambers due to the low operating voltage, which will be required in the high-rate environment of Phase-II. The introduction of the BI RPCs will require also modifications to the BI MDT chambers in the small sectors, which will be replaced with small MDT (sMDT) tubes with reduced thickness, enabling sMDT and new RPCs to fit in the same space as original MDT chambers. A first stage of the BI upgrade has already been done during LS2 with the replacement of BIS7 and BIS8 MDT chambers in small sectors with the BIS78 RPCs and sMDTs.

In the end-caps, the New Small Wheels (NSW) will be operated during Phase-II, exploiting the MicroMegas (MM) and the small TGSs (sTGS) sub-detectors, serving as tracking and trigger chambers respectively. The NSWs have already been installed during LS2, substituting the Small Wheels, made of MDT and CSC chambers, which were operated in Run 2 of Phase-I. Finally, in the end-caps, the EIL4 doublet chambers, covering a region $1.05 < |\eta| < 1.3$ around the NSWs in large sectors, will be replaced with new triplet chambers with a higher readout granularity. With these chambers a more solid 2/3 majority coincidence will be used to trigger muons and the rate of fake triggers induced by low p_T particles generated in the toroid cryostats will be decreased using smaller coincidence windows.

5.1.3 Overview of the Phase-II trigger system

The Phase-II upgrade of the trigger system will modify the current Phase-I system, described in Section 2.2.1, to cope with the high-intensity environment foreseen in the High-Luminosity LHC program.

The Phase-II trigger will be organised in a single Level-0 (L0) hardware trigger, and a second level software trigger called Event Filter (EF). The L0 trigger will have a readout rate of 1 MHz and a maximum latency time of 10 μ s. The EF level, will transfer data to the permanent storage with an output rate of 10 kHz, which is a

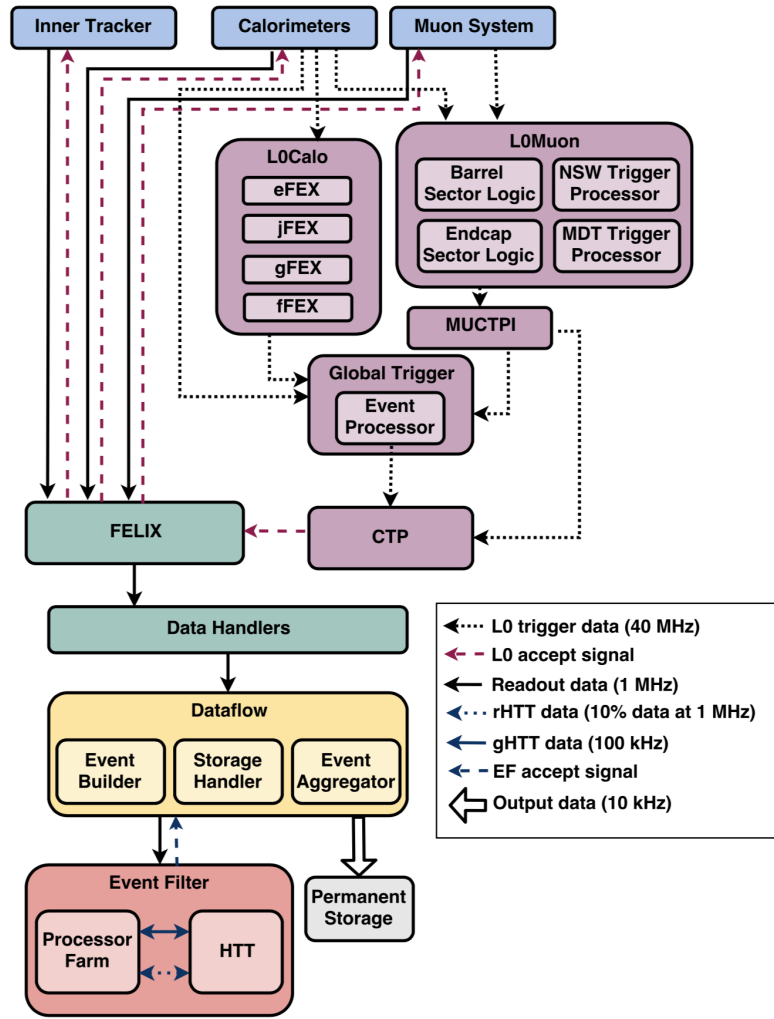


Figure 5.3. Functional architecture of the Phase-II trigger system and its sub-systems. Figure taken from [168].

factor 10 higher than that of the High Level Trigger of Phase-I system. The two trigger levels are interfaced with the Data Acquisition system (DAQ), responsible for buffering, transporting and aggregating events data. Figure 5.3 shows a functional overview of all sub-systems involved in the Phase-II trigger. The trigger systems exploit data coming from the Inner tracker (ITk, pixel and strip detectors), the calorimeters (LAr and Tile) and the Muon system (MDT, RPC, TCG, NSW).

The hardware-based Level-0 Trigger system is composed of the Level-0 Calorimeter Trigger (L0Calo), the Level-0 Muon Trigger (L0Muon), the Global Trigger and the Central Trigger Processor (CTP). The L0Calo sub-system is composed of four feature extractor processors, which recognise specific features from calorimetric energy deposits: the electron Feature Extractor (eFEX), the jet Feature Extractor (jFEX), the global Feature Extractor (gFEX), and the newly introduced forward Feature Extractor (fFEX), specialized in the recognition of high rapidity jets and electrons. The L0Muon sub-system comprises the Barrel and Endcap Sector Logic

processors, the NSW Trigger Processor and the MDT Trigger Processor. The MUCTPI component interfaces the L0Muon sub-system with the Global Trigger and the CTP. The Global Trigger uses full granularity of the calorimeters to refine the trigger objects calculated by L0Calo and L0Muon sub-systems executing topological algorithms to improve rejection of π_0 and e/γ discrimination. The CTP is instead in charge of forming the final L0 decision, taking into account of the menu configuration and prescale factors, and to send a L0A signal via the TTC distribution network to the detector systems.

Data read from the detectors after a L0A are sent to the Front-End LLink eXchange (FELIX), the Data-Handler components, and the Dataflow sub-system, which contains the Event Builder, the Storage Handler and the Event Aggregator components. All these elements together form the DAQ system, which runs on servers and standard networking infrastructure. Finally, the Event Filter refines the trigger objects to cut the rate to its ultimate value of 10 kHz. It is based on CPU-processing farms implementing two HTT co-processors, the rHTT and the gHTT, with regional and global track reconstruction capabilities respectively. The planned physical location of trigger components is the USA15 electronics cavern, where all L0 modular electronics, FELIX and Data Handler will be placed. The Dataflow and EF servers will be installed in the surface-level counting room SDX1.

The major improvements in L0Muon Phase-II system with respect to the corresponding Phase-I version are the addition of the MDT Trigger Processor, enabling to exploit the MDT tracking chambers information to improve the p_T resolution of the trigger candidates, and the addition of the BI RPC chambers. To exploit this newly inserted RPC layer, the trigger algorithm will be modified and will not use any more a fixed pivot plane on the BM RPC chambers. In this way the inefficiencies generated by the acceptance holes in the BM RPCs in small sectors will be recovered, providing a significant improvement to the muon trigger system. Moreover, the readout of data from the detectors subsystems, will be performed through the trigger subsystems boards and not via a dedicated component, as it was done in Phase-I trigger. More specifically, the readout of data from the muon detectors, will be done by a dedicated functionality in the L0Muon barrel and end-cap sector logic, which will collect muon data and send them to the FELIX component. The majority of the original work performed in this thesis on L0Muon trigger concerns the L0 Muon barrel Sector Logic readout, and will be presented in Section 5.3.

5.2 The L0Muon Barrel Sector Logic

5.2.1 System description

The L0Muon trigger exploits hits coincidences across RPC and TGC chambers of the muon spectrometer, the former are used in the barrel region, the latter in the end-cap regions of the detector. The ATLAS detector barrel is divided in large and small sectors, identified by the edges of the RPC chambers across its cylindrical surface. Figure 5.4 shows a section of the muon system in the (x, y) plane in which sectors are shown: small sectors are located in the regions where the toroidal magnet coils are present, while large sectors are located in the spaces between two adjacent magnet coils. The full muon system counts 16 sectors in total: 8 small and 8 large

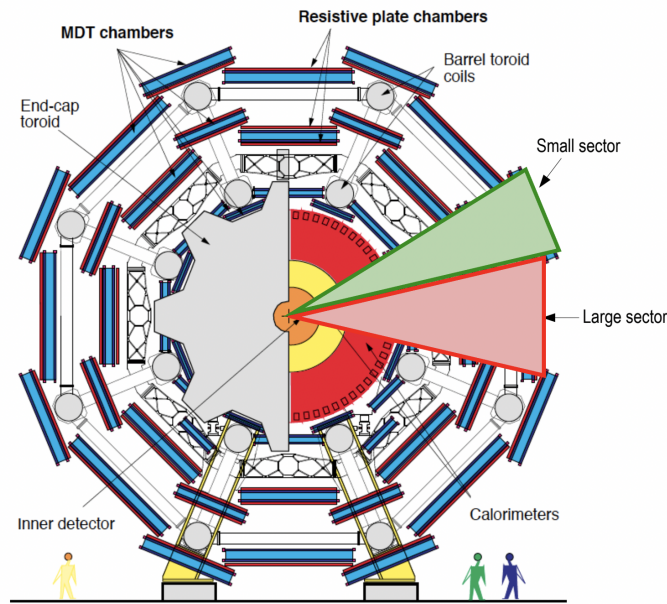


Figure 5.4. Representation of the ATLAS muon system in a (x, y) plane section, with the indication of large and small sectors. Figure adapted from [169].

respectively.

The Barrel Sector Logic (SL) is the electronic board implementing the trigger functionality in the barrel region sectors. It is part of the L0Muon system and is in charge of looking for coincidences across the RPC chambers in one sector and to identify the barrel L0Muon trigger candidates. Each of the 16 sectors of the muon system is divided in two parts, corresponding to ATLAS sides (side A and C). Each part is served by a dedicated SL board, hence a total of 32 boards will be installed in the L0Muon trigger. A similar board with different firmware and features, called the Endcap Sector Logic, is implemented to identify trigger candidates in the end-caps. The work presented in this thesis is focused on the barrel muon trigger, hence we will not consider the Endcap Sector Logic in what follows, and the abbreviation SL will always refer to the barrel Sector Logic.

Figure 5.5 shows a more detailed summary of the detectors and front-end electronics sub-systems involved in the barrel SL. The SL exploits four groups of RPC chambers: the RPC0 chambers are located in the barrel inner (BI) station of the muon spectrometer, the RPC1 and RPC2 are located in the outer and inner part of the barrel medium (BM) station, the RPC3 are located in the barrel outer (BO) station. RPC0 are triplets of chambers: they contain three gas gaps and the passage of one muon can generate up to three hits in the respective gaps. Instead, RPC1, RPC2, RPC3 are doublets of chambers and a muon can generate up to two hits in the relative gas gaps.

Ionisation signals in the chambers are collected by the Data-Collector-Transmitter (DCT) on-detector boards. The DCTs are front-end electronic boards in charge of receiving and sample the data from the RCP chambers, apply a zero-suppression algorithm and transmit the data to the barrel SL. Strips on the BM and BO RPC chambers are divided in two parts (see Figure 5.6), hence DCTs are installed both on

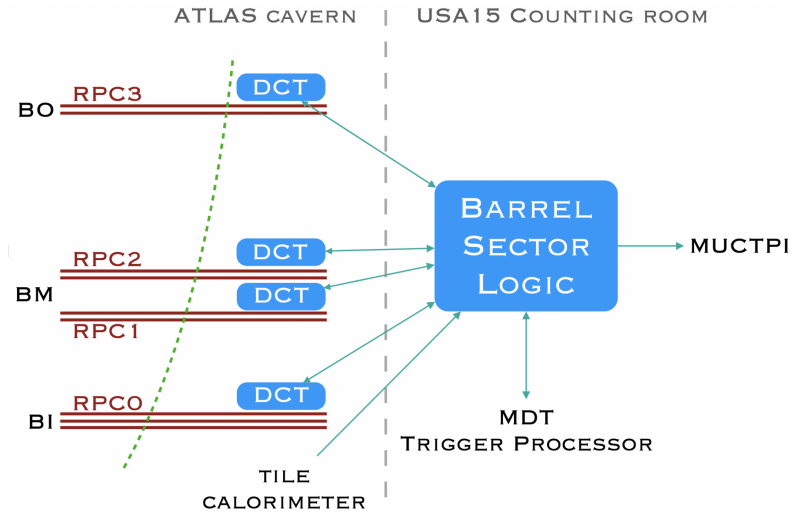


Figure 5.5. Scheme of the L0 Muon Barrel Sector Logic and its connections. Figure adapted from [170].

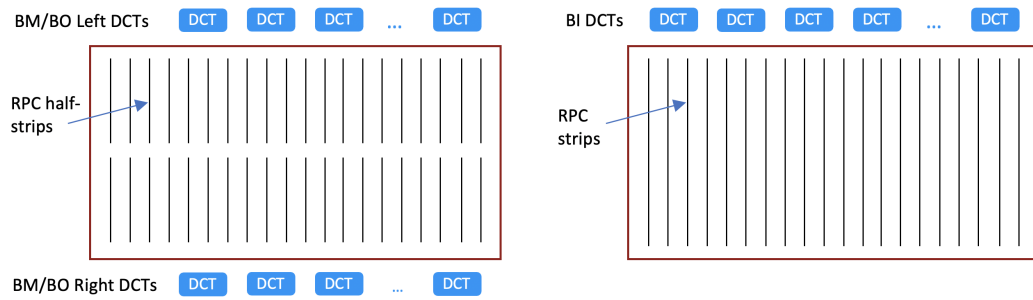


Figure 5.6. Representation of the strips layout in the RPC chambers. BM/BO chambers (left) have half-divided strips, BI chambers (right) have single strips.

the left and right sides of the chambers. Instead, strips of the BI RPC chambers are not divided and DCTs are located only on one side. One SL board is connected to 20 DCTs reading the BM+BO-left-side strips, 20 DCTs reading the BM+BO-right-side strips, 10 DCTs reading the BI strips. A total of $\simeq 1600$ DCT boards will therefore be part of the Phase-II muon trigger front-end electronics. Once collected by DCTs, muon data are transmitted to the SL, which is located off detector in the USA15 experimental cavern. The transmission is implemented via optical fiber connections and data have to be released within the DCT maximum latency. Due to the different physical paths of the transmission lines, the SL receives data relative to the same bunch-crossing with different delays. Such delay differences have to be compensated by the SL, which has to guarantee a fixed latency transmission to the following systems, re-ordering the received data by bunch-crossing ID (BCID).

The barrel SL board is also connected with the MDT trigger processor (MDTTP) and the Muon Central Trigger Processor Interface (MUCTPI). The MDTTP is exploited to refine the estimate of the muon candidates p_T , to reach the resolution of the MDT tracking chambers. Muon candidates are sent from the SL to the MDTTP, which sends back to the SL a trigger confirmation if the candidate is accepted within the improved MDT resolution. The confirmed trigger candidates are sent to the Global Trigger and to the Central Trigger Processor via the MUCTPI interface.

5.2.2 Sector Logic physical board description

Board and FPGAs technical details

The L0 barrel Sector Logic is physically implemented in an electronic board, based on Field Programmable Gate Arrays (FPGAs). An FPGA is an integrated circuit that can be programmed by the user via a hardware description language, to implement the desired functionalities. It consists of an array of configurable logic blocks and interconnects, implemented in a chip, placed on a service board. The L0 barrel Sector Logic is based on Xilinx FPGAs, programmed via the VHDL language.

The physical board is shown in Figures 5.7 and 5.8, reporting the pictures of the first board prototype from different angles and a schematic denoting the major components and ports located on the board. The board hosts a Xilinx FPGA implementing the SL functionalities, namely the Xilinx Virtex Ultrascale+ FPGA, with part number XCVU13P-FLGA2577-1-E. On the same physical board a System on Chip (SoC) module is mounted, based on the Xilinx Zynq Ultrascale+ FPGA, and is used to interface the SL FPGA with external monitoring servers. The SL board is compliant with the ATCA (Advanced Telecommunications Computing Architecture) standard and hosts an IPMC (Intelligent Platform Management Controller) card, used to communicate with the shelf manager. The board is equipped with a power system, distributing the power supply all over its extension, voltage and temperature monitoring sensors, and several Samtec Firefly optical modules to host connections with input/output fibers. Moreover, three RJ45 (Registered Jack 45) and one SFP+ (Small Form-factor Pluggable) ports are available to support data connections via Ethernet and optical fibre respectively.

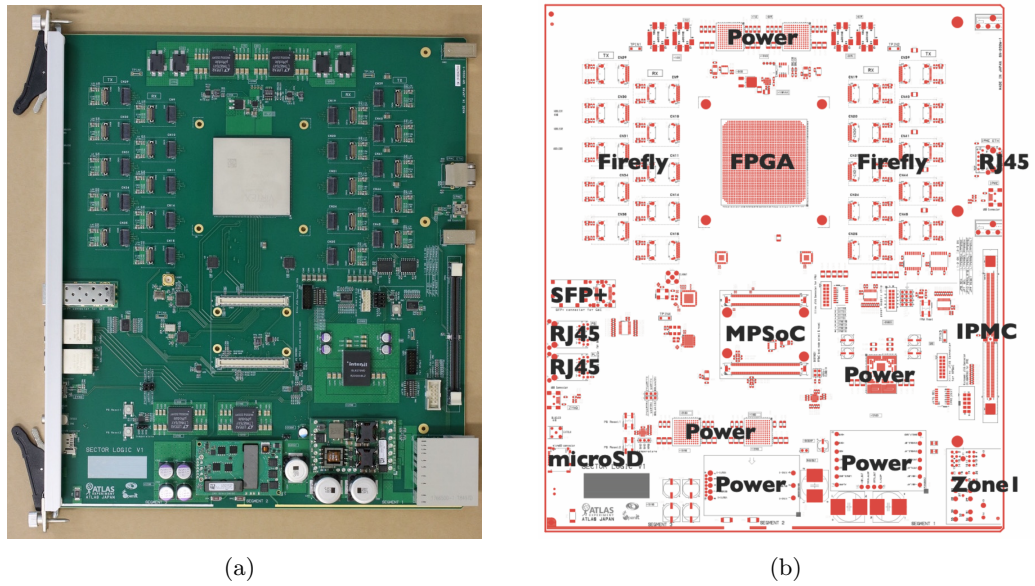


Figure 5.7. The Sector Logic board prototype: (a) top view and (b) schematic of its major components.

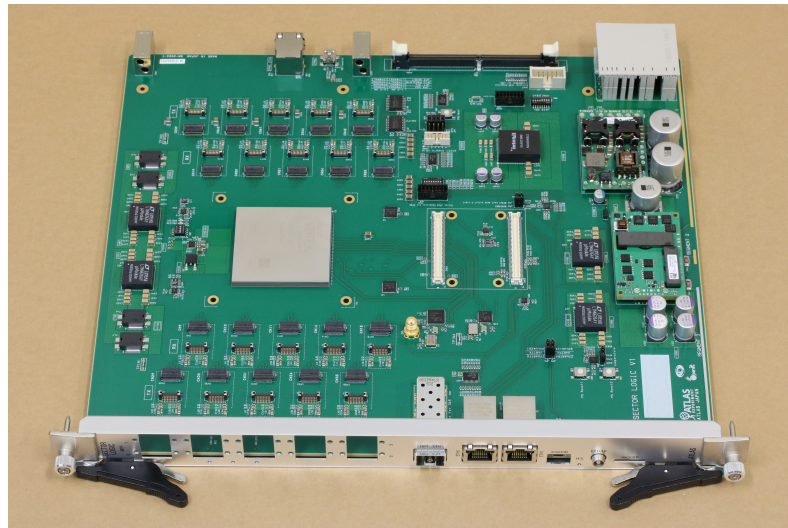


Figure 5.8. The Sector Logic board prototype, seen from the top-side view.

