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DOCTORAL THESIS

Localization of critical raw materials for the GREEN transition based on a 3D lithospheric model

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UNIVERSITÀ DEGLI STUDI DI TRIESTE

Abstract

Dipartimento di Matematica, Informatica e Geoscienze

Doctor of Philosophy

Localization of critical raw materials for the GREEN transition based on a 3D lithospheric model

by Gerardo MAURIZIO

Minerals consumption has increased with the technological advancement we are experiencing and with the green transition, making their exploration and sustainable exploitation a pressing challenge. The localization and the characterization of these resources require the combination of different geophysical and geological techniques. Among these, the inversion of gravity and magnetic data is proving to be a key tool for exploring the Earth's subsurface and identifying promising deposits. However, the inherent ambiguities of potential field data necessitate sophisticated methodologies that integrate geological, geophysical, and probabilistic frameworks to produce robust and interpretable models.

This thesis investigates the application of different inversion techniques in multiple scales of analysis, to enhance the localization of critical raw materials. At the large scale, a Bayesian joint inversion approach is employed to combine seismic tomography and potential field data, generating a high-resolution 3D model of the lithosphere. At the medium scale, the joint inversion applied further refine the subsurface model by focusing on a region with significant resource potential, defining the depth and shape of a crustal batholithic body. At the small scale, the Bayesian joint inversion resolve a localized mineral deposit, tacking in to account for the complexities of geological variability and reducing the ambiguity of potential field interpretations.

Through the integration of interdisciplinary methods and the application of inversion techniques, this research advances both the theoretical and practical aspects of resource exploration. By refining our ability to map the Earth's subsurface at different scales, the thesis contributes to the sustainable development by improving the exploration of the critical raw materials essential for the green revolution.

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Chapter 1

Introduction

The world is experiencing an unprecedented increase in demand for critical raw materials, largely due to the ongoing green transition and the rapid pace of technological advancement. This demand is growing not only because of increased consumption of established materials, but also because emerging applications require new types of minerals that were previously overlooked or underutilized. Consider, for example, the importance that lithium has gained in recent years in the electric battery industry.

The intensification of the activities in the sectors of renewable energy and high-tech electronics have prompted a shift in research priorities within the field of economic geology, through a more profound investigation of the mineral deposits already known, and the identification and exploration of new regions that hold potential for mineral extraction. In this context, geophysics plays an essential role in the exploration process. In particular, the use of gravity and magnetic potential methods allows a non-invasive and broad coverage analysis of the subsurface properties, also resulting to be less expensive than other techniques. What we obtain with these techniques is a specific information about the density and magnetic susceptibility distribution of the materials presents within subsurface. The observation of these fields can be exploited to construct comprehensive models of the lithosphere through the application of inversion techniques, trying as much as possible to resolve uncertainties arising from the process to enhance the precision of the resulting models.

This thesis address the inversion problem by initially exploring the theoretical framework of potential fields and the associated mathematical complexities. The inversion of gravity and magnetic data has been recognized as an ill-posed problem, due to the fact that numerous subsurface configurations can generate equivalent field observations. The thesis evaluates the use of two advanced inversion methodologies as a solution to this problem, utilizing probabilistic approaches and regularization techniques. Additionally, the methods seek to integrate a-priori knowledge derived from geological information and other existing geophysical models to constrain the results of the inversion with other observations. The objective is to develop a model that is as realistic as possible.

Another noteworthy element of the thesis is the discussion of the scale of investigation, as it is acknowledged that varying results can be obtained depending on the resolution of the data. From a geophysical perspective, it is imperative to have a clear understanding of the objectives of the investigation and to be able to predict the outcomes based on the available data. The study employs the inversion technique at various scales to analyze and compare results, thereby ensuring a comprehensive assessment of the inversion process. This methodological approach facilitates the exploration of subsurface features from a regional perspective to the level of individual deposit characterization, providing an understanding of the geological processes.

It is expected that the research will yield a number of multifaceted results. Primarily, the application of advanced inversion methodologies is anticipated to generate more precise and reliable 3D models of the subsurface. These models will further our comprehension of the distribution of density and magnetic susceptibility in the lithosphere, thereby offering new insights into tectonic and magmatic processes that have contributed to the evolution of mineral deposits.