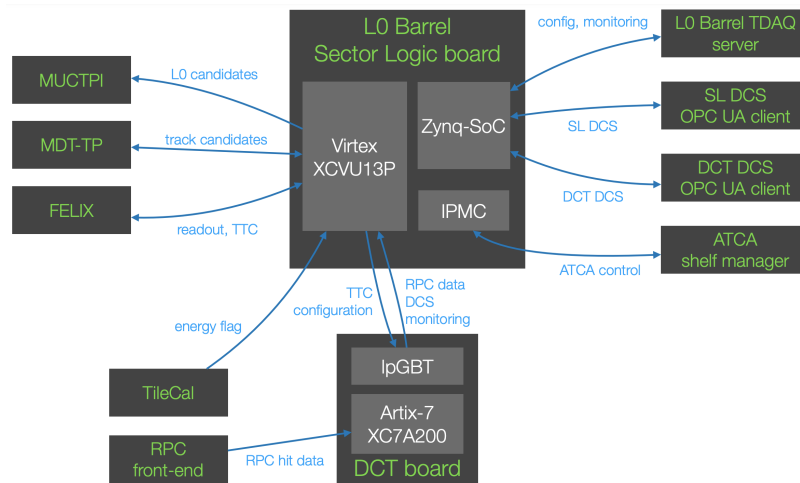


Figure 5.9. Scheme of the barrel SL interconnections with external devices. Details on the FPGAs used are also provided. Figure taken from [170].

Interconnections technical details

Figure 5.9 shows the SL main interconnections linking the board to external systems. Details on the fibres, bandwidths and protocols used are reported in Table 5.2

The bidirectional connection between the SL and the DCTs is supported by 50 optical fibers. The input connections, from the DCT to the SL, transmit the muons data originating from the RPC chambers and the detector control system (DCS) data, reporting the status of the system. The output connections, from the SL to the DCT, instead, transmit the DCS configuration instructions and the timing, trigger and control (TTC) signals, delivering the LHC reference clock, the high level trigger decisions and the synchronized broadcast control commands. Data are encoded along these fibers via the low power Giga Bit Transceiver (lpGBT) protocol, which is implemented on the DCT in the lpGBT chip and in the SL FPGA via the lpGBT-FPGA firmware emulator. The SL is also interfaced with the Tile Calorimeter. This connection is one-directional, from the TileCal to the SL, and is implemented in 6 physical fibers. A connection from the SL to the TileCal is not needed, as the calorimeter system is monitored and controlled via the L0Calo sub-system. The MDT Trigger Processor (MDTTP) and the SL are interfaced via 8 fibers, implementing bi-directional connections. These fibers are used to transmit the L0Muon trigger candidates from the SL to the MDTTP, and receive back the confirmation of the candidate after the high-resolution computation of muon's p_T , obtained within the MDT chambers precision. The SL sends trigger candidates to both the MDTTP of the same sector and to the MDTTPs of the two adjacent sectors and receives back confirmations for both same- and adjacent-sectors MDTTP. Up to three muon candidates can be sent back and forward between the SL and the MDTTPs within the same bunch-crossing. Interface between the SL and the MUCTPI is managed via 4 optical fibers that support the transmission of the L0 trigger candidates to the Global Trigger and Central Trigger Processor. A bidirectional connection is also set between the SL and the FELIX component. The output connection is implemented via 4 fibers and supports the transmission

Table 5.2. Details on the main I/O connections between the barrel SL with external systems.

Ext. system	Type	N fibers	Band (GB/s)	Protocol	Data content
RPC DCT	in	50	10.24	lpGBT	RPC data, DCS data
RPC DCT	out	50	2.56	lpGBT	TTC, DCS commands, configuration
TileCal	in	6	9.6	8b10b	Tile Calorimeter data
MDTTP	in	8	9.6	8b10b	MDTTP trigger candidate confirmation
MDTTP	out	8	9.6	8b10b	SL trigger candidates data
MUCTPI	out	4	9.6	8b10b	L0 barrel trigger candidate
FELIX	in	1	9.6	8b10b	TTC signals
FELIX	out	4	9.6	Full mode	Readout
TDAQ server	in	1	TBD	ethernet	SL/DCT configuration and FPGA firmware
TDAQ server	out	1	TBD	ethernet	SL/DCT monitoring
OPC UA clients	in	1	TBD	ethernet	SL/DCT DCS commands
OPC UA clients	out	1	TBD	ethernet	SL/DCT DCS data
Shelf manager	in	1	TBD	IPMI	ATCA commands
Shelf manager	out	1	TBD	IPMI	ATCA data

of triggered data from the SL readout to the Data Acquisition chain. The input connection instead, supports the propagation of the TTC signal at 40 MHz, from FELIX to the SL, which then propagates this signal to the DCT.

Further connections are in place between the System on Chip (SoC) and the external servers, mainly implementing service and control or monitoring functions. The SoC is connected via ethernet protocol to the external TDAQ server, which receives control and monitoring information. The TDAQ server is also used to upload or modify both the firmware of the SL and of the DCT, which are propagated from the SoC to the SL FPGA via the AXI Chip2Chip [171] bus and the Aurora protocol [172]. The SoC also interfaces with the OPC UA (Open Platform Communications Unified Architecture) clients [173], which receive control and monitoring information on the SL and DCT non-critical parameters, to be sent to the main Detector Control System.

Data formats

Data containing information on the muon hits in the RPC chambers are sent from the DCT to the SL as words of 28 bits. The data format is the following: the first 8 bits encode the ID number of the strip involved in the hit, the following 10 bits encode the bunch-crossing ID number (BCID), the last 10 bits encode the hit time. Data are sent at 320 MHz, with the lpGBT coding. Instead, the data format for the links between the SL and the MDTTP and from the SL to the MUCTPI is 6×32 -bit every 25 ns.

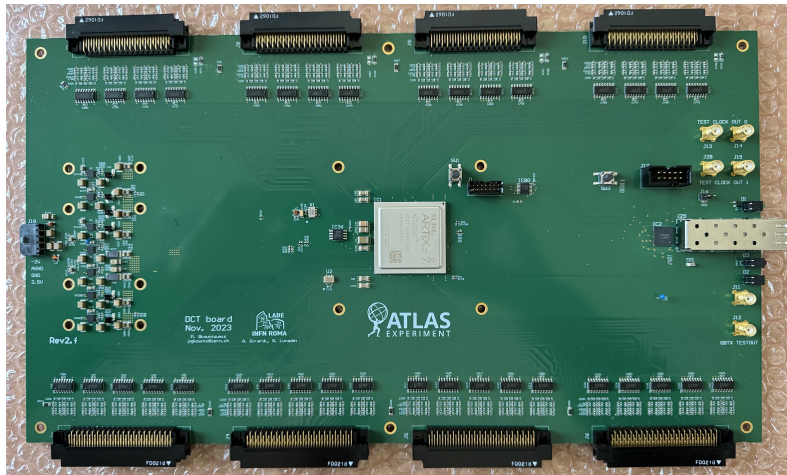


Figure 5.10. The DCT board prototype, seen from the top view.

5.2.3 The DCT board

The SL is processing data transmitted from the Data Collector Transmitters (DCTs). We report for reference some information on this board, for which the design is currently completed. Like the SL, also the DCT is based on a FPGA circuit, mounted on a board. In particular, the Xilinx Artix-7 XC7A200 FPGA is used to implement the DCT firmware. Figure 5.10 shows the DCT board prototype. Together with the FPGA, the board hosts also high-speed receivers, to acquire the data from the RPC chambers front-end electronics, the lpGBT chip implementing the data transmission protocol, and optical transceivers to send the data to the SL.

5.3 Readout of the Barrel Sector Logic

The barrel Sector Logic readout represents the original contribution given by the author to the L0 Muon Phase-II upgrade, since I have been in charge of the design, simulation and implementation of the full readout logic as part of this thesis project.

The readout is a necessary functionality that needs to be deployed in each trigger system. A trigger system is used to select interesting events, among the huge amount of non relevant ones for the physics analyses. The online events selection, based on requirements on the physics objects, benefits to the front-end electronics which has to cope with a decreased data rate to be acquired and saved on the permanent storage. Since the execution of the trigger algorithm on the analysed data requires time, a readout system needs to be used to store them temporarily, while the trigger takes the decision. Without a readout system, the triggered data would be lost and hence it would not be possible to propagate them in case of positive trigger decision.

The main difference between the Phase-I and the Phase-II systems is that in Phase-II data will be sent from the detectors to local readouts, implemented in each L0 sub-component, and from these ones they will be sent to FELIX, in case of a L0 trigger. In Phase-I, instead, data were transferred directly from the detectors to the FELIX system, which was serving as readout for all ATLAS sub-systems involved in the trigger. We discuss in the following the readout for the L0Muon barrel SL.

Table 5.3. Details of the input/output signals of the readout firmware.

Signal	IN/OUT	Type	N bits	Data content
BMBO DCT Left	IN	bus	20 x 28 bits	Muon data from DCTs
BMBO DCT Right	IN	bus	20 x 28 bits	Muon data from DCTs
BI DCT	IN	bus	10 x 28 bits	Muon data from DCTs
Trigger words SLR1	IN	signal	256 bits	Trigger candidates data from SLR1
Trigger words SLR2	IN	signal	256 bits	Trigger candidates data from SLR2
BMBO Left output	OUT	signal	32 bits	Muon data sent to FELIX
BMBO Right output	OUT	signal	32 bits	Muon data sent to FELIX
BI output	OUT	signal	32 bits	Muon data sent to FELIX
Trigger words output	OUT	signal	512 bits	Trigger cand. data sent to FELIX
Clock 320	IN	signal	1 bit	Clock signal
Clock 240	IN	signal	1 bit	Clock signal
Clock 40	IN	signal	1 bit	Clock signal
L0A	IN	signal	1 bit	L0 trigger accept signal

5.3.1 Conceptual design of the readout logic

The conceptual scheme of the entities used to implement the L0Muon barrel SL readout in the FPGA is displayed in Figure 5.11, and a detailed summary of all the input and output signals of the readout logic is reported in Table 5.3. The readout is implemented by the `top_readout` object, which is composed of the `data_readout` and `cand_readout` entities, designed through the Vivado toolkit [174] which will be introduced in Section 5.3.2. The `data_readout` entity is itself made of three instances of the `top_memory` entity: the first two receive data from the 20 BM/BO Left DCTs and 20 BM/BO Right DCTs respectively, while the last one manages the data sent by the 10 BI DCTs. The `cand_readout` entity, instead, receives the trigger candidates data from the trigger logic located in super-logic regions 1 and 2 (SLR1, SLR2) and propagates them to the FELIX system, as will be further described afterwards.

DCT data arrive continuously with fluctuating latencies to the `data_readout` entity, and are stored in memory. When a L0-Accept (L0A) signal is raised, the data corresponding to the triggered bunch-crossing ID (BCID) are released on first three output fibers (two for BM/BO Left and Right respectively, one for BI). If, instead, data reside in memory for a time greater than the L0 maximum latency time of $10\ \mu\text{s}$ (i.e. the maximum time allowed to the trigger to issue a positive decision), they are deleted. Correspondingly, also the trigger candidates data arrive to the `cand_readout` entity and are released after a L0A on the fourth output fiber. The readout logic is designed to work with a clock frequency of 240 MHz, which sets the frequency at which all the firmware processes are executed in the logic. Data are coming from the DCTs with a higher frequency of 320 MHz, hence specific dual-clock FIFO buffers are used to and decrease the input data rate to 240 MHz, after suppressing the null incoming words. Some additional FIFO memories (denoted as `FIFO_L0A` in Figure 5.11) are used to manage situations in which two L0As are raised with a time separation lower than the time needed to release triggered data

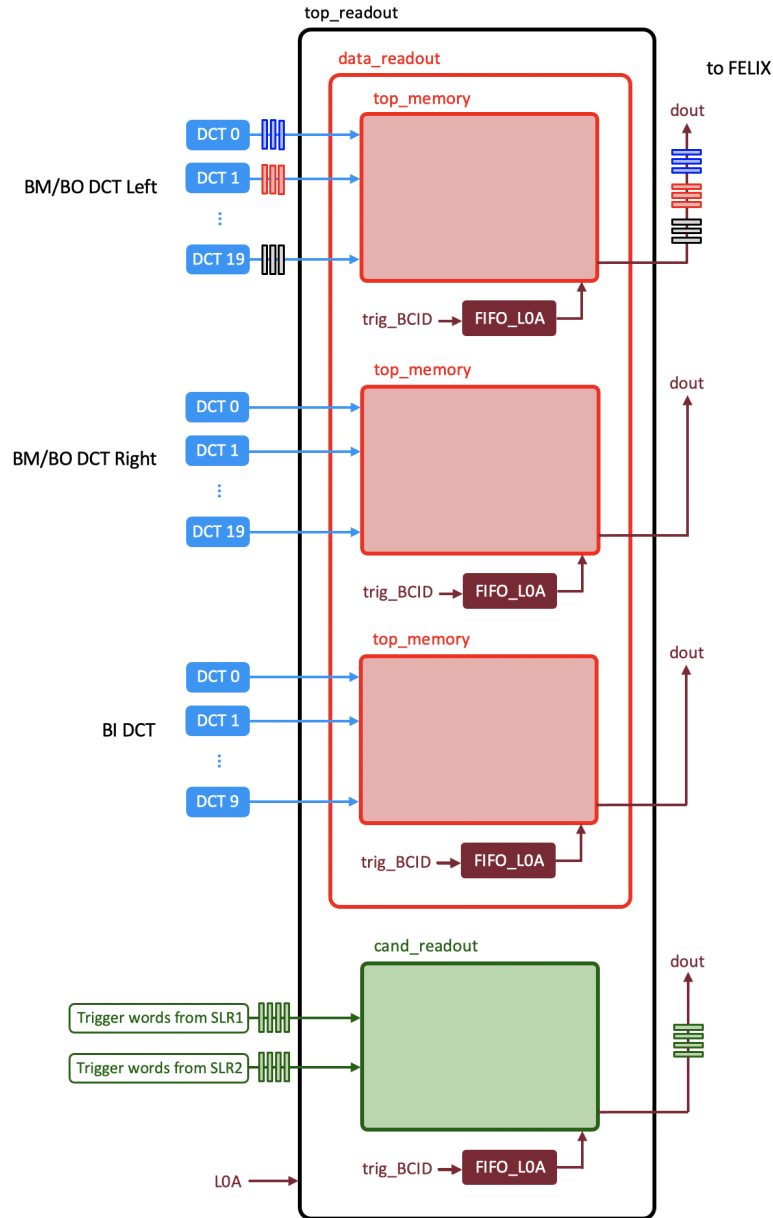


Figure 5.11. Scheme of the L0 Muon barrel SL readout, encoded in the `top_readout` entity. Some of the major input/output signals are also represented.

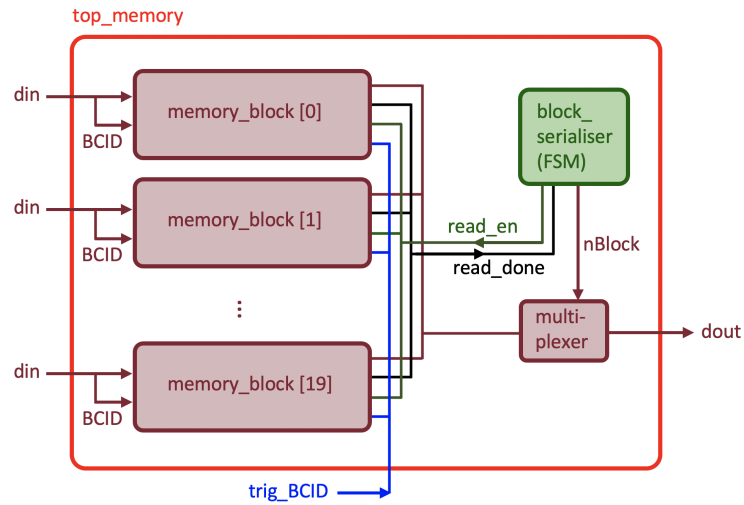


Figure 5.12. Scheme of the `top_memory` entity and its constituents.

from the readout memories. When a L0A signal arrives the triggered BCID is stored into the `FIFO_L0A` memories which then send the triggered BCIDs to the readout logic. In this way the triggered BCIDs are kept in a buffer and near-in-time triggered BCIDs are processed exploiting periods of lower trigger frequency. The average time to release the trigger data has anyhow to be lower than the average time separation between two triggers, which is fixed by the L0 output frequency of 1 MHz.

Together with the readout functionality, the `data_readout` entity is also implementing the auxiliary function of *ordering* the data with respect to the DCTs. Data associated with a given BCID arrive from each DCT with fluctuating latency, since DCTs are physically located in different places of the detector and can have buffers with different occupancy (determined by the different frequency of muons passing by). This yields different delays along the transmission, and therefore data arrive in the SL readout without being ordered with respect to the DCTs. When data of the same BCID exit the SL readout, instead, they are propagated in a sequence ordered with respect to DCT number: first will be released data of DCT0, then of DCT1, and finally of DCT19. This automatically compensates the DCTs latency fluctuations.

The data format of the words exiting the `data_readout` entity has 32-bits, containing information on the number of strip of the RPC detector which registered the signal, the BCID corresponding to the muon's passage, and the hit time. Bits are divided as follows: 2 bits empty, 8 bits for the strip ID, 12 bits for the BCID, 10 bits for the hit time. Instead, the data format of the words exiting the `cand_readout` entity is 512 bits. The 12 bits for the BCID are required to be compliant with the FELIX data format requirements.

The `top_memory` entity

The `top_memory` entity, shown in Figure 5.12, is the basic component constituting the SL readout logic. It is mainly made of n instances of the `memory_block` entity, each one corresponding to its relative DCT.

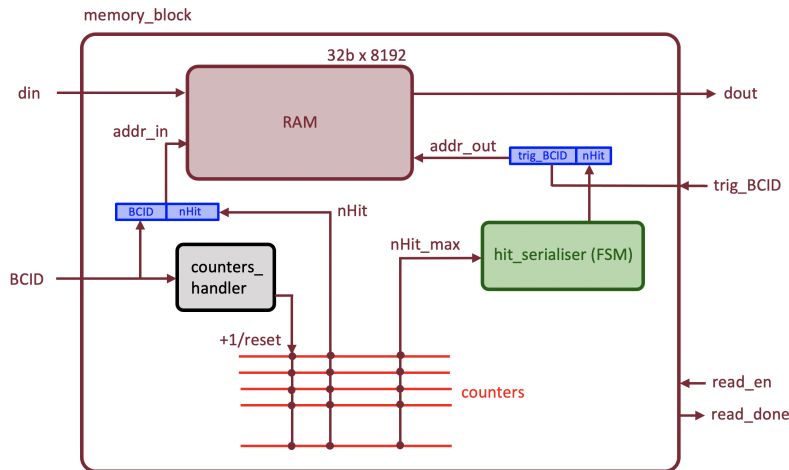


Figure 5.13. Scheme of the `memory_block` entity and its constituents.

Data continuously flow from the DCTs to the memory blocks and are stored according to the BCID to which they are referred, which is extracted directly from the appropriate bits of the input words. When L0A arrives, data stored in each memory block and corresponding to the triggered BCID are extracted and sent on the output fiber. The data extraction is ruled by the `block_serialiser` finite state machine. The block serialiser points one by one each memory block through the `read_en` signal and activates the flushing of the triggered data. When a memory block completes the data release the `read_done` signal is raised and the block serialiser starts processing the next memory block, until the last one. Data are routed through n output signals, which are then merged into a single output fiber by a `multiplexer` entity, operated via the `nBlock` signal.

Notice that the `top_memory` entity is implementing the ordering functionality: data are registered in the memory blocks with fluctuating latency, while the same data are extracted and sent to the output fiber ordered by DCT number.

The `memory_block` entity

The `memory_block` entity, represented in Figure 5.13, is in charge of storing the data coming from a single DCT. It is mainly based on a dual readout RAM memory, implemented as a built-in object in the toolkit used to design this firmware, i.e. the Vivado Design Suite (see Section 5.3.2 for more details). The RAM memory is sized to store the full amount of data expected to be delivered by the DCT. Since on average a maximum of 16 words are expected to arrive from the DCT for each of the possible 512 bunch crossing IDs, the depth of the memory is fixed to 8192 words. The number of considered BCIDs is determined by the number of bunch crossings comprised within the $10\ \mu\text{s}$ latency, at a bunch crossing rate of 40 MHz. The RAM width is 32-bits, equal to the number of bits of the incoming words.

Input data referred to the same bunch-crossing ID have to be stored in contiguous memory locations of the RAM. This is achieved by constructing the address of the input words properly: the first part of the address is equal to the words' BCID, while the second part is a counter taken from a series of 512 `counters` (one for each

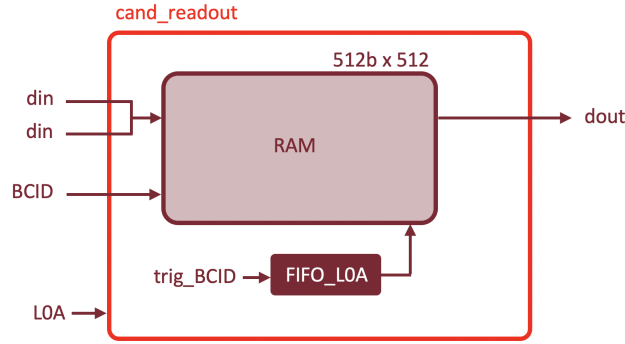


Figure 5.14. Scheme of the `cand_readout` entity and its constituents.

possible BCID), managed by the `counters_handler` entity. When the `read_en` signal is raised, the data corresponding to the triggered BCID have to be flushed. This is also achieved making use of a composite output address: the first part of the address is equal to the triggered BCID number, the second part is assigned by the `hit_serialiser` entity, which generates a counter from 1 to the number of hits stored in memory `nHits_max`. After flushing all the triggered words, the `read_done` signal is raised.

In parallel to the input and output functionalities, the `memory_block` entity also implements the reset functionality to delete all words which resided in memory more than the L0 latency time of $10\ \mu\text{s}$. More specifically, this is implemented by the `counters_handler`, which deletes data corresponding to BCID $k = j - 480$, when j is the current BCID ($10\ \mu\text{s} = 400$ BCIDs, and a 20% tolerance is added).

The readout for trigger candidates

The trigger algorithm utilises the information encoded in the raw DCT data to evaluate if a muon with p_T higher than the trigger threshold is present in the event (see Section 5.4 for details). The algorithm produces as output 4 words of 128-bits each which, in case of positive trigger decision, have to be sent to the FELIX system. To enable this, the `cand_readout` entity is used, in order to store the trigger words during the elaboration time and transmit them in case of a trigger. The readout for the trigger words is simpler, since data are not coming in parallel from different DCTs and there is not a variable number of words associated to the same BCID.

The `cand_readout` entity, shown in Figure 5.14, is based on a single RAM memory. The width of the RAM is set to 512-bits, to read in parallel the 4 words of 128-bits each. The depth of the RAM is also 512, to have one memory location for each possible BCID. The trigger candidates words are received through two 256 bit signals, which are merged together and propagated in output in a single signal of 512 bits. An auxiliary `FIFO_LOA` is present to manage situations in which two `LOA` signals arrive with a time separation lower than the time needed to release output words, similarly to what was done in the `top_memory` entity. The input address simply corresponds to the BCID associated with the input words, while the output address corresponds to the triggered BCID.

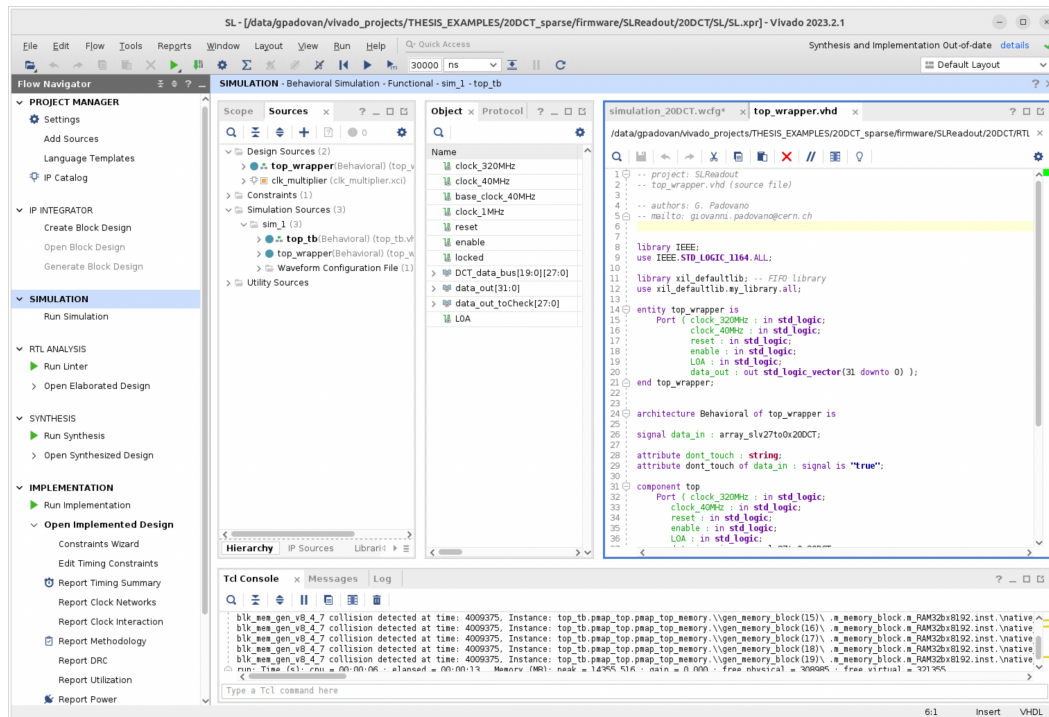


Figure 5.15. Main view of the Vivado Design Suite user interface.

5.3.2 The Vivado design suite

The conceptual design presented in previous section has to be encoded in a firmware to be implemented into the FPGA physical board, described in Section 5.2.2. To accomplish this task I used the Vivado Design Suite [174], distributed and maintained by the company Xilinx, to support firmware implementation of the FPGA boards produced by the same company.

Figure 5.15 shows the main screen of the Vivado Design Suite user interface. Several menus and panels are available to accomplish all the required tasks and deliver a finalised firmware to be uploaded in the physical FPGA board. The left-hand side panel collects the menus providing access to the main functionalities: the “project manager” menu, displaying generalities on the status of the project and on the selected physical FPGA, the “simulation”, “synthesis”, and “implementation” menus, which enable the run of the main steps of the pipeline. The right-hand side box, enables the writing of firmware via VHDL language. Here the user builds the custom entities via the hardware description language, combining them also with Vivado built-in entities, available through the IP generator tool. The two upper-central boxes show the list of entities involved in the project, both custom and built-in, displaying also their hierarchical organisation. The lower box, instead, displays all error and warning messages, and presents also a command line to provide in-line instructions, to be expressed in the TCL syntax.

The firmware development pipeline is characterised by several steps, described in the following:

- **simulation:** after writing the firmware code in VHDL the top-level entity

(i.e. the entity which contains all the other entities involved in the project) is positioned on a *test bench*, which is a simulation entity having no input and output signals. The top-level entity inputs are connected with test signals handled within the test bench, while the outputs are monitored via a waveform display screen. In this way the user can inspect the output signals and verify that they correspond to the expected waveforms;

- **synthesis:** after a successful simulation the synthesis algorithm is run. The synthesiser translates the VHDL instructions into a series of elementary logic ports (AND, OR, NAND, XOR, flip-flops etc.) which realise the circuit described in VHDL. The output of the synthesis step is therefore a logic circuit, which can be placed in an FPGA array of logic ports;
- **implementation:** in this last step, the logic circuit generated in the synthesis step is actually placed in the real physical connections of the considered FPGA board. Each required logic element is assigned to a particular logic connection of the board, taking into account of the total available connections and of the physical distance between each couple of connection end-points. The implementation algorithm is an optimiser, which considers all the possible logic ports placements, and selects the most feasible one. After a successful implementation a bit-stream can be generated, to be directly uploaded in the FPGA board.

At implementation stage some *constraints* can be enforced by the user, requiring that some internal signals are placed on specific connections on the FPGA's interface ports, or requiring that a specific entity or a part of the firmware is placed in a defined region of the FPGA array. These requirements are expressed as statements in a constraint file, and are used either to verify external requirements needed in the project or to help the optimiser to converge towards an optimal solution in the logic placement. During the implementation step *timing errors* can arise, generated by signals that cannot propagate between two assigned end-points within a time lower than the clock cycle. All timing errors have to be solved to obtain a successful implementation and most of them can be addressed empirically, either changing the constraints, or adding flip-flops to divide signals connecting far end-points or simplifying the logic, for example decreasing the inter-connectivity between entities.

The Vivado built-in entities

Figure 5.16 shows the FIFO and Block-RAM (BRAM) built-in entities, that are available in Vivado via the IP generator tool and have been used in this project to build the SL readout logic.

The FIFO entity. The FIFO entity [175], displayed in Figure 5.16(a), represents a standard First-in-first-out memory: data are orderly saved in memory and exit from memory in the same order as they entered. Data are inserted in memory via the `din` signal and read as output from the `dout` signal. The `wr_en` and `rd_en` signals are auxiliary and have to be asserted when writing and reading data from the input and output ports respectively. The `full` and `empty` signals, instead, report

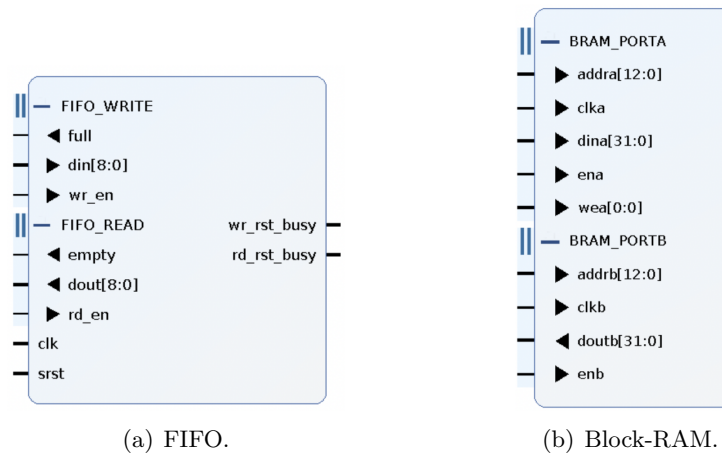


Figure 5.16. Representation of Vivado built-in objects: (a) FIFO memory (b) Block-RAM memory.

auxiliary information on the status of the FIFO memory, the first one warning that all the locations are occupied with data, the second one telling that they are all available. The `clk` and `srst` signals apply the clock and the reset of the entity respectively. During reset operations the entity cannot be used and the `wr_rst_busy` and `rd_rst_busy` signals are raised.

The Block-RAM entity. The Block-RAM (BRAM) entity [176] is a random access memory, constituted of a series of locations accessible in any desired order via their address. The major input/output signals are displayed in Figure 5.16(b): input and output data are inserted and extracted respectively on the signals `dina` and `doutb`, and the addresses to point to the reading and writing memory locations are provided via the `addra` and `addrb`. The `ena` and `enb` auxiliary signals have to be raised when I/O operations are underway in the respective ports, while the `wea` signal has to be raised to let port A be an input port. The `clka` and `clkb` signals are used to provide the clocks for operations on side A and B of the BRAM.

5.3.3 Reduced simulation with 20 DCTs

I performed a first simulation and implementation of the readout firmware, using a reduced version of the system, made by only 20 DCTs connected to a single `top_memory` readout entity. The aim of this study is to test the firmware with a fictitious and controlled input in order to verify that the output data are consistent, as well as attempt a first firmware implementation and verify that it can be supported by the available resources of the chosen FPGA.

Simulation

Figure 5.17 reports a snapshot of the most significant signals as they are captured by the Vivado Design Suite waveform viewer. From direct inspection of the waveforms, the most important features of the firmware can be noted.

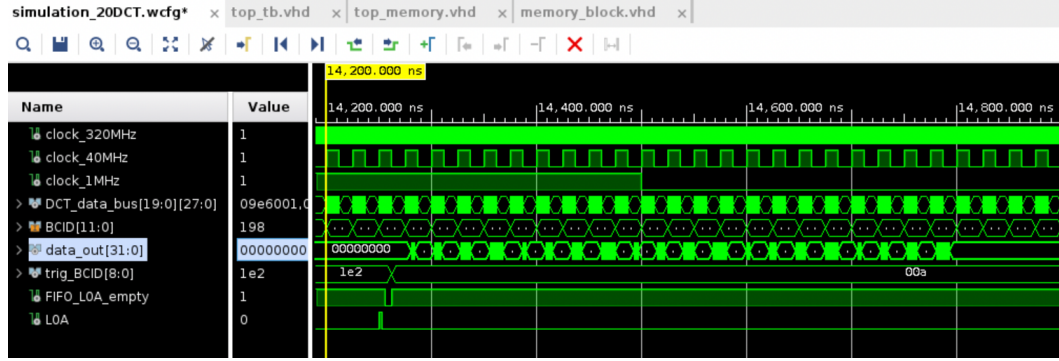


Figure 5.17. Simulated waveforms for the reduced firmware with 20 DCTs.

Three clock signals are used, with different frequencies: `clock_320MHz`, `clock_40MHz`, `clock_1MHz`. The first one is the base clock used to run the readout logic¹, the second represents the LHC bunch-crossing frequency, the last one generates the L0A signals, which are foreseen at the average frequency of 1 MHz for the Phase-II L0 trigger. The input data are fictitious and are generated by a `data_generator` entity. This entity produces a bus of 20 signals, one for each DCT, reporting a sequence of words designed to be easily recognisable in the output. The bus of input signals is denoted in Figure 5.17 as `DCT_data_bus`. When a L0A signal arrives the triggered BCID, represented by the `trig_BCID` signal, is sent as input in the `FIFO_L0A` memory. The entry of the triggered BCID word in memory can be verified looking that the `FIFO_L0A_empty` signal is not anymore raised to 1. Afterwards, the `trig_BCID` word is sent to the `top_memory` entity which starts to flush the triggered data in output. A sequence of 20 groups of words can be visualised on the output signal `data_out`, each one corresponding to words originated from one DCT and stored in the respective `memory_block` entity.

From inspection of the `data_out` signal it can be noted that the release of output words is affected by some delays originated from the internal operations of the logic. In particular, 9 counts of the 320 MHz clock pass between the raise of the L0A signal and the emission of the first word on the `data_out` signal. These clocks are needed to transfer the information on the triggered BCID to the `top_memory` entity and to start the `block_serializer` finite state machine. Moreover, 6 clock counts pass between the emission two adjacent groups of data on the `data_out` signal. These clock counts are needed by the `top_memory` entity to move the pointer between the two adjacent `memory_blocks` through the `read_en` and `read_done` signals. The total amount of lost clocks (i.e. clocks corresponding to auxiliary operations) is therefore $n_{\text{tot}} = 9 + 20 \times 6 = 129$ clocks.

Figures 5.18 and 5.19 show in more detail the structure of input and output data respectively. In Figure 5.18 the generated data words corresponding to the `<00a>` BCID are observed. They consist in a bus of 20 parallel signals, containing words with a clearly recognisable pattern. In Figure 5.19 it is shown the output sequence when

¹Notice that in this study a 320 MHz base clock is used, instead of the 240 MHz clock. This causes no qualitative differences both in the simulation and in the implementation. The final implementation of the full barrel SL firmware, reported in Section 5.5, is done with a 240 MHz base clock.

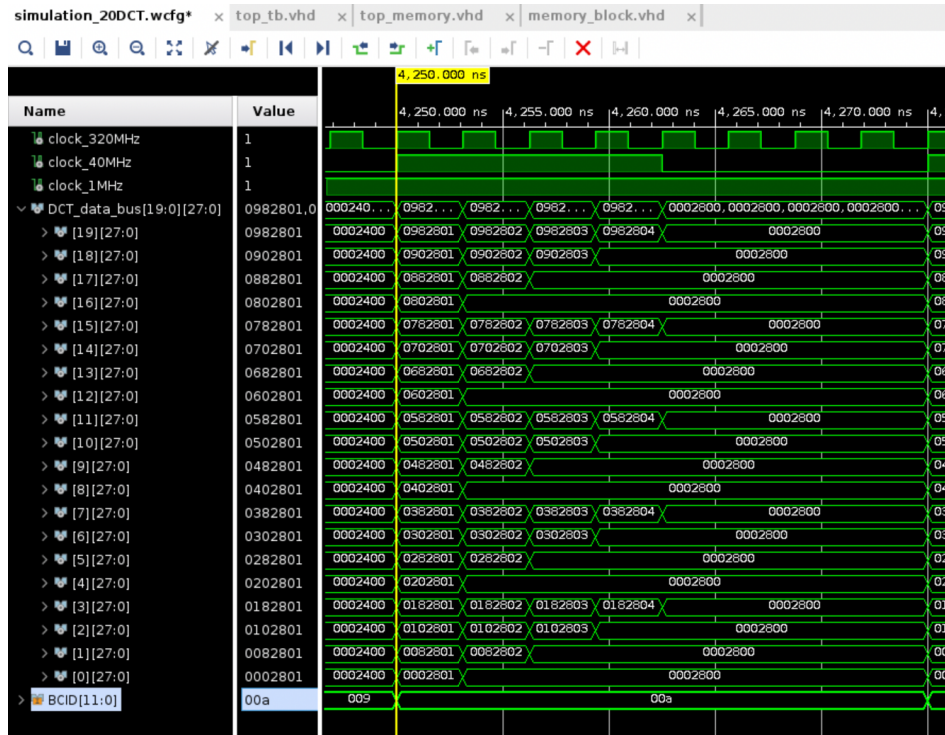


Figure 5.18. Detail of the input data sent to the readout logic in the 20 DCTs simulation. Data correspond to the BCID <00a>.

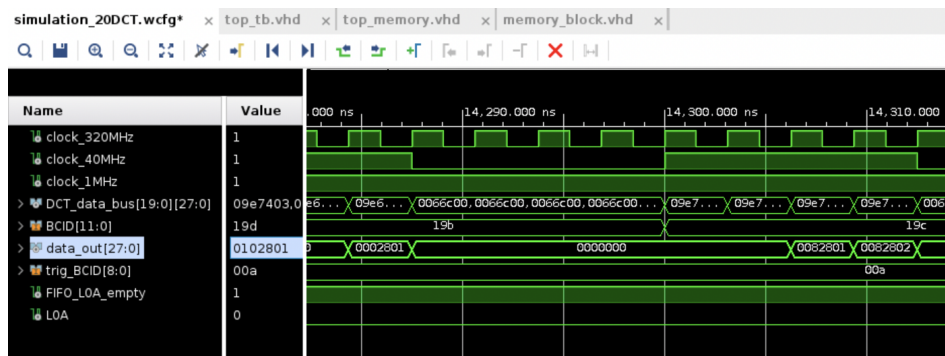


Figure 5.19. Detail of the output data extracted from the readout logic in the 20 DCTs simulation. Data correspond to the triggered BCID <00a>.



Figure 5.20. Representation the implemented readout logic into the FPGA board, for the 20 DCTs case study.

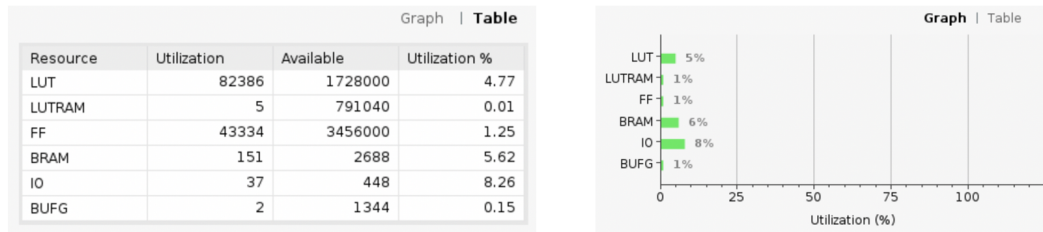


Figure 5.21. Resources occupation for the implemented logic in the 20 DCTs case study, reported in the form of table (left) and graph (right).

the same <00a> BCID is triggered: from direct inspection the emission of the data word <0002801> can be seen, extracted from the first `memory_block`, followed by the two words <0082801> and <0082802> extracted from the second `memory_block`.

Implementation and resources estimate

The synthesis and implementation of this firmware have successfully been done, using the Xilinx Virtex Ultrascale+ xcvu13p-flga-2577-1-e FPGA. The options `Flow_PerfThresholdCarry` and `Performance_ExtraTimingOpt` have been used for the synthesis and implementation respectively as they guarantee a more optimised handling of timing violations, at the expense of a little higher resources occupancy.