Secondly, an analysis of the results derived from varying investigative scales will permit to evaluate the differences between extensive regional solutions and the detailed local solutions necessary for the characterization of a mineral deposit. This methodology aspires to formulate a systematic analytical procedure that commences with a comprehensive examination of a region deemed prospective for mining, progressively delving into enhanced levels of accuracy, until the delineation and description of new mineral deposit. Finally, the work is intended to contribute to the broader goal of sustainable resource management by valuing exploration techniques that are both scientifically rigorous and economically viable. In doing so, it supports the strategic objectives of the green economy by facilitating the discovery and sustainable exploitation of the critical raw materials that are essential for modern technological applications. The structure of the thesis is designed to explore the theory and the methodology of the potential fields inversion, and to show practical applications. The opening chapter offers a comprehensive review of the economic geology, highlighting its fundamental concepts. The information present in the chapter is mainly derived from the course of Economic Geology held by the University of Pisa, and from the course of Mineral Deposits held by the Freie Universität in Berlin. The chapter also provides an accurate review of some of the minerals considered most interesting for the economic development. The second chapter provides an exhaustive review of potential field theory, explaining the principles behind gravitational and magnetic measurements, and the inherent difficulties of the inversion process. The chapter delineates the principles of the two inversion techniques employed for the study. Following this theoretical foundation, the subsequent chapter presents a series of case studies that demonstrate the application of the developed methodologies in various geological settings. These case studies are presented in a progressive manner, beginning with a large-scale inversion that captures the regional lithospheric structure, and moving through a medium and a small-scale application that focus on specific mineral deposit. Each case study is discussed in depth, with detailed analysis of the data, the inversion process, and the geological interpretations that emerge from the models. In the final chapter, a comprehensive overview of the preceding case studies is provided. Concurrently, the results are generalized by incorporating a consideration of the employed methodologies and the scale of investigation. Additionally, the chapter provides a comprehensive discussion of the contributions of this work to the domain of economic geology and explores potential avenues for future research that could further augment our ability to locate and evaluate critical raw material deposits.

In summary, the thesis proposes a framework for the application of different geophysical inversion methods with a comprehensive, multi-scale exploration strategy. Through a detailed exploration of economic geology and inversion theory of potential fields, and through the application of these methods to different case studies at different scales of investigation, the research aims to refine the approach to mineral exploration. This work aims to make a significant contribution to the field of economic geology, thereby supporting the sustainable development of resources critical to the global green transition.

Chapter 2

Mineral Exploration And Its Impact On The Economy

The information present in this chapter was discussed in the course of Economic Geology held by the University of Pisa, and in the course of Mineral Deposits held by the Freie Universität Berlin. Main reference books have been "Ore Deposit Geology" by Ridley (2013), "Ore Geology and Industrial Minerals: An Introduction" by Evans (1993), and "Economic Geology: Principles and Practice" by Pohl (2011). The three books are also mentioned inside the text.

2.1 Introduction to Economic Geology

Human societies fundamentally depend on the Earth's resources for their survival and development. From metals like iron, copper, and gold, that have marked the evolution of human history, to non-metallic minerals, up to the fossil fuels like petroleum and natural gas, these resources form the backbone of modern civilization.

Economic Geology is a sub-discipline of the geosciences dedicated to the study of these vital mineral resources. It covers all the aspects involved in describing and understanding these resources, from genesis to exploration and ore processing, covering also their practical application in industry and society. Main objective of Economic Geology is to bridge theoretical geoscience and practical mining by providing insights into the genesis of ore deposits, methods for their discovery, and techniques for efficient extraction.

In recent periods, the role of this discipline has become critically important, with the growing global demand for raw materials necessary to face the green transition and the movement to more environmentally sustainable energy sources. Trends show that demand will continue to increase, especially in those nations that are now experiencing economic growth, such as China. The challenge of economic geology is primarily to identify new mineral (ore) deposits and ensure a sustainable mining in the future, both from a quantitative point of view, taking advantage of the technological growth of the recent period and of the scientific knowledge of certain areas which increases with the demand, and from a qualitative point of view, identifying the consequences of a prolonged extraction.