The implementation result is graphically shown in Figure 5.20: the adopted FPGA is schematically represented and the colored area indicates the logic ports utilised to implement the firmware. No constraints have been imposed on the position of the logic ports, hence the logic has been placed in the FPGA in the most convenient position according to the optimiser criteria. The occupied resources estimate is reported in Figure 5.21. The occupancy is low: a total of 5% of Look-up-tables (LUT) and 6% of block-RAM (BRAM) resources are utilised to implement the firmware.

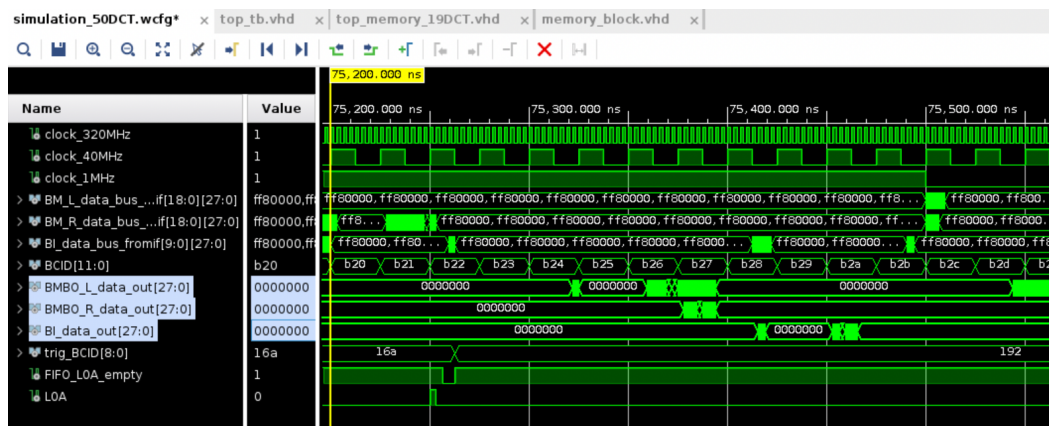


Figure 5.22. Simulated waveforms for the reduced firmware with all the 50 DCTs.

5.3.4 Full simulation with 50 DCTs

To test the readout firmware to its full extension I have run a second simulation and implementation of the complete version of the firmware, constituted of three replicated `top_memory` entities serving 20+20+10 DCTs which correspond to the BM/BO Left, BM/BO Right and BI front-ends respectively. The simulation has been executed using “real” data, obtained from a Monte-Carlo simulation of the DCTs. The implementation served to demonstrate that the complete readout logic with 50 DCTs has an occupancy compatible with the available resources on the FPGA.

Simulation

A snapshot of the most important signals visualised through the Vivado Design Suite waveform viewer is reported in Figure 5.22. The input signals are now represented by three buses, each one collecting the simulated data of respectively 20, 20 and 10 DCTs. As in the reduced simulation discussed in Section 5.3.3, the L0A signal is raised and the triggered BCID, represented by the `trig_BCID` signal, is registered in the `FIFO_L0A` memory. Afterwards, the output data are released along three independent signals, denoted with `BMBO L data out`, `BMBO R data out`, `BI data out`.

Since the logic is based on the same entities as in the reduced case with 20 DCTs, also the delays generated by the auxiliary operations on internal signals are the same. In particular, 9 clock counts are necessary to obtain the emission of the first data word after a trigger and 6 clock counts are necessary to move the pointer from one `memory_block` to the following. Hence, a total of 129 clocks are needed in the auxiliary operations to extract data on the `BMB0_L_data_out` and `BMB0_R_data_out` fibers, while 69 clocks are needed on the `BI_data_out` fiber. According to the signals simulation, the readout system on average is able to flush in output the data corresponding to a triggered BCID in a time shorter than the time between two L0As. This demonstrates the design of the readout system is correctly sized and will not generate back-pressure on the rest of the trigger system.

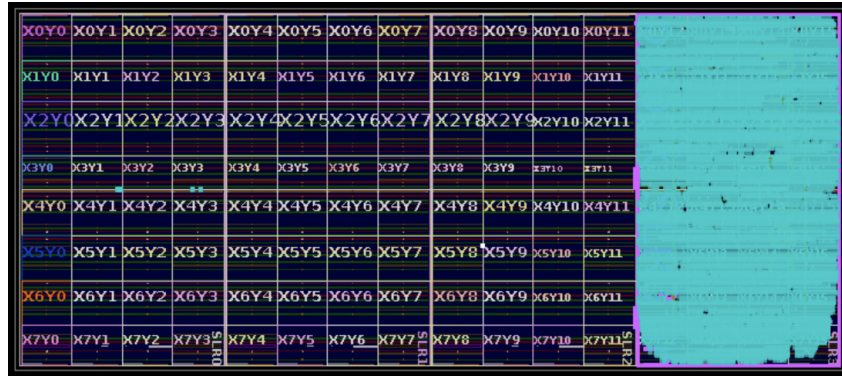


Figure 5.23. Representation the implemented readout logic into the FPGA board, for the 50 DCTs case study. The logic is constrained in the SLR3.

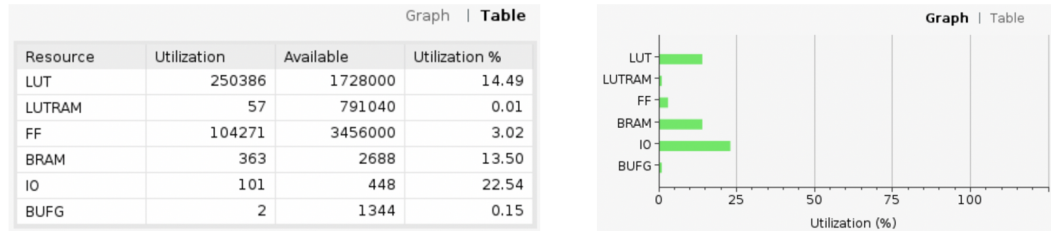


Figure 5.24. Resources occupation for the implemented logic in the 50 DCTs case study, reported in the form of table (left) and graph (right).

Implementation and resources estimate

The implementation of the complete firmware has been performed, using the same options `Flow_PerfThresholdCarry` and `Performance_ExtraTimingOpt`, reported in Section 5.3.3. In this implementation a constraint on the logic placement has been introduced. The Xilinx Virtex Ultrascale+ FPGA is divided into four regions, called *super logic regions* (SLR), and denoted with SLR0, SLR1, SLR2 and SLR3. The super logic regions are highly connected areas of the FPGA, which are linked among each others via data buses enabling the information transfer from one SLR to the adjacent one. The readout firmware has been constrained to be placed all in the SLR3, in order to leave the other SLRs empty for the trigger and I/O firmware placement.

The implementation result is displayed graphically in Figure 5.23, where the FPGA is represented (including its separation in four SLRs) and the colored area denotes the readout logic circuitry. Figure 5.24 reports quantitative results on the utilised resources. The estimated resources are consistent with the implementation of the partial readout with 20 DCTs, since they are approximately tripled. More specifically, the implementation requires the occupation of the 14% of the total available Look-up-tables (LUT) and of the 13% of the total block-RAMs (BRAMs) available in the FPGA.

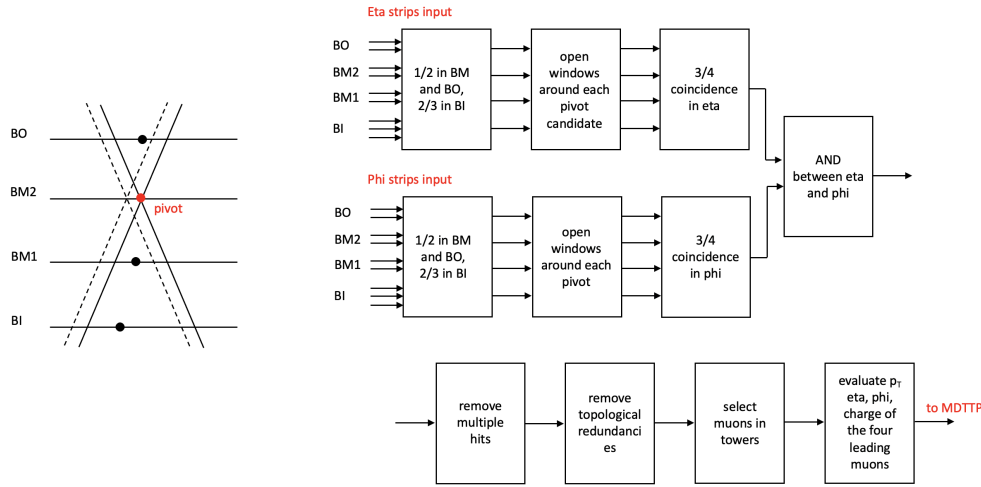


Figure 5.25. Schematic representation of the Phase-II barrel muon trigger algorithm. On the left an example of topological redundancy of two muon candidates reconstructed from the same hits is shown.

5.4 The trigger algorithm

The execution of the trigger algorithm to search for events with high p_T muons is the main functionality of the SL. A preliminary firmware has been developed and implemented in the FPGA to measure its occupancy.

The barrel muon trigger algorithm is based on selecting events in which at least one muon is present with p_T above a defined threshold. The p_T evaluation cannot be done with off-line quality, but is done as an approximate estimate, searching for hits in defined *coincidence windows* opened between the RPC chambers. The Phase-I trigger algorithm was based on defining a *pivot* hit in the BM2 station and opening coincidence windows towards the BM1 and BO chambers to look for additional hits. The acceptance holes due to the magnet toroid support structures in BM1 and BM2 were severely limiting the efficiency of this algorithm, since one hit on the BM2 layer was necessarily required by construction. The Phase-II trigger algorithm exploits the newly installed BI chamber to recover such acceptance inefficiencies and is structured to not require necessarily a hit on the BM2 chamber.

Figure 5.25 summarises the main steps of the Phase-II algorithm for the barrel muon trigger. First of all, a reduction logic merges the hits collected on the different gas gaps of each RPC station. An OR logic is applied between the two gas gaps of the doublet chambers (BM1, BM2, BO), while a 2/3 majority is applied on the three gas gaps of the BI chamber. Then, starting from each strip on the BM2 chamber, which is taken as *pivot*, coincidence windows are open towards the upper BO chamber and the lower BM1 and BI chambers and a 3/4 majority coincidence is required among the stations. These coincidences are run in parallel for both the eta and phi coordinates, and an AND between the two results is taken.

The procedure described so far can generate multiple muon candidates corresponding to the same hits, hence some redundancy suppression strategies have to be deployed. A first type of double counting can be generated by multiple hits

released by the same muon on adjacent strips. The multiple hits can induce the reconstruction of multiple muons corresponding to the same physical muon. To avoid this, all couples of hits located on the same RPC plane within a distance of three strips are merged in a single hit. A second type of double counting can be induced by hits topology. Hits across the four stations, produced by one muon, can induce multiple reconstructed muons, as shown in the left part of Figure 5.25. To avoid this redundancy, all muon candidates couples, whose pivots on the BM2 are at a distance less than three strips are reduced to one. The candidate with the highest number of hits is selected, and, in case of the same number of hits, the one with lowest eta is selected. Moreover, to avoid having several muon candidates in the same spatial region, the barrel is divided in 20 separate regions, called *towers*, and only the leading p_T muon in each tower is selected. Finally, the trigger algorithm produces as output four muon candidates, which are determined as the ones with highest p_T among the muons passing the previous selections. For these muon the kinematic coordinates (eta, phi, p_T) and the charge are calculated and encoded in four words of 128-bits, which are sent to the MDTTP. The whole algorithms takes 21 clock cycles at 320 MHz to run.

5.5 Complete firmware implementation

The complete firmware has been collected and implemented into the chosen FPGA (the Xilinx Virtex Ultrascale+) to demonstrate that the device is suitable to support this firmware project. To prepare the complete implementation, the trigger and readout firmwares have been integrated, together with additional logic supporting the input/output (I/O) interfaces with the external boards as well as secondary operations.

5.5.1 I/O interfaces and firmware floorplanning

The scheme of the I/O interfaces of the SL is summarised in Figure 5.26. The FPGA is equipped with 8 transmission quads in each super logic region (SLR), for a total of 32 quads. Each quad collects 4 GTY transceivers, supporting connections with the optical fibers.

Transceivers installed on the SLR0 support the connection between the SL and the BI DCTs, as well as the connection with the Tile Calorimeter, the end-cap SL, and FELIX. The BI DCT data are received on bi-directional connections that are used also to send monitoring commands to the RPCs, while the connections with TileCal and FELIX are uni-directional and are used to receive complementary calorimetric information and the TTC signal respectively. The transceivers in the SLR1 and SLR2 support the connections with the BM-BO DCTs and with the MDTTP and the MUCTPI systems. Data are received from the DCTs, are elaborated by two instances of the trigger algorithm firmware running respectively in the SLR1 and the SLR2, and are sent to the MDTTP. If candidates are accepted, they are sent to the MUCTPI from the SLR2. The BI and calorimetric information is propagated via internal connections from the SLR0 to the SLR1 and SLR2 in order to be available to the two trigger firmware instances. The whole data received from BI, BM1, BM2, BO DCTs in SLR0, SLR1, SLR2 is propagated to the SLR3, where the readout

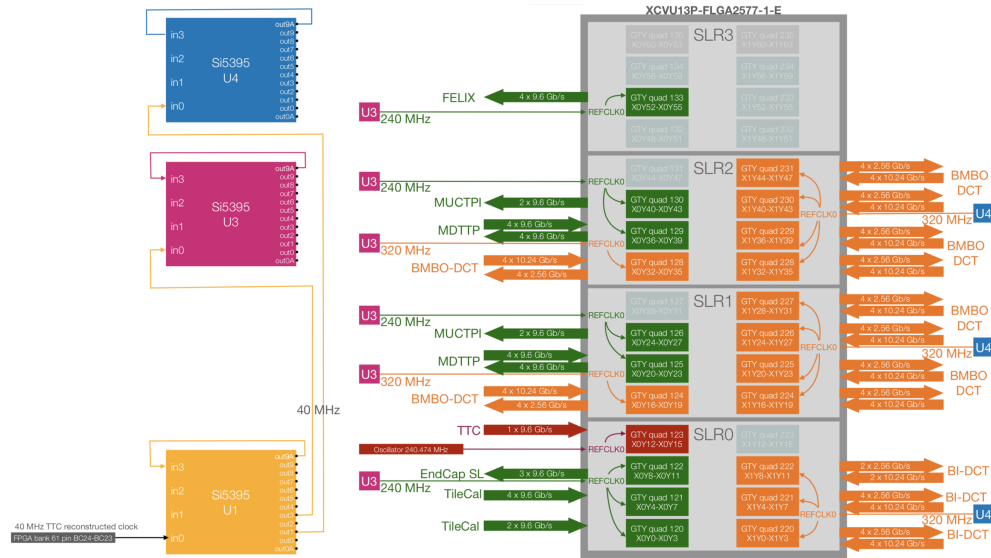


Figure 5.26. Scheme of the FPGA transceivers and their usage in the SL I/O interfaces.

firmware is constrained. Here a connection to the FELIX system on four different optical fibres is available, in order to transmit data to the DAQ system in case of positive trigger. This transmission is implemented via internal FIFO memories and flip-flops in a pipelined architecture, which have the function of separating the data transmission along the whole length of the FPGA in intermediate steps, in order to avoid timing violations.

Two clock domains are determined into the FPGA. The trigger firmware as well as connections between the SL and DTCs are operated at 320 MHz, while the readout firmware and connections with the MDTTP and the MUCTPI work with a 240 MHz clock. The transition between these two clock domains is managed through dual clock FIFO memories, which can operate with two different clocks in the input and output ports respectively.

5.5.2 Complete implementation results

The complete implementation results are shown graphically in Figure 5.27 and quantitatively in Figure 5.28. The firmware placement has been technically operated instantiating four `pblock` entities, collecting the instances to be placed in each SLR. The implementation has been performed with the `Flow_PerfThresholdCarry` and `Performance_ExtraTimingOpt` options of the Vivado Design Suite optimiser, which limit the raise of timing violations. After several attempts, no timing violation has been observed and a sustainable resources budget has been obtained.

The 35% of the total available Look-up-tables are required to implement the firmware, and only the 17% of the block-RAMs (BRAM) is utilised. Moreover, a non negligible percentage (14%) of flip-flops are occupied. It can be seen that the region with the higher occupancy is the SLR3, which is hosting the firmware implementing the readout functionality. This occupancy is consistent with the results discussed in Section 5.3.4. The resources occupancy is considered acceptable for this first

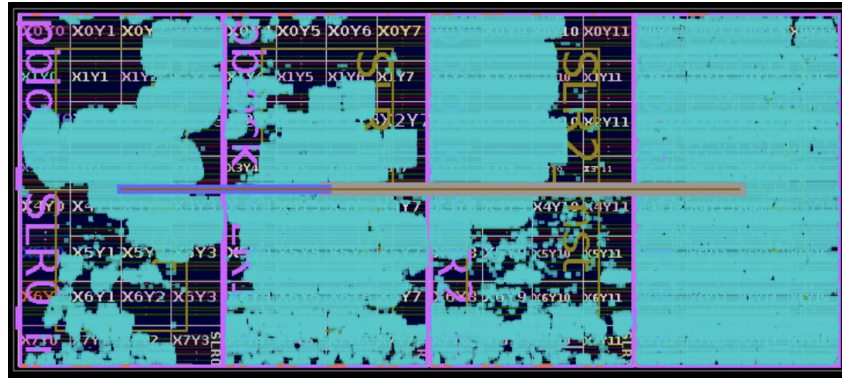


Figure 5.27. The complete SL firmware implemented in the FPGA.

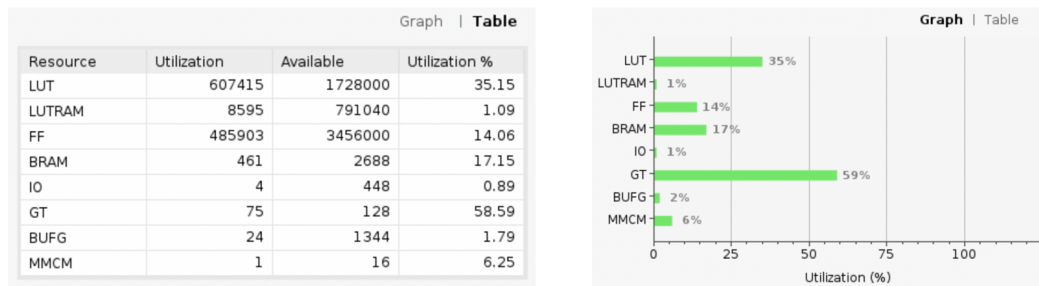


Figure 5.28. Resources occupation for the complete SL firmware, reported in the form of table (left) and graph (right).

implementation of the project and further optimisations are left for future studies.

5.6 Towards a testing campaign: current checks and future developments

A prototype of the Sector Logic board has been designed and produced in parallel to the development of the firmware described in this chapter. Some preliminary hardware tests on the SL prototype have been performed so far, which will be more extensively conducted in the years to come to finalise the SL design and progress towards commissioning and integration of the full system.

The hardware tests have been conducted in the CERN Laser Room, located at Point 1, and corresponding to room 2175-R-B03 according to CERN Maps [177] numbering convection. The room presents a rack, with two shelves compliant with the ATCA scheme, equipped with powering systems and connections to an external server used to control the experimental setup. Figures 5.29 and 5.30 show a collection of pictures taken during the preliminary testing campaigns in summer and autumn 2023, representing respectively the SL prototype mounted in the rack in the experimental room, and the prototype positioned on a desk for cross-checks.

We describe here in brief the preliminary tests performed and give some perspective on the upcoming future testing campaigns. As a first check, a voltage test has been performed on the SL prototype (see Figure 5.30(a)), dismantled from the rack.

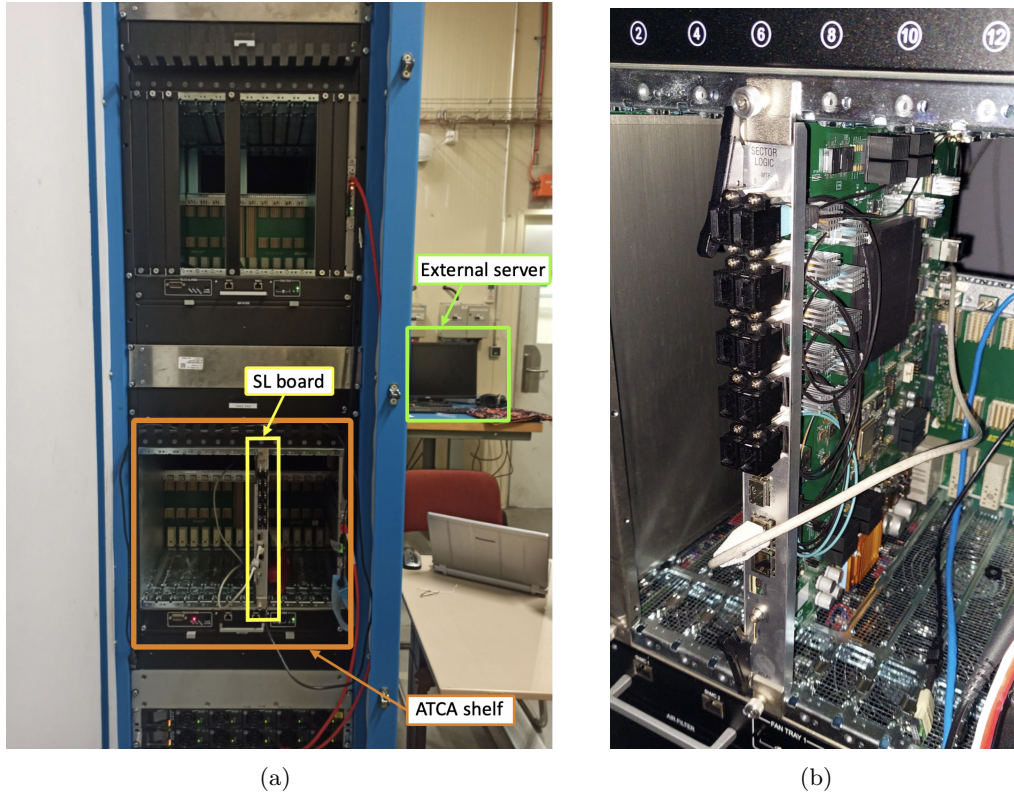


Figure 5.29. The testing experimental setup in the CERN Laser Room at Point 1: (a) rack with two ATCA shelves and (b) the Sector Logic mounted on one ATCA blade.

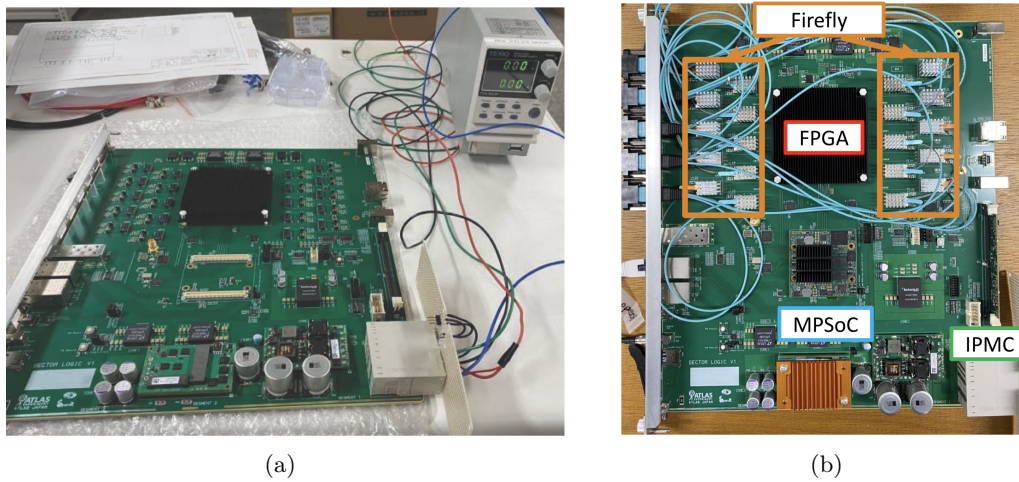


Figure 5.30. Pictures of the SL hardware preliminary tests: (a) power supply test and (b) mount test.

A voltage generator has been connected to the board, sending to the power supply chain the $V = -48$ V tension. The supply voltage has then been measured with a voltmeter in characteristic points of the supply chain and was found consistent with the nominal design values. Subsequently, a mount test has been performed, integrating the full board set-up, as shown in Figure 5.30(b). The MPSoC (System on Chip) and IPMC external cards, have been mounted successfully on the main board. Moreover, the Firefly modules used to link the optical connections and the heatsinks used to dissipate the thermal power have been integrated without encountering mechanical issues.

Once cross-checks on the dismounted board have been completed, the prototype has been integrated in the experimental rack, as shown in Figures 5.29(a) and 5.29(b). The board has been located on a central ATCA blade in the second shelf of the rack and powered. Further checks have been performed to control that the board is successfully controlled from the external server via the shelf manager. More in detail, the external server has been connected via the ATCA shelf manager to the IPMC chip on the board and test words have been routed through the connection to verify its status. Also the control of the MPSoC has been tested, successfully booting CentOS 7 on the chip from remote and re-booting the system from the reset button located on the board.

Finally, first studies have been performed to move towards more complex testing configurations, involving jointly the SL and DCT prototypes. A communication test has been prepared to check the up- and down-link connections between the SL and the DCT boards via the lpGBT protocol. The possibility to use this protocol in the configuration required to connect the DCT and the SL was already demonstrated in an independent standalone test, performed with two Xilinx Kintex-7 KC705, as reported in Ref. [178]. The physical SL board, installed in the experimental rack in the Laser Room, has been connected to a DCT emulator and a bit-error-rate test has been performed to check the DCT-SL transmission link, showing no errors within a 24 hours run.

Future testing campaigns will reiterate this last set-up in more complex and comprehensive configurations. First of all, a connection and transmission test will be performed utilising the SL prototype connected with the real DCT prototype, instead of its emulator, to perform the bit-error-rate test. Then the trigger algorithm implemented in the SL firmware will be tested, sending to the SL hits coincidences from multiple DCTs, to check if the algorithm is able to reconstruct the trigger coincidence. This test will be replicated both with multiple DCT emulators and with real prototype boards. Finally, the connection between the SL board prototype and the FELIX board will be checked, providing also a test of the readout firmware developed as main contribution to the upgrade project within this thesis.

Chapter 6

What's next? Tau leptons at High-Luminosity LHC and future colliders

In this brief review chapter I report an overview on the role of tau leptons in the High-Luminosity LHC program and future colliders. This summary has also the aim of connecting together the main results delivered in the thesis in a broadened context and to evaluate their relation with the future landscape of particle physics.

Tau lepton final states constitute nowadays an effective tool to probe the structure of the Standard Model flavor sector. With the start of the High-Luminosity LHC program in 2029, the Large Hadron Collider will be transformed from a high-energy to a high-luminosity machine, operating at the intensity frontier and starting an era of precision study of the Standard Model observables. In the very long term CERN is evaluating the possibility to construct a new collider for the precision study of the Higgs and electroweak gauge boson properties, matching Europe's ambition to operate next frontier accelerating complex in the high energy physics community. Tau leptons will play a even more central role in this middle and long-term horizon, since they also constitute a powerful final state for the precision study of the Higgs boson and its couplings.

6.1 Tau leptons among the High-Luminosity LHC physics drivers

The first phase of the operations of the Large Hadron Collider has driven the landscape of particle physics to a very peculiar condition. On the one hand, the Higgs boson has been discovered, completing the long-predicted matrix of particles and interactions of the Standard Model. On the other hand, almost no LHC signal has been found in the following years, pointing to an absence of new physics phenomena at least in the energy range up to 1 TeV. The High-Luminosity LHC program aims to go beyond this landscape, investigating the Standard Model properties with the highest precision achievable by the current accelerating machine. New physics is

Table 6.1. Overview of some of the physics drivers for the High-Luminosity LHC, including examples of the investigated final state processes. Table adapted from Ref. [168].

Category	Physics driver	Process
Precision Higgs measurements	Couplings to fermions	$H \rightarrow \tau\tau, H \rightarrow \mu\mu, ttH, H \rightarrow bb$
	Couplings to W/Z , cross-sections	$H \rightarrow \gamma\gamma, H \rightarrow WW \rightarrow \ell\nu\ell\nu, H \rightarrow ZZ \rightarrow 4\ell$
	Self coupling	$HH \rightarrow bb\tau\tau / bb\gamma\gamma / 4b$
	Scalar Higgs vs. BSM composite	$H \rightarrow \ell\ell', ZH \rightarrow \ell\ell + \text{inv.}$
Precision Standard Model measurements	Forward-backward asymmetry	$Z \rightarrow ee, Z \rightarrow \mu\mu$
	Vector-boson scattering	$WWjj, WZjj$
	Top mass and cross-sections	$t\bar{t}$ production
Flavour physics	Lepton Flavour Violation	$\tau \rightarrow \mu\mu\mu$
	Searches for FCNC in top decays	$t \rightarrow u/c + H/Z$
	Rare B -meson decays	$B \rightarrow \mu\mu, B_s \rightarrow J/\psi + \phi$

expected to show up either as a sensible anomaly, identified in the high precision measurement of some Standard Model observable, or as a pattern of deviations, interpreted as the low energy imprint of some new phenomenon in the higher energy range.

The High-Luminosity LHC program aims to cover a wide range of physics goals (see Table 6.1), which include unveiling the paradigm of the electroweak symmetry breaking with the precision study of the Higgs boson and its couplings and of the Higgs field potential. The study of the Higgs sector will be complemented with the measurement of Standard Model quantities, with a prominent role played by the investigation of the flavour sector, of the rare B -mesons decays and of the search for lepton flavour universality. Searches for elusive exotic phenomena (e.g. WIMPS, Heavy Neutral Leptons, SUSY, etc.) or lightly coupled dark-sectors will also be included in the program.

Tau leptons will play a crucial role in this context. In fact, being the most massive leptons, they are characterised by the highest coupling to the Higgs boson, and therefore constitute an optimal final state to investigate the properties of this particle with the High-Luminosity dataset. As shown in Table 6.1, physics analyses in the channels $H \rightarrow \tau\tau$ and $HH \rightarrow bb\tau\tau$ will provide precision measurements of the Higgs coupling to third family leptons and of the Higgs potential respectively, which will improve our understating of the electroweak symmetry breaking mechanism. Tau leptons are also optimal final states for studying the flavour sector, since they are produced in rare B -mesons decays into taus pairs, in single tau final states originating from the $b \rightarrow c\tau\nu$ transition, and are also involved in optimal channels to build ratios for testing the lepton flavour universality.

Drawing this broadened context also offers the possibility to qualitatively evaluate its relation to the results delivered in this thesis. The implementation of measurements and searches involving tau leptons in the final state, like the one presented in this thesis in Chapter 4, are a crucial step to test analysis strategies involving single- and di-tau channels (leptonic, semi-leptonic, hadronic), and will constitute the benchmark for the future implementations.

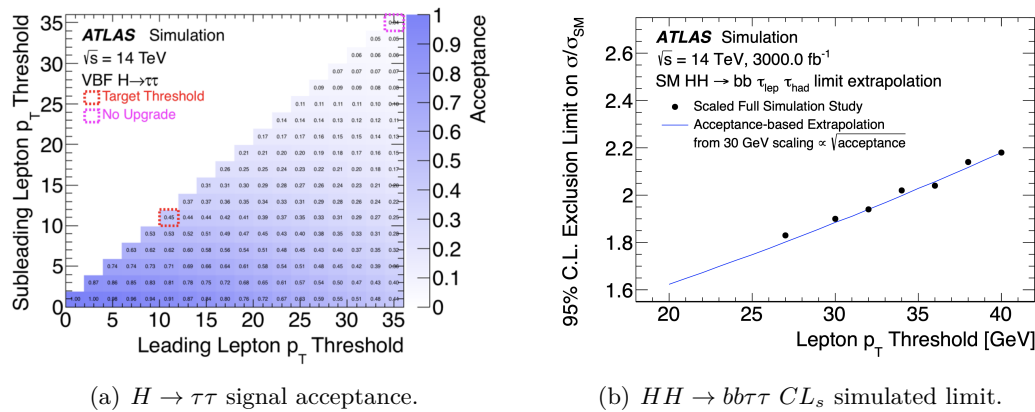


Figure 6.1. Impact of the lowering of the light leptons trigger thresholds in tau-related physics analyses of the High-Luminosity LHC program: (a) the $H \rightarrow \tau\tau$ measurement and (b) the $HH \rightarrow bb\tau\tau$ search. Figures from Ref. [168].

Also the improvements in the methodologies for the rejection of the fake taus background, like the Fake Factors method presented in Chapter 3 of this thesis, as well as the advancements in the tau leptons reconstruction and calibration techniques, will be relevant to reduce the experimental uncertainties at the same level of the statistical uncertainties foreseen in the High-Luminosity phase.

Finally, the upgrade of the muon trigger system, detailed in Chapter 5 of this thesis, will have an impact too on all the measurements in tauonic channels in which there is at least one tau decaying leptonically into a muon. As shown in Figure 6.1, the lowering of the trigger thresholds, which is obtained in the upgraded system during Phase-II, enables to increase by a large factor the acceptance of the $H \rightarrow \tau\tau$ signal and to probe the di-Higgs production $HH \rightarrow bb\tau\tau$ with the highest sensitivity, highly impacting the potential of these two core analyses of the future High-Luminosity LHC physics program.

6.2 Tau leptons in future colliders

The High-Luminosity LHC program is foreseen to reach its end at around the year 2041, and the high energy physics community is already discussing about what the next accelerating machine will be for continuing the study of elementary particles and interactions. Recently, a consensus is starting in the community in aiming for the construction of a 80-100 km long circular collider - the Future Circular Collider (FCC) [179] - to be hosted at CERN laboratories in Geneva area, matching Europe's ambition to operate the next worldwide particle accelerator for the study of fundamental interactions.

The Future Circular Collider, has been conceived to start as a luminosity-frontier electron-positron machine (FCC-ee), with a centre of mass energy up to 365 GeV, later evolving into an energy-frontier hadron collider (FCC-hh), reaching the unprecedented collision energy of around 100 TeV. This multi-stage approach has the enormous advantage of enabling the implementation of different and complementary physics programs, using the same tunnel infrastructure, and leading to a sensible

reduction of the technological risk. Moreover the duration of the program, as well as the possibility to build several experiments on a circular machine, offers a sufficiently wide and challenging project to engage the whole particle physics community for the next decades, giving to the FCC the potential to become next CERN flagship project.

The highest priority for the operation of the FCC-ee will be the high precision study of the Higgs sector, characterising the Higgs boson couplings to leptons and quarks and the Higgs boson self-coupling, leading to a high precision measurement of the Higgs potential and unveiling the intimate nature of the Higgs itself and of its mass. Among the several results achievable, the FCC-ee machine could have the potential to probe the Higgs coupling to electrons, shedding light for the first time on the origin of the mass of the particles we are made of. The study of the Higgs will be complemented by a broad and extensive program of Standard Model precision measurements, covering the study of electroweak, QCD, top processes and deserving a peculiar attention to the flavour sector of the Standard Model.

Tau leptons, once again, will play a fundamental role in this broadened context. Given their privileged coupling to the Higgs boson and their prominent position in the context of the Standard Model flavour measurements, they will constitute the building blocks of optimal final states to implement a wide spectrum of measurements included in the FCC program. The study of tau leptons, the implementation of analyses with taus in the final state as well as the studies to improve the tau reconstruction techniques, constitute therefore nowadays not only an interesting and rewarding field of research, but also a strategic topic in the future landscape of particle physics.

Chapter 7

Conclusions

The Standard Model (SM) of particle physics is currently the most accurate description of elementary particles, but it is not the ultimate theory of Nature, and searches for new physics are currently ongoing, looking for some beyond the Standard Model physics signature. Tau leptons are playing a crucial role in this quest for new physics since they can be used to test beyond Standard Model scenarios in which lepton flavour universality is violated in the third family of leptons and quarks.

A search for leptoquark particles via the di-tau Drell-Yan process has been presented in this thesis, using the 140 fb^{-1} dataset of pp collisions collected by the ATLAS experiment at the LHC, recorded with a centre-of-mass energy of $\sqrt{s} = 13 \text{ TeV}$. The main aspects of the analysis have been covered: the analysis strategy definition and the events selection, the main backgrounds modelling, the uncertainties evaluation and the statistical interpretation. The analysis led to the exclusion of vector leptoquark models, in a region of phase space which is extremely near to the region preferred by the B -physics flavour anomalies. This points out that a considerable improvement can be achieved in re-running this analysis with an increased dataset, as for example the LHC Run 3 and the High-Luminosity LHC datasets. Projections show that the amount of data which will be registered at the end of the High-Luminosity LHC program will be enough to obtain a complete exclusion of the B -anomalies preferred phase space region, and will therefore provide a significant advancement in the understanding of these anomalies and their eventual connection with leptoquark particles.

Some effort in the thesis has been devoted to the development of an experimental technique for the data-driven estimate of the background of hadronic jets misidentified as fake hadronic taus: the Fake Factors Method. In this context, it has been demonstrated that such technique can be extended to di-tau final states, considering the combinatorial possibilities in which a fake event can be generated with two taus.

A part of the thesis has also been dedicated to the L0Muon trigger upgrade project for the Phase-II High-Luminosity program. The readout functionality of the Sector Logic has been fully designed, simulated and implemented. This functionality is in charge of acquiring in memory data while the trigger algorithm is processing the accept/reject decision and to release in output the data in case of positive trigger decision. The readout firmware has been simulated and implemented in a Xilinx Virtex Ultrascale+ FPGA and integrated with the trigger and I/O interfaces

firmwares. The occupancy of the complete firmware has been measured, resulting equal to 35% of the total resource of the chosen FPGA, and demonstrating the feasibility of such firmware implementation.

Taus are playing and will continue to play an important role in the LHC physics program both in the ongoing Run 3 and in the future High-Luminosity LHC program. The Phase-II muon trigger upgrade will also benefit to the measurements of the leptonically decaying taus into muons. The precision study of the Standard Model flavour sector as well as the study of the Higgs boson properties via its decays into taus ($H \rightarrow \tau\tau$), and of the di-Higgs production via tau and b -quarks final states ($HH \rightarrow b\bar{b}\tau\tau$) are among the core physics motivations of the High-Luminosity LHC program, and even motivate the construction of an enlarged collider, the Future Circular Collider (FCC), which the European Strategy of Particle Physics is nowadays evaluating to endorse. For this reason the improvements in the measurement techniques and the physics analysis strategies involving the tau leptons constitute core topics for the development of the High Energy Physics research field and for continuing the search for new physics via the precision study of the Standard Model.

Appendix A

Unfolded differential measurement of the di-tau Drell-Yan process

I report in this appendix a preliminary measurement of an unfolded differential cross section of di-tau production, which has been developed within the same analysis team performing the search for leptoquark particles presented as main topic of this thesis (see Chapter 4). The unfolding framework has been mainly developed by other members of the analysis team. I learned this part of the work during a dedicated visiting period at the University College London, which was main responsible for the unfolding development, and I am currently able to understand the main features of the measurement and to run the unfolding framework.

A.1 Introduction and motivations

The study of the Drell-Yan process constitutes a relevant part of the ATLAS Standard Model physics program, since it enables detailed tests of the Standard Model predictions, as well as the extraction of fundamental parameters, deeply probing the structure of the electroweak interactions. This process constitutes also a relevant background in several searches and measurements, motivating the need of a precise estimate of its cross section.

ATLAS has performed several cross section measurements of the Drell-Yan process using channels with electrons and muons in the final state. Particularly, inclusive cross-sections at 7 TeV and 13 TeV have been measured in Refs. [181] and [182], and differential cross sections have been evaluated both in the Z peak di-lepton invariant mass range [183], and in the low- and high-mass ranges [148, 149, 184]. Nevertheless, the current status of the art still lacks an extended set of measurements of the Drell-Yan process using the tauonic final states, which are also sensible to eventual anomalies associated with lepton-flavour violating new physics. In fact, integral cross sections for the $pp \rightarrow Z/\gamma^* \rightarrow \tau\tau$ process have been measured at $\sqrt{s} = 7$ TeV [143, 144], but still no differential cross section measurement has

currently been published. The di-tau Drell-Yan process has been exploited to measure a few electroweak parameters [113], but still others, like the forward-backward asymmetry or the weak mixing angle, have been measured only exploiting di-electron and di-muon final states [185].