A mineral deposit represents a natural aggregation of substances within the earth's crust that could have economic value (Ridley, 2013). It highlights any unusual concentration of minerals. What we are most interested in are ore deposits, which are natural concentrations of economically valuable metals, minerals, or rocks that can be profitably extracted. This makes the concept of "ore deposit" variable in time: something that is not an ore deposit in this period may be an ore deposit in future, and vice versa. This happens because many issues could change over time: technological advancement, extraction costs and percentages that can be extracted, knowledge about quantities, and the economic value of the ore itself. As an example, we could think of the demand for lithium, which has increased dramatically in recent years, leading to a significant boost of its extractive interest. These ore deposits are distinct from mineral occurrences, which may be of scientific interest but lack the economic viability for exploitation.

Ore deposits are formed through complex geological processes that enrich elements or compounds far beyond their average crustal abundance. These enrichments result from dynamic interactions within the Earth's crust, mantle, and surface systems. Key processes include endogenic processes like magmatic differentiation and hydrothermal activity or exogenic processes like sedimentation and weathering. Economic geology seeks to understand these processes to better locate and utilize such deposits.

Economic geology does not merely aim to describe the Earth's mineral wealth but also seeks to optimize its extraction and utilization. The mining cycle includes:

- Exploration: the use of geological, geophysical, and geochemical techniques to locate new deposits.
- Evaluation: Assessment of mining feasibility through reserve estimation, grade determination, and cost analysis.
- Exploitation: implementation of mining methods specific to a certain deposits, managing waste and environmental impacts.
- Closure and Rehabilitation: Ensuring sustainable post-mining land use and addressing long-term environmental concerns.

Materials investigated can be divided into two different categories: Metallic minerals, which are minerals extracted from rocks in a pure way, by more delicate and expensive processes, and industrial minerals, which are geological materials with low-medium commercial value, as they require low cost to produce. An example of industrial minerals are sands, or gypsum. Whether or not a deposit is economic depends on numerous factors, often not geological. Based on the economic importance, we can divide deposits into resource and reserves. A resource includes an area of the deposit which is uncertain in geological knowledge, or certain concerning the ore presence but uncertain about the economic return of the potential extraction. Defines the amount of a geologic commodity in such a form that economic extraction is feasible. A reserve is a part of the resource which is well geologically identified, and with an ore presence which can guarantee a profit. From a resource a commodity can be economically and legally extracted at the time of determination. A reserve can itself be divided into three subcategories. It can be "measured" when the materials has quality and quantity well determined ($\pm 20\%$) from quantitative data, "indicated" when minerals quality and quantity are known from quantitative data and partly from reasonable inferences, and "inferred" when the deposit is identified but under-explored, and whose quality and quantity of the ore are supposed from geological projections (Evans, 1993).

Whether a mineral falls into one or the other category depends on two different factors: Feasibility, based on economic, engineering, and environmental factors (i.e., the economic value of an ore, the cost of extraction and disposal) and the degree of Geological Assurance, which indicates how well the deposit is known, how it has been defined, how certain is the presence of the ore of interest at the site (i.e., what surveys have been done, geophysical accuracy, etc.). A summary graph is shown in Figure 2.1.1.

The resource can become a reserve and vice versa, basically depending on legislative factors, economic variations, or geological knowledge. High feasibility and high geological security allow the resource to become a reserve.

All these topics, covered by the Economic Geology, are used to characterize the attractiveness of an area for the extraction of a determined mineral.

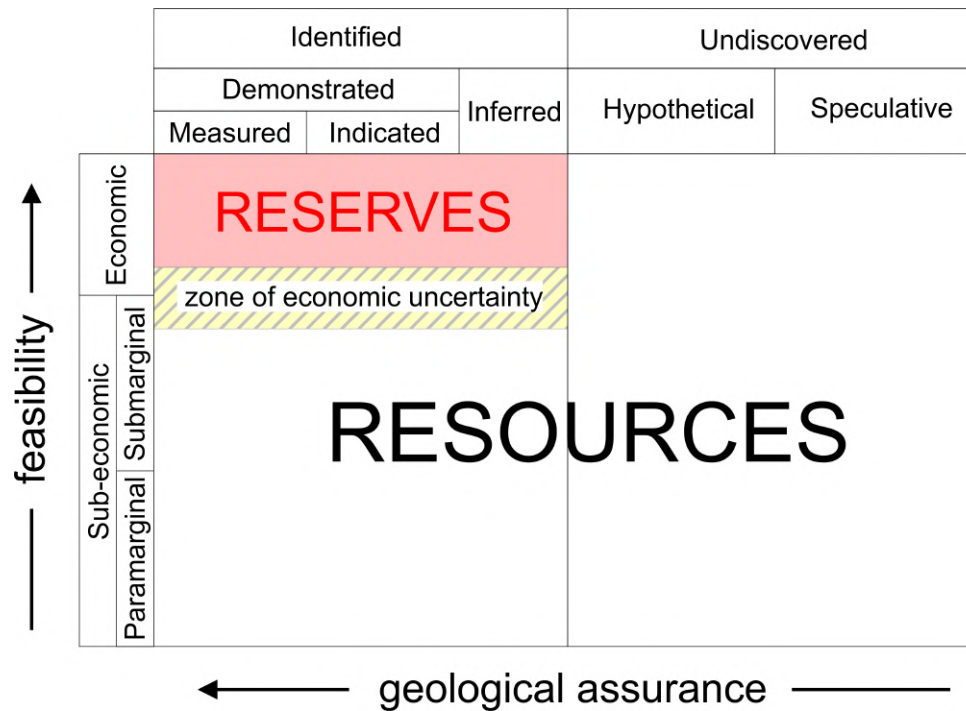


Figure 2.1.1: Variability in the definition of an ore deposit between resource and reserve, based on the economic, engineering and environmental feasibility and the degree of geological assurance. The figure was readapted from Evans (1993).

2.2 Ore deposits classification

Classification techniques are fundamental in the approach to ore deposit geology, serving to organize the vast number of known deposits into coherent groups for a faster and better knowledge of the mineral.

Ore deposits could be categorized using various attributes, each tailored to specific practical or theoretical needs. These include:

- **Commodity-Based:** classification focused on the element or mineral extracted, a standard chemical classification.
- **Host Rock:** classification which considers the primary geological formation where the ore occurs (e.g., carbonate-bearing sedimentary rocks).
- **Tectonic Setting:** classification which analyzes structural and stratigraphic context (e.g., deposits in back-arc basins).

All of these previous classifications can be used to define our mineral, but generally the most widely used classification is the one based on the genetic process of the deposit, which divides the ore based on the formation process (Ridley, 2013). The main processes that can lead to the formation of a deposit are magmatic processes, hydrothermal processes, and sedimentary-surface processes.

Magmatic processes lead to deposits formed by chemical and mineralogical processes that occur directly within magmas during the cooling of molten rock, through segregation of immiscible fluids rich in chemicals or crystallization where the elements may partition into mineral or immiscible fluid phases. Depending on the type of magma we will have different mineralization: metals like nickel, and platinum often originate from ultramafic magmas, while granitic systems may host tin and tungsten deposits. These deposits are commonly associated with large igneous bodies or with specific tectonic settings, like mid-ocean ridges or subduction zones.

The hydrothermal process involves the interactions in which large amounts of heated fluids move through rocks, leading to the complexation, circulation, and deposition of minerals. It includes phenomena such as mineral precipitation from solutions and the alteration of host rock minerals. These fluids may originate from magma or other external sources, and frequently create vein-type deposits abundant in metals like gold, as well as porphyry systems.

Finally, considering sedimentary process, mineral concentration is due to near-surface mechanical or chemical processes during sediment deposition, as well as to the action of weathering. These typically involve the surface concentration of metals like aluminum in bauxite, or nickel in lateritic soils, or a secondary enrichments in already existing accumulations. It may also include placer deposits, formed by physical sorting of dense minerals, or by chemical sedimentation, like the Banded Iron Formations. Evaporites deposits, of gypsum or lithium, are another example of this accumulation process (Ridley, 2013).

By examining a specific tectonic environment, we can predict the occurrence of a certain mineralization. Subduction zones generally produce porphyry copper and gold deposits, continental rifts are associated with rare earth elements and alkaline magmatic systems, while mid-ocean ridges host volcanogenic massive sulfide (VMS) deposits (Pohl, 2011).

To distinguish various types of processes, we need to examine certain characteristics of the deposits. Initially, we should evaluate the nature and distribution of mineralization, which involves analyzing the host rock that contains the ore deposit, the existing structures, and the three-dimensional distribution of the deposits through fieldwork or core analysis. Subsequently, we can proceed to conduct a chemical and mineralogical analysis of the ore, identifying chemical indicators of the formation process along with the temperatures and pressures at which the minerals originated. Figure 2.2.1 presents a Temperature-Depth graph illustrating the formation zones of several major mineral groups.