I present in this appendix preliminary results for an unfolded differential cross section measurement of the di-tau production from LHC $pp \rightarrow \tau\tau$, inclusive of the Drell-Yan production, $pp \rightarrow Z/\gamma^* \rightarrow \tau\tau$, as well as all other processes generating two taus in the final state. The measurement is performed using the ATLAS full Run 2 dataset of 140 fb^{-1} at a centre of mass energy of $\sqrt{s} = 13 \text{ TeV}$. The fiducial cross section is measured differentially in the di-tau invariant mass $m_{\tau\tau}$ in the high mass range and is inclusive in an arbitrary number of b -jets in the final state. The fully hadronic channel, in which both taus decay into hadrons, is exploited and the impact of ATLAS events reconstruction is unfolded in order to provide distributions that are detector invariant.

Beyond its intrinsic interest in completing the picture of the high-mass di-lepton production, this measurement has also an interest in the context of the searches for new physics, and particularly in the field of the extensions of the Standard Model flavour sector addressing the B -physics anomalies, described as main topic of this thesis. In fact, the precision measurement of the $pp \rightarrow \tau\tau$ cross-section in the high mass tail opens to the possible detection of an anomalous deviation, constituting the signature of a high-scale new physics with preferential coupling to tau leptons. This new physics signature could be interpreted - among the others - with the leptoquarks models reported in the detector-level search described in Chapter 4 of this thesis.

The di-tau precision cross-section measurement can therefore be seen as an alternative, more general and model-agnostic strategy to search for a high-scale new physics with flavour-dependent coupling to leptons and quarks. The di-tau spectrum, once measured, offers also the possibility to easily construct further observables potentially sensible to anomalies like the forward-backward asymmetry, to build lepton flavour universality tests, or to implement model-dependent searches directly at particle-level, without the need to repeat time-consuming detector simulations.

This appendix is organised as follows. After a brief introduction on the unfolding procedure given in Section A.2, a preliminary measurement of the di-tau differential cross-section is given in Section A.3. Optimisation and tests against possible sources of bias in the unfolding are described in Section A.4, and conclusions and perspectives on future developments are given in Section A.5.

A.2 The unfolding procedure

Physics measurements in high-energy particle detectors are based on the evaluation of distributions of physical observables. These consist of histograms, collecting data in bins of finite width, each one characterised by its events yield.

Due to the detector experimental effects, the measured distributions are distorted and modified by the finite resolutions and the inefficiencies. We therefore have to distinguish between two types of objects: the reconstruction-level (or detector-level) histograms, representing the distributions actually measured by the detector, and the truth-level (or particle-level) histograms, which are the underlying distributions,

generated by the physical process, that would have been measured by an ideal detector. While the reconstruction-level distributions are the only ones accessible in data by a real experiment, the truth-level distributions are of high interest in Standard Model measurements, since they can be compared with theory predictions and with results from other experiments. The *unfolding* is the process of computing, from a measured reconstruction-level distribution, its corresponding truth-level, factoring out the detector effects.

A.2.1 Simple inversion unfolding

The major effect causing the difference between the reconstruction-level distribution and its corresponding truth-level is the events migration between neighbouring bins, caused by the finite experimental resolution. Events in a given truth-level bin can migrate in a preceding or following bin due to an experimental under- or over-estimation of the measured quantity.

If we denote as t_j the particle-level bins and r_i the detector-level bins, we can represent events migrations with a matrix R_{ij} that encodes the probability of mapping an event in each bin at particle-level to a bin at reconstruction-level:

$$P(r_i) = \sum_j R_{ij} P(t_j) . \quad (\text{A.1})$$

where we denote with $P(r_i)$ and $P(t_j)$ the probabilities of events falling in bin i of detector-level histogram and bin j of particle-level histogram. The matrix R_{ij} is commonly called *response matrix* (or folding matrix) and encodes the knowledge of the detector. In running an unfolding procedure we want to transform the distribution measured at detector-level into the particle-level one. This could in principle be done by inverting Eq. (A.1)

$$P(t_j) = \sum_i R_{ji}^{-1} P(r_i) = \sum_i U_{ji} P(r_i) , \quad (\text{A.2})$$

where U_{ji} is the unfolding matrix, defined as the algebraic inverse of the response matrix.

However, the matrix inversion is not always possible, and fluctuations associated with low statistics can lead to instabilities in the inversion process. For this reason this unfolding procedure is not commonly used.

A.2.2 The iterative Bayesian unfolding

The commonly used unfolding method in high energy physics is the Bayesian iterative unfolding, proposed by G. D'Agostini in Ref. [186, 187], and based on the construction of the unfolding matrix through the Bayes theorem and the concept of conditional probability.

Within this method we identify the R_{ij} element of the response matrix as the conditional probability that an event is reconstructed in the detector-level bin r_i , given that it was generated in particle-level bin t_j , $R_{ij} = P(r_i|t_j)$. Similarly, the element of the unfolding matrix U_{ji} is the conditional probability that an event was originated in particle-level bin t_j , given that it has been reconstructed in the

detector-level bin r_i , $U_{ji} = P(t_j|r_i)$. Making use of the Bayes' theorem we can compute the elements of the unfolding matrix from the reconstruction matrix as

$$P(t_j|r_i) = \frac{P(r_i|t_j) \cdot P(t_j)}{\sum_k P(r_i|t_k) \cdot P(t_k)} , \quad (\text{A.3})$$

where $P(t_j)$ are the *prior* probabilities, representing the experimenter a-priori knowledge of the particle-level distribution. Typically the prior is chosen equal to the Monte Carlo predictions, encoding the best knowledge of the process previous to the measurement. However, since the MC simulations are not ideal and always present a certain grade of mis-modellings, the prior assignment introduces a bias into the unfolding procedure.

To reduce the bias D'Agostini proposed to iterate the unfolding, using each calculated posterior as prior for the next iterations:

$$P(t_j|r_i)_n = \frac{P(r_i|t_j) \cdot P(t_j)_{n-1}}{\sum_k P(r_i|t_k) \cdot P(t_k)_{n-1}} , \quad (\text{A.4})$$

where $n \geq 1$ is the number of iterations, and the prior is chosen as

$$P(t_j)_n = \begin{cases} P(t_j)_{\text{MC}} & n = 0 \\ P(t_j|r_i)_n & n \geq 1 \end{cases} ,$$

Within this approach, the event yields of the unfolded distribution are defined as

$$N(t_j) = \sum_i N(r_i)_{\text{obs}} \cdot P(t_j|r_i)_{n_f} , \quad (\text{A.5})$$

where $N(r_i)_{\text{obs}}$ are the event yields observed in data and n_f is the number of unfolding iterations. The optimal value of n_f is determined balancing the fact that fewer iterations yield a stronger bias from the initial prior, while a high number of iterations increases the total uncertainty associated with the unfolding procedure (see Section A.4.2).

When doing the measurement, data are selected with cuts on kinematic variables, defining the *fiducial region*. The fiducial region is defined to be included into the phase space region accessible by the detector and at the same time as extended as possible. Beyond the events migration due to resolution effects, reconstruction-level distributions are also distorted due to detector inefficiencies and fake events. More in detail, detector inefficiencies account for all the particle-level fiducial events which do not pass the fiducial selection at detector-level, whereas fake events are non-fiducial events at particle-level which mistakenly resulted in passing the detector-level fiducial selection. To account for these effects the expression in Eq. (A.5) is modified as follows:

$$N(t_j) = \frac{1}{\epsilon_j} \sum_i f_i \cdot N(r_i)_{\text{obs}} \cdot P(t_j|r_i)_{n_f} , \quad (\text{A.6})$$

where ϵ_j is the reconstruction efficiency of bin t_j , representing the fraction of events in the particle-level bin t_j passing also the detector-level fiducial selection, and f_i is the fiducial fraction of bin r_i , representing the fraction of events in the detector-level bin r_i passing also the particle-level fiducial selection.

A.3 Unfolded differential cross section in di-tau invariant mass bins

A preliminary measurement of the unfolded differential cross section of the $pp \rightarrow \tau\tau$ process is reported, exploiting the events in the fully hadronic channel, in which both final state taus decay hadronically. As this part of the analysis is still ongoing, results are preliminary and fully based on Monte Carlo simulation. They are presented as a current status of the ongoing measurement, reporting the results achieved so far.

A.3.1 Objects and events selection

The cross section measurement is based on two separate selections: the detector-level selection, acting on reconstructed objects and their kinematic features, and the particle-level selection, acting on truth objects, available in the Monte Carlo simulation only.

Detector-level selection

The detector-level selection for the cross section measurement is exactly the same as the one of the leptoquark search analysis presented in Chapter 4 of this thesis. Objects are pre-selected according to the criteria discussed in Section 4.4.1 and the fully hadronic channel triggers are applied, as reported in Table 4.4. Events are finally selected in the detector-level fiducial region by applying the fully hadronic channel selection criteria, listed in Table 4.5.

Particle-level selection

The particle-level selection is determined reflecting the detector-level criteria as closely as possible, as this choice minimises the extrapolation from the observed detector-level data to the inferred particle-level cross sections and decreases the model-dependence introduced in the final particle-level measurement.

Specifically, hadronic tau lepton candidates are required to have $p_T > 20$ GeV and $|\eta| < 2.47$ and electron candidates must have $p_T > 7$ GeV and $|\eta| < 2.47$, excluding the crack region $1.37 < |\eta| < 1.52$. Similarly muons are required to have $p_T > 7$ GeV and $|\eta| < 2.5$. Both electrons and muons should be “prompt”, hence should not have an hadronic origin beyond the initial state protons. Jets at the particle-level are built from stable particles using the anti- k_T algorithm [93] with $R = 0.4$ and are required to have $p_T > 25$ GeV. They are considered fiducial b -jets if they contain at least one b -hadron with $p_T > 5$ GeV. Events are finally selected in the particle-level fiducial region if they satisfy at particle-level requirements similar as those listed in Table 4.5 for the detector-level selection: they must contain two fiducial hadronic taus, with opposite charge sign and di-tau invariant mass $m_{\tau\tau} > 100$ GeV. Moreover, the leading tau must have $p_T > 90$ GeV, while the subleading $p_T > 60$ GeV.

Events are considered inclusively, independently of the number of b -jets in the final state and independently of the process which produced the two taus in the final state (Drell-Yan, $t\bar{t}$, multi-boson or any other source).

A.3.2 Evaluation of the unfolding inputs

The unfolding inputs are evaluated using Monte Carlo simulation of the signal process $pp \rightarrow \tau\tau$. In this study we consider only the dominant production modes for di-tau final states, the Drell-Yan and $t\bar{t}$ production, modelled via SHERPA 2.2.11 [125] and POWHEGBOX v2 [134] respectively (see Section 4.3.2 for details). The inputs to the unfolding are:

- **Response matrix.** It is the matrix representing the detector response; its elements are the probability of events being reconstructed in bin r_i , given they are originated in truth-bin t_j . It is evaluated from Monte-Carlo simulation as:

$$R_{ij} = P(r_i|t_j)_{\text{MC}} = \frac{N(r_i \cap t_j)}{N} , \quad (\text{A.7})$$

where the N considered events are required to pass both the detector- and particle-level selections.

- **Reconstruction efficiency.** It is defined for each particle-level bin and is the fraction of events in bin t_j that pass also the detector-level selection (i.e. that fall in *some* bin r_i). It is evaluated from Monte Carlo simulation as:

$$\epsilon_j = \frac{\sum_i N(r_i \cap t_j)}{N(t_j)} . \quad (\text{A.8})$$

- **Fiducial fraction.** It is defined for each detector-level bin and is the fraction of events in bin r_i that pass also the particle-level selection (i.e. that originate in *some* bin t_j). It is evaluated from Monte-Carlo simulation as:

$$f_i = \frac{\sum_j N(r_i \cap t_j)}{N(r_i)} . \quad (\text{A.9})$$

The fake rate can also be defined, and is the complementary of the fiducial fraction: $\text{fake}_i = 1 - f_i$.

- **Purity.** It is similar to the fiducial fraction, but evaluates the fraction of events in bin r_i that originate *exactly* from the corresponding particle-level bin t_i :

$$p_i = \frac{N(r_i \cap t_i)}{N(r_i)} \quad (\text{A.10})$$

An analogous quantity, the stability - measuring the fraction of events in particle-level bin t_j falling in the same detector-level bin r_j - can be defined, but is usually not involved in the unfolding process.

The response matrix to unfold the di-tau invariant mass distribution is shown in Figure A.1. It is highly diagonal, with in-diagonal elements close to unity, $P(r_i|t_i) \gtrsim 0.9$. The migration matrix assumes low non-null values only in the bins around the diagonal, meaning that minor migrations happen mainly between adjacent $m_{\tau\tau}$ bins and that the binning has been chosen sufficiently coarse to cover the experimental resolution.

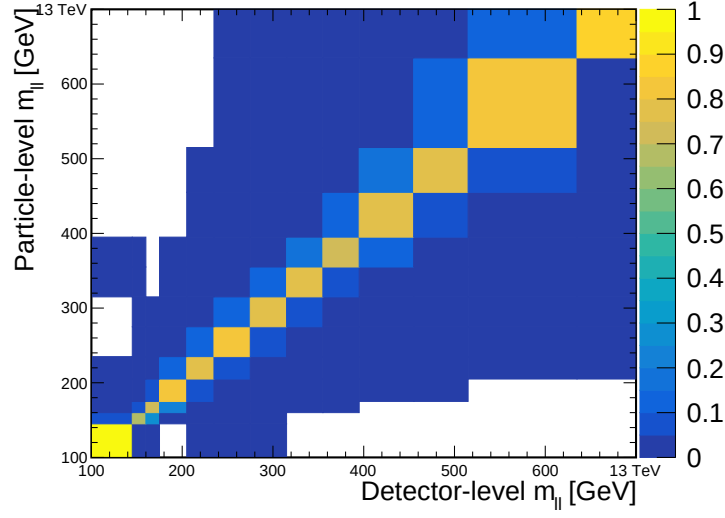


Figure A.1. Response matrix R_{ij} evaluated from Monte Carlo simulated events in bins of the di-tau invariant mass.

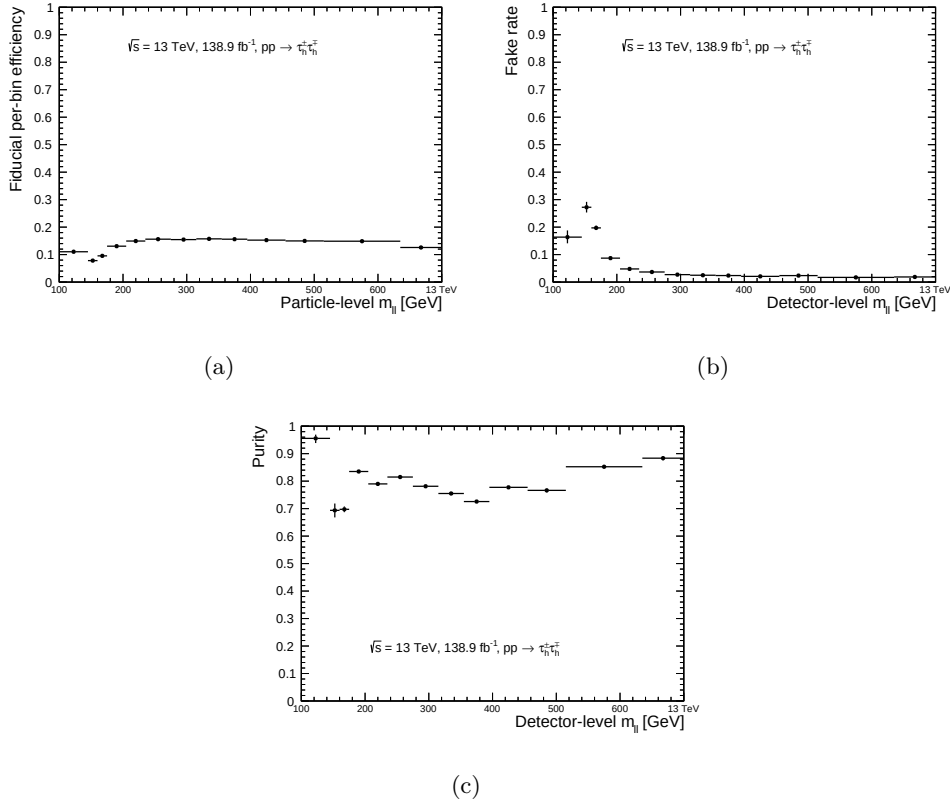


Figure A.2. Unfolding inputs evaluated from Monte Carlo simulated events in bins of di-tau invariant mass: (a) reconstruction efficiency, (b) fake rate, (c) purity.

The reconstruction efficiency and the fake rate are shown in Figure A.2(a) and Figure A.2(b) respectively, the latter being the complementary to one of the fiducial fraction. The reconstruction efficiency is generally small and around $\simeq 10\%$ across the $m_{\tau\tau}$ bins. This is due to a combination of the trigger efficiencies and the lepton identification and reconstruction efficiencies, causing a large part of the events satisfying the truth-level selection to be discarded at detector-level. The fake rate is on average very small, with a slight increase in the proximity of the fiducial region boundaries, caused by spurious events entering the detector-level fiducial region due to the finite experimental resolution.

The purity is also evaluated, and reported in Figure A.2(c). This quantity has been used to define the $m_{\tau\tau}$ binning. Specifically, bins have been chosen to be sufficiently coarse to yield a purity of at least 65% and to contain at least 30 events, in order to limit statistical fluctuations.

A.3.3 Results

Since at the time of writing the data distribution is blinded in order to prevent the analyzer bias in the finalisation of the leptoquark search presented in Chapter 4, the unfolding has been performed using a pseudo-data distribution, based on the Monte Carlo expectations on the real data distribution.

The pseudo-data distribution has been obtained fluctuating bin-by-bin the yields of the signal Monte Carlo stack assuming a Gaussian model with mean equal to the Monte Carlo yields and standard deviation equal to the Monte Carlo uncertainty. Statistical uncertainties have been attributed to the unfolded distribution. These have been computed by generating N toy pseudo-data distributions, by varying the pseudo-data yields with a Poissonian model with mean λ and standard deviation $\sqrt{\lambda}$, and assigning in each bin an uncertainty equal to the standard deviation of the N results, evaluated with respect to the nominal unfolded distribution.

Figure A.3 shows the resulting unfolded pseudo-data distribution, representing the expected differential cross-section measurements in bins of $m_{\tau\tau}$. Agreement is observed with the truth-level Monte Carlo distribution of Standard Model di-tau events, showing the overall consistency of the study.

A.3.4 Impact of the systematic uncertainties

It is import to assess the impact of the experimental uncertainties on the unfolded distribution, to identify which ones are the most relevant with respect to the cross section measurement.

For each considered experimental systematic the varied response matrix, reconstruction efficiencies and fiducial fractions have been evaluated from the associated varied Monte Carlo, and a corresponding varied unfolded distribution has been obtained. The experimental uncertainty is quantified as the difference between the varied unfolded distribution and the nominal one. All ATLAS standard experimental uncertainties have been processed and the subset of the most impactful has been identified via a pruning procedure. To evaluate the impact of the statistical uncertainty, N toy pseudo-data distributions have been generated with Poissonian variations,

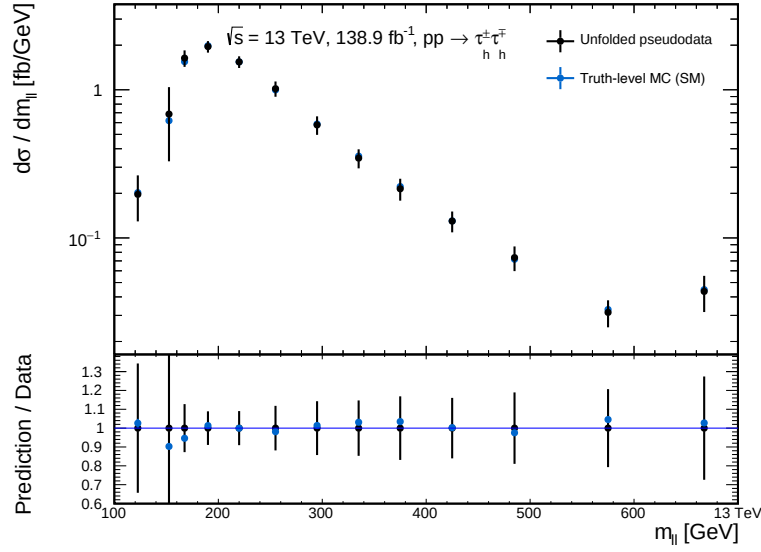


Figure A.3. Expected unfolded fiducial differential cross section of the $pp \rightarrow \tau\tau$ process in bins of di-tau invariant mass, compared with the Standard Model truth-level Monte Carlo distribution.

and the uncertainty has been assessed bin-by-bin as the standard deviation of the N unfolded distributions with respect to the nominal one.

Figure A.4 shows the uncertainties breakdown on the expected differential cross section, where the experimental uncertainties have been combined with a quadrature sum in different categories. As can be noticed, the precision of the measurement in the high-mass range is expected to be limited by statistics and by the experimental uncertainties on hadronic taus reconstruction.

A.4 Tests and optimisations of the unfolding framework

Once developed the unfolding framework has to be tested to confirm its consistency and to ensure the limitedness of the possible sources of bias in the unfolded distributions. The optimal number of unfolding iterations has also to be determined for the specific case under study.

A.4.1 Technical closure test

The first trivial check that has to be performed when developing an unfolding framework is the technical closure test. This test is the equivalent of the Asimov fit in the exotic searches, and aims to cross-check that the unfolding code is consistent. The reconstruction-level Monte Carlo is unfolded to particle-level using the nominal response matrix, reconstruction efficiencies and fiducial fractions, evaluated with the same Monte Carlo. A perfect closure of the unfolded distribution with the truth-level prediction is expected, after one iteration of the unfolding. If this is not the case, it means that some technical mistake has been made in the developed framework.

Figure A.5 shows the results for the technical closure test, for the unfolding

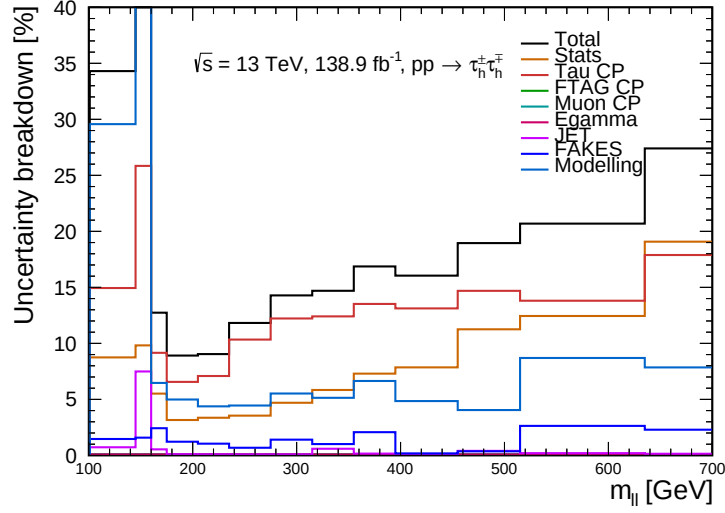


Figure A.4. Impact of the systematic and statistical uncertainties on the unfolded differential cross section.

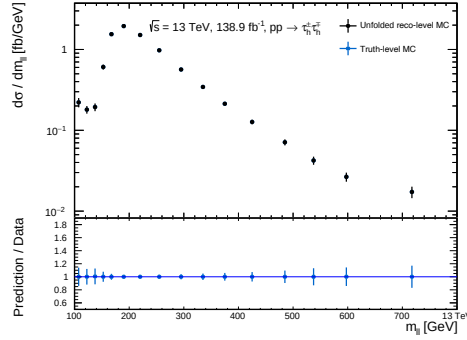


Figure A.5. Technical closure test of the unfolding procedure. The unfolded reco-level Monte Carlo distribution is compared to the corresponding truth-level.

discussed in this appendix. The closure between the unfolded and the truth-level distribution is observed, as expected.

A.4.2 Optimisation of the number of iterations

The number of iterations of the unfolding procedure is usually chosen balancing the fact that a high number of iterations decreases the bias of the unfolded distribution towards the prior, but at the same time increases the statistical error on the result. We discuss here the optimal number of iterations by determining these two quantities.

In order to quantify the bias a re-weighted Monte Carlo model is utilised. Specifically, bin-by-bin weights are determined in order to deform the truth-level distribution according to the linear model $f(m_{\ell\ell}) = A \times m_{\ell\ell}$, where A is a factor of order unity. Such weights are applied to the nominal Monte Carlo weight of each simulated event, yielding re-weighted truth- and reco-level distributions. The re-weighted

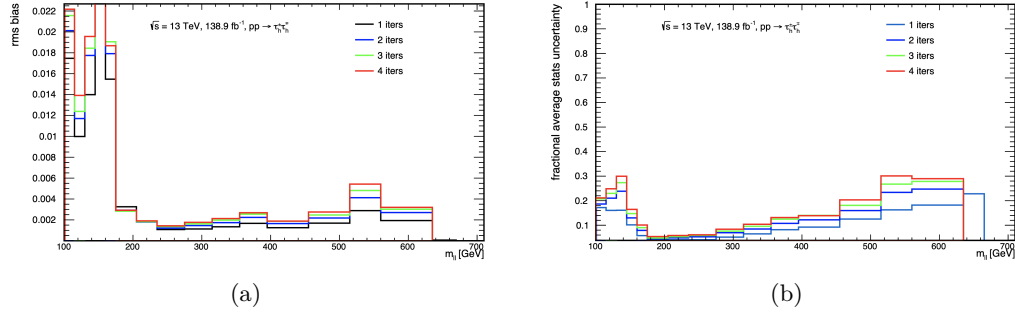


Figure A.6. Quantities used to optimise the number of the unfolding iterations: (a) the unfolding bias and (b) the statistical uncertainty on the unfolding.

reco-level distribution is then unfolded and compared to the re-weighted truth-level distribution. The bias in each bin i is measured as

$$\text{Bias}_i = (U_i - P_i)/P_i, \quad (\text{A.11})$$

where U_i is the yield of the unfolded histogram and P_i is the corresponding yield in the truth-level histogram. The bias is evaluated multiple times with $N = 2000$ Gaussian fluctuated reco-level distributions and the standard deviation of the biases is determined, taking as reference the re-weighted truth-level distribution.

Similarly, the statistical uncertainty on the unfolding is assessed using $N = 2000$ reco-level distributions obtained from the nominal one applying fluctuations within the pre-unfolding statistical uncertainty. Each distribution is unfolded and the standard deviation of the results with respect to the nominal unfolded distribution is taken as statistical uncertainty on the unfolding.

Figure A.6 shows the bias and the statistical error on the unfolding, as a function of the number of unfolding iterations. As can be seen, the total uncertainty is dominated by the statistical component, hence a lower number of iterations is optimal. Therefore, the decision is made to use two unfolding iterations, which is the minimum number of iterations possible in an iterative unfolding process.

A.4.3 Tests against sources of bias

The unfolding procedure is intrinsically subject to bias, since the Bayesian approach produces unfolded distributions that tend to be distorted towards the chosen prior, i.e. towards the Standard Model truth-level Monte Carlo distribution. Despite the distortions can be decreased by several iterations of the method, the limitedness of the remaining bias has to be checked and eventually taken into account with proper dedicated uncertainties.

Signal injection test

The measurement of the cross-section in the high di-tau mass range is sensible to the potential presence of beyond-Standard Model (BSM) signals, which could be revealed also in the unfolded spectrum at particle-level. Therefore, we want to test

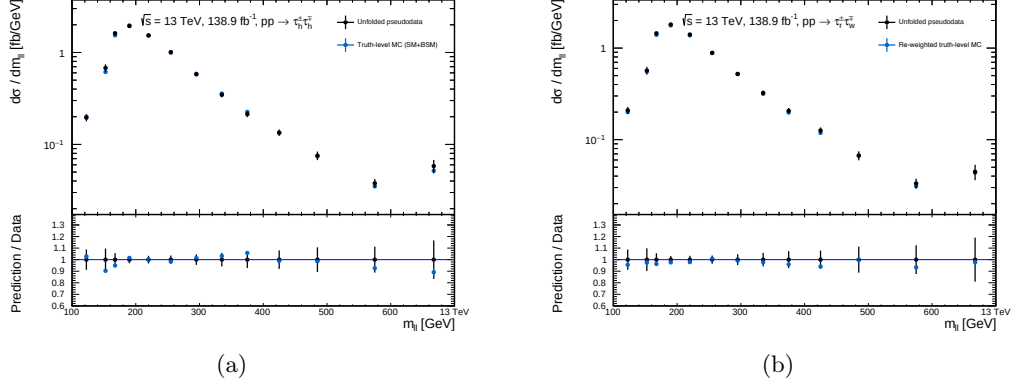


Figure A.7. Tests to assess the potential biases present in the unfolded distributions: (a) signal injection test and (b) di-tau p_T re-weighting test.

the robustness of the unfolding framework in preserving such signals at particle-level, despite its intrinsic bias towards the Standard Model predictions.

To do this, a simulated BSM signal is injected in the Monte Carlo stack, representing vector leptoquark (LQ) events with $m_{LQ} = 1.5$ TeV and coupling $|\beta_L^{b\tau}| = 1$ (see Section 1.4.1 of Chapter 1 for details on the model). The Monte Carlo reco-level distribution is then taken as pseudo-data and unfolded using the pure Standard Model response matrix, efficiencies and fiducial fractions, and finally compared to the SM+BSM truth-level distribution. A good agreement between the two distributions is observed, as shown in Figure A.7(a), meaning that the bias towards the SM-only prediction is limited.

Di-tau p_T re-weighting test

An additional source of bias in the unfolded distribution can potentially come from mis-modellings present in the Monte Carlo distributions of other kinematical variables - different than the one used for the differential bins - especially if they are used in the fiducial region definition. A test has been performed to assess if potential biases are induced in the unfolded distribution, originating from mis-modellings in the $p_T^{\tau\tau}$ distribution.

To this purpose, weights have been determined as the ones that re-scale the bin-by-bin the $p_T^{\tau\tau}$ reco-level distribution to match perfectly the data. These weights have been applied on an event-by-event basis to the Monte Carlo simulation, generating re-weighted reco- and truth-level $m_{\tau\tau}$ distributions. Finally the reco-level distribution has been taken as pseudo-data and unfolded using the nominal response matrix, efficiencies and fiducial fractions. The unfolded distribution has been compared to the truth-level distribution to assess any potential bias from the difference between the two. As shown in Figure A.7(b) a good agreement has been observed between the two distributions, meaning that this source of bias is negligible.

A.5 Conclusions and outlook

A preliminary measurement of the unfolded differential cross section in the di-tau invariant mass has been presented. The unfolding framework has been developed, optimised and tested against possible sources of bias, and the impact of the major experimental systematics on the unfolded cross section has been evaluated. Since the data used for this measurement are currently blinded to prevent the analyser bias in the associated detector-level leptoquark search presented in Chapter 4, all the results obtained so far rely on Monte Carlo simulation and correspond to expectations.

The first step towards the finalisation of the unfolded cross section measurement will therefore be to plug the ATLAS Run 2 data into the developed unfolding framework, once their unblinding is approved by the Collaboration. Specifically, the unfolded data distribution has to be evaluated and the optimisation of the number of iterations and the bias tests have to be repeated, to check that results are compatible with the ones obtained so far with pseudo-data. Finally, a more complete assessment of the systematic uncertainties on the unfolded distribution will be provided, including also the modelling uncertainties on the signal and background processes.

Once the differential cross section measurement in bins of di-tau mass is completed, in the long term we plan to produce additional cross section measurements, differential in other variables, as for example the di-tau transverse momentum $p_T^{\tau\tau}$ and rapidity $y_{\tau\tau}$, which will provide additional insight in our understanding of the Drell-Yan process and its eventual connection with new physics scenarios.

Appendix B

Muon desk operations in the ATLAS control room

I refer in this appendix the activities I have done as muon desk shifter in the ATLAS Control Room during the detector operations. I served as muon desk shifter during the Run 3 operations in the years 2023 and 2024.

The ATLAS operations are an important part of the experimental program and deal with the online acquisition of data recorded by the detector during the pp collisions delivered by the Large Hadron Collider. The operations are managed by the ATLAS run coordinators, which work together with the detector systems run coordinators, the sub-systems experts on-call and the ATLAS crew.

The ATLAS crew operates in the ATLAS Control Room, located in Building 3162 (see CERN Maps [177]), and is the team in charge of monitoring the progress of the online data acquisition. The crew is composed of several members, called *shifters*, working under the coordination of a *shift leader*. The shifters have different roles and duties, and together cover the monitoring of the whole variety of ATLAS sub-systems and functions. Three shifters (the muon shifter, the inner detector shifter, the calorimeters shifter) monitor the main hardware sub-systems, and are accompanied by the trigger shifter and the run control shifter, monitoring the data-acquisition and maneuvering the run start/stop respectively. A data quality shifter and a shift leader in matter of safety (SLIMOS) are also present to account for the online cross-check of the acquired data and for all safety issues.

When the year data taking starts, the ATLAS crew is present in the Control Room 24-hours a day until the year-end technical stop (YETS), and members alternate in shifts of 8-hours duration. A typical year-long data taking starts in March and ends in November of the same year.

B.1 Set-up and duties of the muon desk shifter

The muon shifter sits in the ATLAS Control Room at the muon desk, located in the rear left part of the room (see Figure B.1 for some pictures), and operates through several monitoring tools displayed on three screens.

When the shifter arrives in the control room at the beginning of its time slot,

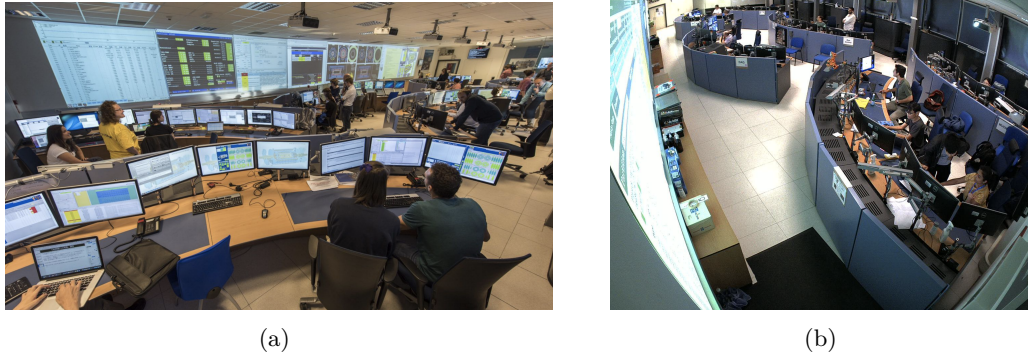


Figure B.1. The ATLAS control room and its desks: (a) close-up view of the muon desk and (b) overall view from one of the online monitoring cameras.

its first duty is to make the handover with the previous shifter and learning from him about issues and critical events happened in the preceding hours. Then, before starting its operations, he is supposed to have a quick read of two online pages available on the muon desk screens, the plan of the day and the muon whiteboard, reporting respectively information on the foreseen ATLAS operations on the current day and instructions of immediate use for the shifter about the muon sub-systems.

The main tasks which the muon shifter has to accomplish are three. First of all, he has to monitor the hardware of the detector to check for eventual problems occurring in the chambers of the muon system, through the Detector Control System tool. Secondly, he has to monitor the data acquisition process, checking that all the data recorded by the muon chambers are collected to be sent to the acquisition chain, through the DAQ interface. Finally, he has to perform an online cross-check of the acquired data, to verify that they are roughly consistent with expectations and of good quality for the offline physics analyses.

Together with these three main tasks, the muon shifter performs in parallel some side and complementary activities. In particular, he has to monitor the shifter assistant, which is a tool issuing information messages, alerts and warning, instructing also the shifter about the actions to be taken in case of errors. Moreover, he has to monitor and write on the ELisA online logbook, in which all relevant issues about ATLAS sub-systems are posted. Finally, he writes a shift summary and a run summary, containing respectively relevant information about the shift (detector status, warnings encountered, any event of particular relevance) and about the run.

B.2 The Detector Control System and Data Acquisition

The Detector Control System (DCS), represented in Figure B.2, is the interface which allows the shifter to monitor the hardware status of the physical chambers constituting the muon system and to be advertised for critical situations. It is composed of two parts: the DCS finite state machine and the DCS alarm screen.

The DCS finite state machine (see Figure B.2(a)) reports in a series of graphical

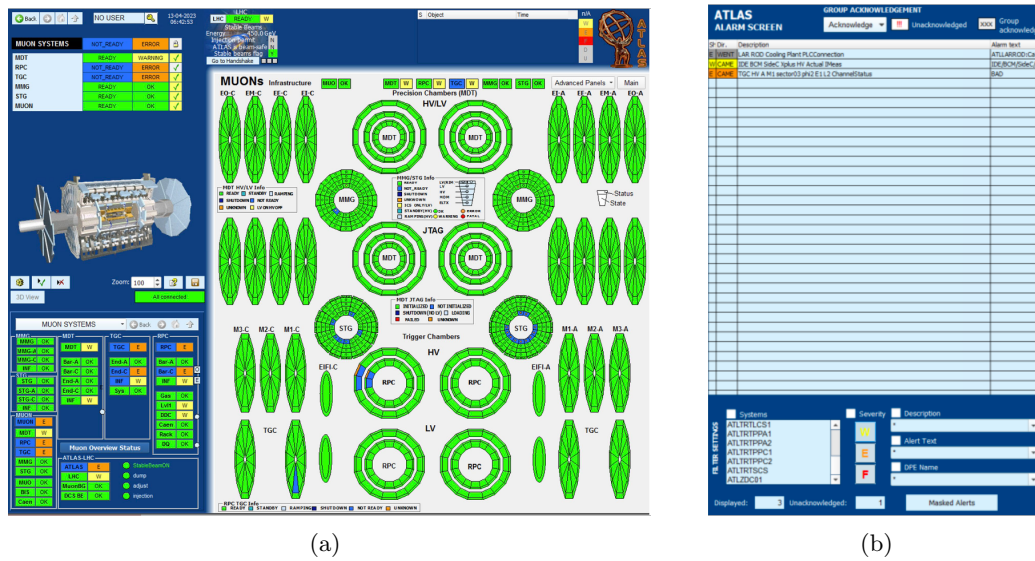


Figure B.2. Screen view of the Detector Control System (DCS): (a) the DCS finite state machine and (b) the alarm screen.

schemes the status of all the muon system chambers. It constructed as a navigable interface, in which the shifter can go through obtaining information about the status of the high voltage systems and gas systems, the chambers temperature, and other critical parameters. In the DCS finite state machine the status of the muon sub-systems is reported (NOT_READY, STANDBY, READY, etc.) together with a flag (ERROR, OK) telling whether the status is correctly reached or not. At the beginning of an LHC operational cycle, in the absence of the beam, the status of the muon sub-systems is set to STANDBY, corresponding to a decreased voltage of all the muon chambers. Then, when the proton bunches filling and the energy ramp are done, the stable beams condition is assessed and the muon chambers status is set to READY, corresponding to the nominal high voltage value. It should never happen the beam is injected in the LHC when the muon system is in the nominal high voltage status: to prevent this the muon shifter has to explicitly refer to the shift leader that he can authorize the beams injection after having checked that none of the muon sub-systems is in the READY state.