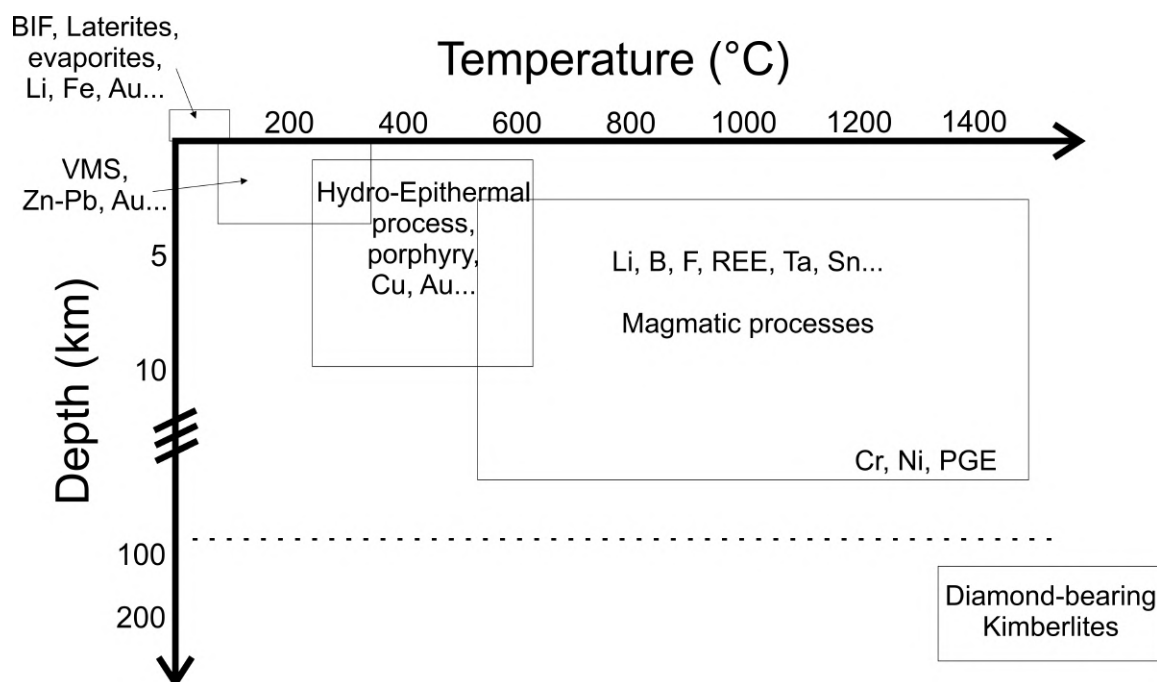


Figure 2.2.1: Depth and Temperature conditions for the genesis of principal ore deposits. The figure was readapted from the slides of the course in Economic Geology, from the University of Pisa.

Other more specific analyses can also be carried out, like a study of the isotopic composition, which can help to date ores and the ore process, and an examination of the fluid inclusion, as to determine the composition of fluids which is dependent on the ore. Recent advances in geosciences have refined the understanding of ore-forming systems and have deepened insights into how metals are concentrated.

Each of these formation processes discussed in this chapter reflects distinct geological, chemical, and physical conditions that drive the concentration of valuable minerals.

2.3 Critical raw materials

Critical raw materials (CRMs) are materials vital to the European Union's economy that are at risk of supply interruptions for various reasons. Initiated in 2008, the European Union campaign targets the reduction of the disparity between energy material production within Europe and imports from other countries (Grohol & Veeh, 2023). Additionally, it seeks to improve the recovery of secondary materials by promoting a more circular mining economy.

Whether an element belongs to the category of CRMs depends essentially on two factors: Economic Importance and Supply Risk (Grohol & Veeh, 2023).

The Economic Importance (EI) shows how useful a mineral could be for the development of the economy. It is calculated based on the importance of a given material in the EU for end-use applications and on the performance of available substitutes in these applications. Not to be confused with its economic value (e.g. gold has a low Economic Importance, while cobalt and tungsten have much higher values).