The DCS alarm screen (see Figure B.2(b)) reports instead a series of warnings and error messages associated with issues in the muon system, together with information on the priority of the error (minor, critical) and a description of the problem and of the eventual actions required. The muon shifter has to monitor the alarm screen and solve the reported errors either acting as stated in the error description, or looking for information in the shifter assistant, or calling the relevant expert. It can happen that some errors do not require actions, as they are known and unavoidable problems which do not prevent the ATLAS operations, or because are due to temporary fluctuations of some parameters. In the first case, the error is typically reported on the muon whiteboard, with the instruction to ignore and to mask it. Instead, typical examples of issues connected to parameters fluctuations are the high temperature errors for some parts of the muon system. In this case, the muon shifter can recognize

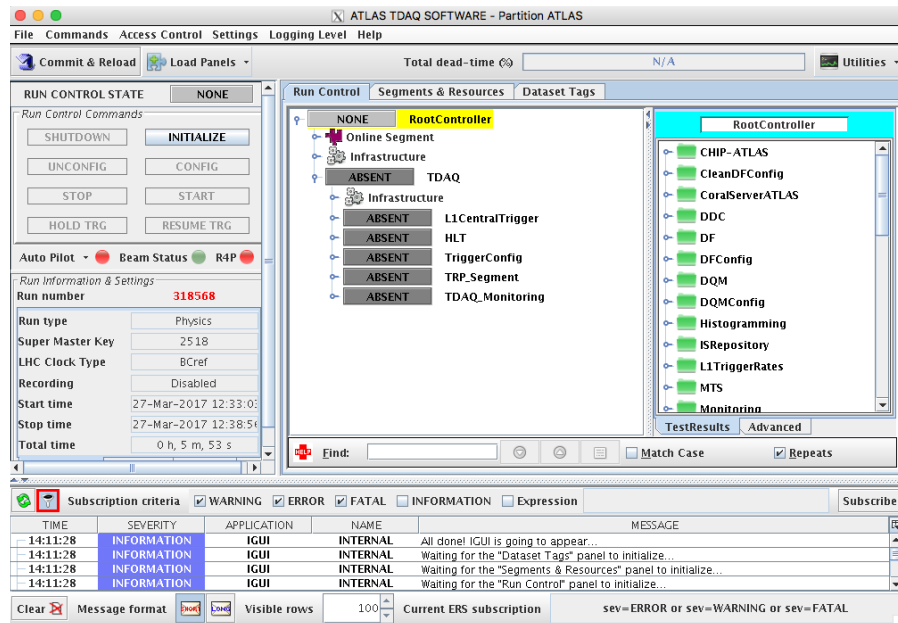


Figure B.3. The DAQ Interactive Graphical User Interface (IGUI).

if the issue is just a temperature fluctuation looking at the temperature versus time trend through the options of the DCS alarm screen.

The Data Acquisition Interactive Graphical User Interface (DAQ IGUI), represented in Figure B.3, is instead the tool which the muon shifter uses to monitor the data acquisition. This interface is common to all desks of the control room and is used by the run control desk to start/stop the runs and to define which detector sub-systems are part of the data acquisition partition. The muon shifter uses this interface as a monitoring tool only (i.e. without the permission to issue any command), with the aim of checking the status of the data acquisition process through the muon chambers. More in detail, he has to check whether the muon system is included or not in the partition, consistently with the plan of the day, and identify errors issued in the DAQ IGUI panel connected with the data acquisition process and involving the muon system, which he has to report and solve with the relevant expert.

B.3 Data Quality assessment

The data quality assessment is the complementary duty which the muon shifter has to accomplish, together with monitoring the detectors and the data acquisition chain. To produce the histograms used for data quality, a specific processing infrastructure is set-up running on raw data coming directly from the detector. The raw data are propagated from the read-out drivers (RODs) and the trigger calibration stream through the Gnam online software framework, and from the trigger express stream through the Athena framework, to be pre-processed. Then, they are visualised to the muon shifter in histograms available into two navigable tools: the Online Histogram Presenter (OHP) and the Data Quality Monitoring Display (DQMD).

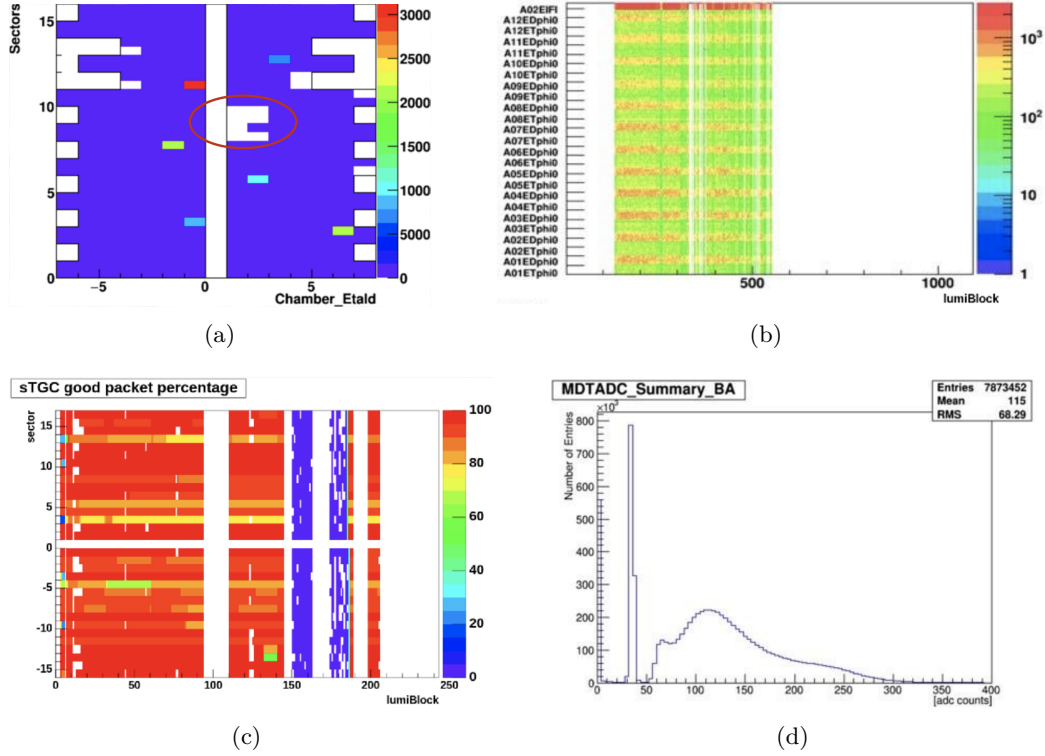


Figure B.4. Examples of data-quality plots monitored by the muon desk shifter: (a) Resistive Plate Chambers (RPC) occupancy, (b) Thin Gap Chambers (TGC) occupancy as a function of luminosity blocks, (c) good data packet percentage in Small TGC e-links, (d) shape histogram for the Monitored Drift Tubes (MDT) ADC counts.

Despite the sub-detectors constituting the muon spectrometer are different, the histograms used for the data quality assessment are of few types and fall in three main categories. The first category includes the occupancy histograms. In these histograms the acceptance of the muon detectors is represented and, the muon shifter has to verify that there are no acceptance decreases caused by issues in the muon chambers. Figure B.4 shows examples of occupancy plots. In particular, Figure B.4(a) reports the occupancy of the Resistive Plate Chambers (RPC) in the rapidity versus sector number plane, showing an acceptance hole which requires further investigation by the relevant experts. Figure B.4(b), instead, represents the Thin Gap Chambers (TGC) occupancy, as a function of time counted in units of luminosity blocks. Some occupancy drops are shown in small intervals of time, which do not correspond to issues as they are expected due to the chambers re-synchronisations and trigger pre-scale keys changes. The second category of data quality plots covers all histograms representing chambers electronics synchronization and related errors. An example of plot belonging to this category is shown in Figure B.4(c), representing the percentage of good transmitted data packets on the e-links of the small-TGCs. It can be seen that, as a function of luminosity blocks (i.e. of time), the good packets percentage is high in all sectors except for some ones having a $\simeq 70\%$ fraction of good packets and representing minor defects. At a certain time, the good packets fraction is drastically

reduced, requiring the intervention of experts. The third category of plots collects distributions of characteristic variables of the muon detectors (e.g. ADC counts, hits and timing distributions, charge distributions, etc). An example of plot belonging to this category is shown in Figure B.4(d), representing the ADC counts distribution for the Monitored Drift Tube Chambers of the muon spectrometer. In this case the muon shifter has to look at the shape of the distribution and check its agreement with a reference histogram presented in the online monitoring tool.

The data quality assessment is a very import task since it directly impacts the reliability of the dataset which will be delivered to the ATLAS physics analyses to perform measurements and searches. For this reason, muon shifters are not the only ones in charge of accomplishing this task, which is performed also by the other sub-detector systems shifters (inner detector and calorimeters) and by the data quality shifter. After the data acquisition, specific data quality experts and physics signature experts also analyse the features of the new dataset before signing-off for the inclusion of the collected data in the Good Runs Lists.

Appendix C

HEPScape! The High Energy Physics Escape Room

I describe in this appendix an outreach project I participated to during the years of the PhD course, about a thematic escape room on high energy physics. I participated to the construction of the first “Hepscape!” prototype in 2021, and joined several runs of the activity in festivals and fairs in the period 2021-2023. The activity has spread nowadays over several institutes in Italy.

C.1 An escape room for outreach and education

Escape rooms are a playful activity which has become quite popular in recent years. An escape room is an environment in which the visitors are challenged with a series of quizzes and puzzles they have to solve in order to leave the room. They typically have an underlying theme (e.g. detective stories, ancient history), and a moderator is often present to guide visitors through the experience.

Escape rooms were originally conceived as fun attractions, but have also been used by adult co-workers for team building exercises, since the participants have to work together towards a common goal. Recently an interest has grown in using escape rooms also for educational and outreach purposes [188]. In fact, for their characteristics, escape rooms are able to stimulate people’s curiosity through active learning, developing in parallel soft skills like critical thinking, organisation and teamwork abilities. The visitors are stimulated with puzzles and question, which require to return an immediate feedback on the information they receive, maximising their memorisation of notions.

In 2021 I participated to proposing a thematic escape room on high energy physics, “Hepscape!” [189], together with other two Ph.D. students in Rome University and researchers from INFN Rome. “Hepscape!” is an escape room for outreach purposes, to be used in science festivals, fairs and laboratories open days. The visitors enter the room and have the impression of moving underground in the Large Hadron Collider (LHC) tunnel, where they are puzzled with quizzes and games telling them about the CERN laboratories, the LHC and its experiments. They are taught about



Figure C.1. Pictures of the “Hepscape” setup: (a) indoor configuration in a room and (b) outdoor setup in a gazebo.

the basic notions on elementary particles and how they are accelerated into colliders, and finally learn about the Higgs boson and how it has been discovered. The escape room has been prepared for a general public, and is available in two versions, one adapted to young children (approximately 8-11 years old) and one for teenagers and adults.

C.2 Description of the activity

“Hepscape!” has been conceived as a portable kit which can be transported, installed and run by a minimum of three people. Each iteration of the activity can host approximately 20 visitors, and takes around 30-40 minutes.

C.2.1 Required equipment and setup

The escape room can be installed indoor in a physical room, or outdoor in a gazebo, as shown in Figure C.1. The total required space is around 25 m². At the entrance of the room a desk is placed, with one person standing in order to welcome visitors and distribute them work helmets, like in a real LHC underground visit. Several decorative posters are also available, and a PVC curtain showing the LHC tunnel is mounted at the entrance of the indoor version.

The set-up inside the room is shown in Figure C.2. Some tables are hosting three projectors controlled by a laptop: one pointing to the main wall, and the other two pointing to the side walls. Six LED lights are installed to draw visitor’s attention to particular parts of the environment, along the visit. The laptop and the lights controller are handled by one or more moderators, which sit in one of the two side desks. Several posters are distributed in the room, containing information which is needed to solve the quizzes: the periodic table of elements, a picture showing the structure of the atom, and another one representing the structure of the proton into quarks. Additional material (LHC control room badges, small balls representing quarks and other particles, a balance) are put on a shelf. People are told to sit in the



Figure C.2. Layout of the equipment and setup inside the escape room.

centre of the room on some pillows, and one moderator, which will act as storyteller through the visit, stands near the main screen and moves in the room guiding the visitors through the games.

C.2.2 The games

The visit starts as soon as all the people are seated inside the room. The storyteller makes a brief introduction to the context, telling about the activity, and giving general information about CERN laboratories and particle physics. Then, a video is projected simultaneously on the three walls, simulating the descent of the visitors in the LHC tunnel with an elevator, inside one of wells to access the underground areas.

Visitors have to solve three main games in sequence (see Figure C.3 for a representation of some of them). At the end of each game they have to find a lock hidden in the room, which they can open with a numeric combination related to the solution of the preceding game. Once each lock is opened, they found inside some explanation with scientific content, together with a missing piece of the puzzle representing the CMS experiment, which they have to complete along the visit. In the first game, the visitors have to guess the depth of the LHC tunnel. The game is differentiated with respect to the age group: adults have to solve a system of symbolic mathematical equations, while children solve a shorter and simpler enigma. In the second game, participants discover that the superconducting magnets of the LHC are based on an Nb-Ti alloy, solving a crossword. Then, they have to search for those elements in the periodic table and use their atomic numbers to open the lock related to the second game. The third game is about the Standard Model: using plastic balls representing particles, adult visitors have to identify the quark constitutes of the proton, while children have to discover the structure of the atom. Once the three games are completed, a video of proton-proton collisions inside LHC is projected, with the guide giving information on how particles are generated, decay and are detected in the experiments. The visitors are told about the Higgs boson and have to identify an event in which an Higgs decays into four muons. They look

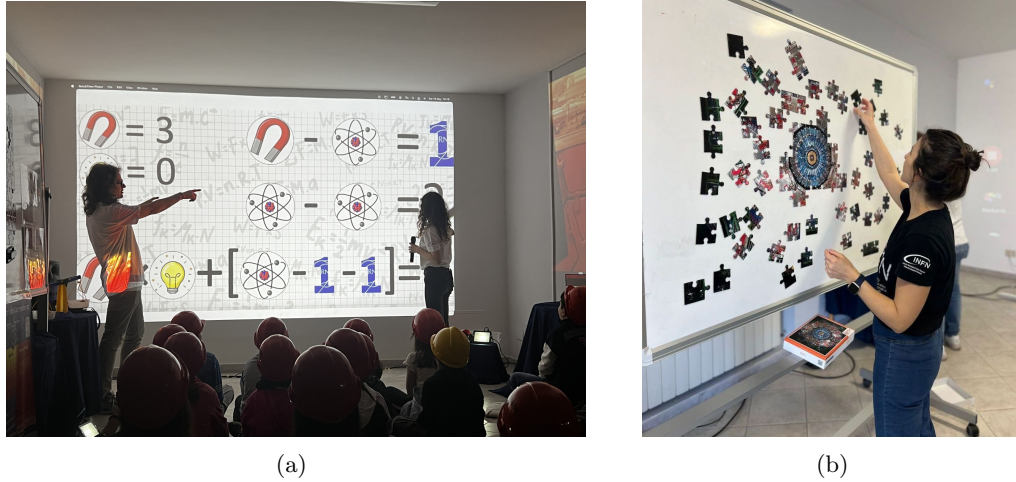


Figure C.3. Pictures of some of the games proposed during the activity: (a) the numeric quiz and (b) the puzzle of CMS experiment.

at events displays and count the number of muons in each analysed event, until they identify the Higgs candidate.

The “Hepscape!” experience terminates with the video of the Higgs discovery announcement, as recorded in the CERN main auditorium on the 4th of July 2012. At the end of the visit, a brief discussion session is offered, in which participants can ask questions to the moderator about their curiosities on particle physics and the life of a physicist at CERN.

C.3 Evaluating the impact: “Hepscape!” across Italy and beyond

After its start in 2021 the “Hepscape!” project has immediately demonstrated its potentiality in terms of impact on the visitors and dissemination across a wide range of public, also thanks to its conception as a portable kit, which is easy to transport and mount in different places.

C.3.1 Visitors satisfaction

The visitor’s satisfaction is assessed via a simple feedback questionnaire that participants are asked to fill at the end of the activity. The survey is composed of two questions: the age of the participant and its satisfaction, quantified in a scale from 1 to 5.

Figure C.4 shows the results of the survey as they were collected at the Genova Science Festival in 2022. The left figure shows the satisfaction for people participating as school groups guided by their teachers. The central figure, instead, shows the satisfaction of individuals, which came at the festival by their own initiative. Finally, the right figure shows the combination of the data from the preceding two categories. As can be noticed in the case of school visitors a very high satisfaction was reached

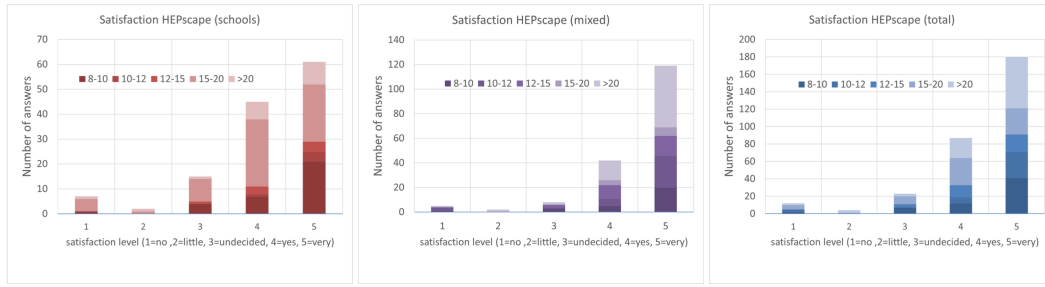


Figure C.4. Statistics of visitors satisfaction survey at the Genova Science Festival (2022) for: school groups (left), individuals (centre), and total audience (right).

for young children and adults, which can be attributed to the fact that “Hepscape!” was always run in the version adapted to the age group of the participants. A non-negligible tail on unsatisfied visitors is present, which is explained thinking that in school classes there can always be a fraction of people in the group which is not interested in science, but is visiting the festival as part of the class. Instead, individual visitors are almost always satisfied, since they all most likely have a personal interest in science which led them to book the activity. It can be noticed that a small percentage of unsatisfied children visitors is present. This can be attributed to the fact that in this case the escape room was always run in its version for adults.

The overall satisfaction rate, averaged across all visitors, is 4.4/5 which quantifies the high success of this initiative among the public

C.3.2 Dissemination and future plans

The “Hepscape!” project started in Rome in 2021. I participated to the construction of the first prototype, which was built and run in the inner garden of the Rome Physics department, with funding from the INFN Rome section and from an “Avvio alla terza missione” outreach project granted by Sapienza university to me and other two Ph.D. students.

After the prototype validation, the activity was presented to the public as an attraction in the European Researchers Night in September 2021, and subsequently at the Genova Science Festival and at the Frascati Open Labs 2022. After these initial runs, other Italian institutes have shown interest in this activity, which was therefore reproduced in Perugia and Padova INFN sections. Figure C.5 shows the overall dissemination of the activity through several festivals in Italy in the period 2021-2023, which comprehensively was offered to more that 4500 visitors. In 2024 the INFN outreach committee recognised “Hepscape!” as an outreach project of national interest and endorsed the activity with a stable annual financing. The project was also reported to the high energy physics community in international conferences and was presented at Lepton Photon 2021 conference [191] and ICHEP conference in 2022 [190] in Bologna. The overall dissemination of this outreach activity is remarkable, and this can certainly be attributed to the playful approach used to convey the scientific notions, as well as the fact the “Hepscape!” has been conceived as a portable kit, which is easy to learn and to reproduce in other interested

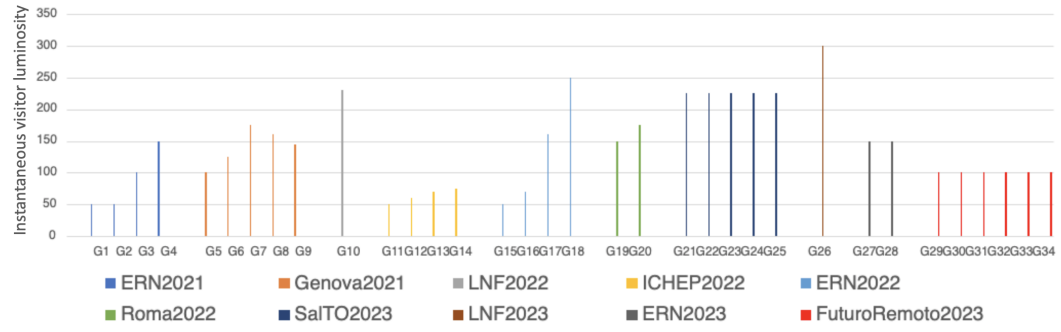


Figure C.5. Dissemination of the “Hepscape!” activity in Italian science festivals in the period 2021-2023. The number of participants per day is shown for every run of the activity in a different location.

institutes.

In the future we plan to translate the “Hepscape!” games into English and other languages, including the language of signs, to make the activity more inclusive and implementable with an international public. The possibility to collaborate with the International Particle Physics Outreach Group (IPPOG) is under development, to eventually run “Hepscape!” at CERN, for example during the annual CERN Open Days.

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