Supply Risk (SR) represents the possibility that a resource may stop being extracted and is calculated based on factors that measure the risk of a disruption in supply of a specific material. This may depend on the abundance of a material in specified areas, but also from other geopolitical conditions as trade restrictions and agreements or import reliance (e.g. rare earth elements have a very high supply risk, because they are present in small concentrations in the minerals, and the minerals that contain them are abundant only in a few areas of the Earth).

The list of CRMs is established on the basis of the raw materials which reach or exceed a thresholds for both parameters (Grohol & Veeh, 2023). The thresholds are set at $SR \geq 1.0$ and $EI \geq 2.8$. In Figure 2.3.1 and in the Table 2.3.1 are shown the CRMs for the 2023.

Table 2.3.1: Critical raw materials list of 2023 compared with the list of the 2020. Table was taken from Grohol and Veeh (2023).

2023 CRMs vs 2020 CRMs			
aluminium/bauxite	gallium	phosphate rock	vanadium
antimony	germanium	phosphorus	arsenic
baryte	hafnium	PGM	feldspar
beryllium	HREE	scandium	helium
bismuth	lithium	silicon metal	manganese
borate	LREE	strontium	copper
cobalt	magnesium	tantalum	nickel
coking coal	natural graphite	titanium metal	indium
fluorspar	niobium	tungsten	natural rubber
Legend:			
Black: CRMs in 2023 and in 2020.			
Red: New CRMs added in 2023, not present in 2020.			
Blue: 2023 declassified CRMs, present in 2020.			

We will now examine into a detailed analysis certain CRMs which, for various reasons, are among the most significant and researched, and have also been the focus of our study.

2.3.1 Lithium

Lithium and in the recent period became a crucial element for modern technologies and a symbol of the green transition. Its unique properties, coupled with its abundance and diverse applications, make it essential for various industries and a critical resource for a greener future.

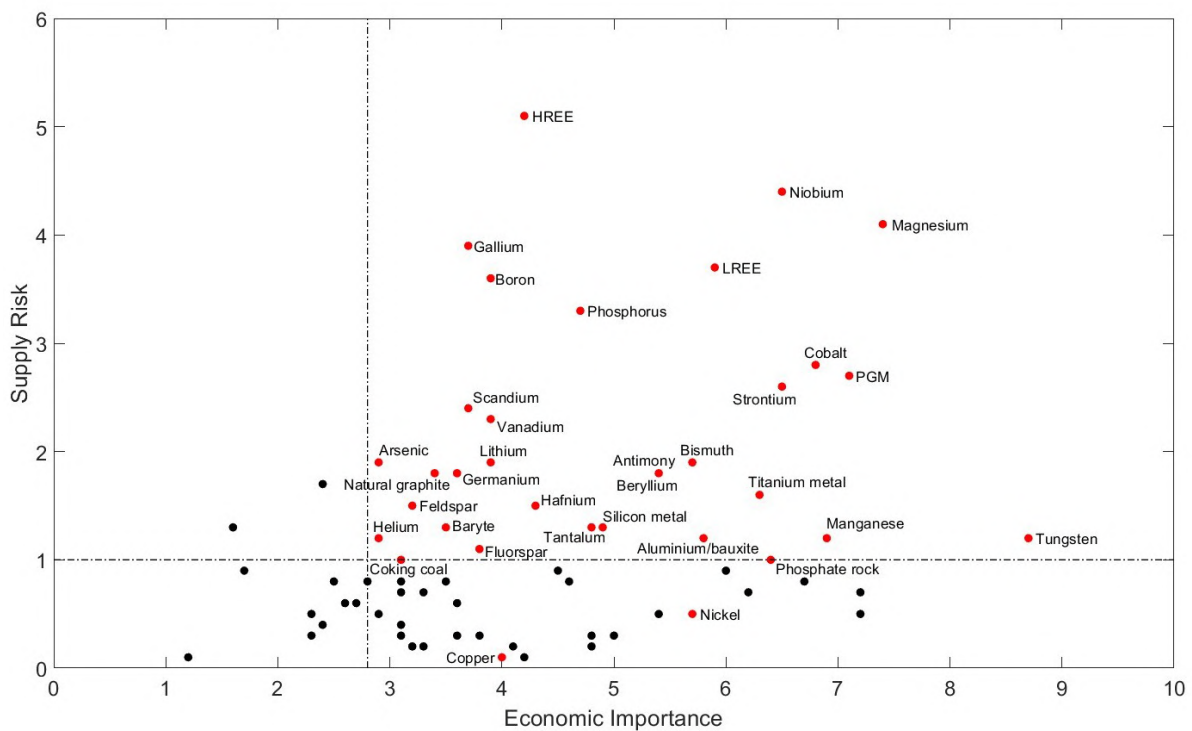


Figure 2.3.1: Critical raw materials list expressed as a function of Economic Importance and Supply Risk, resulting from the last EU criticality assessment, in 2023. In red are the elements that exceed both thresholds set by the committee. Copper e Nickel do not exceed the established threshold but are on the list as strategic raw materials. Figure was readapted from Grohol and Veeh (2023).

Lithium (Li) is the third element in the periodic table. It is a soft, silvery-white metal and an alkali metal. It is the lightest of all solid elements, with a very low density (Bradley et al., 2017). It concentrates in igneous rocks, especially granites, and moves into brines during weathering. Brines are the principal form in which we find lithium on Earth. They formed in arid basins, where lithium-rich groundwater concentrates through evaporation. Brines currently dominate the global production of lithium. Major deposits are in South America, primarily in Chile and Argentina (Bradley et al., 2017). We can find important percentages of lithium also in a variety of minerals present in pegmatites. Spodumene ($\text{LiAlSi}_2\text{O}_6$) is potentially the most exploited lithium source due to its high concentrations, although lithium is also derived from petalite ($\text{LiAlSi}_4\text{O}_{10}$) and lepidolite ($\text{K}(\text{Li},\text{Al})_3(\text{Si},\text{Al},\text{Rb})_4\text{O}_{10}(\text{F},\text{OH})_2$). Main production is due to the brine evaporation, which occurs by pumping lithium-rich brine to evaporation ponds where sunlight concentrates the lithium (Bradley et al., 2017). Nowadays also the extraction of lithium minerals from pegmatites is starting to become relevant. Deposits do not have a strong magnetic signal but are associated with unique geological formations.

Contrary to popular belief, lithium is not in short supply in the Earth. Its concentration in the Earth's crust is about 20 ppm, making it the 30th most abundant element. It has recently become a critical material for its strategic importance, so in the last period it has become more studied, and knowledge about the deposits is new and increasing (Bradley et al., 2017).

Lithium has diverse uses that span multiple industries, but it is universally recognized for the lithium-ion batteries which power a wide range of devices from smartphones to electric vehicles, and are considered crucial for reducing greenhouse gas emissions. It is also widely used in ceramics and glass production as it enhances its durability and thermal resistance. In 2013, 35% of lithium consumption was for ceramics and glass, 29% for rechargeable batteries. Now, as the world transition to renewable energy takes place, the main purpose of lithium

is changing and its importance continues to rise. It plays a central role in green transition technologies and its demand is projected to grow significantly. With global resources exceeding 39 million metric tons, lithium is poised to meet future needs.

2.3.2 Rare Earth Elements

Rare Earth Elements (REEs) comprise a group of 15 lanthanide elements, along with scandium and yttrium, known for their unique chemical and physical properties that are critical for modern technologies. Despite their name, REEs are relatively abundant in the Earth's crust but are rarely concentrated enough to form economic deposits. Their specific characteristics enable their use in defense, energy and industrial applications, driving global efforts to secure and develop new sources (Van Gosen et al., 2017).

These elements are traditionally divided according to their atomic number (Z) into:

- Light Rare Earth Elements (LREEs): Lanthanum (Z = 57) through europium (Z = 63).
- Heavy Rare Earth Elements (HREEs): Gadolinium (Z = 64) through lutetium (Z = 71), plus yttrium.

For his properties, scandium cannot be classified as either an LREE or HREE.

Although LREEs are more abundant and widely used, HREEs are rarer and have critical applications in high-tech industries.

REEs are primarily found in several key minerals, each of which serves as an important source for their extraction. Most significant are the bastnaesite, which is the primary ore mineral for REEs at China and USA major deposits, the monazite, which is often found in placer deposits and weathered laterites, and the loparite which is a source of both niobium and LREEs (Van Gosen et al., 2017). Deposits often show gravity and magnetic anomalies due to associated dense minerals or unique geological formations.

All the main processes previously seen can result in the accumulation of REEs. We can find REEs in carbonatites, which could host high concentrations of LREEs, while alkaline rocks are associated with HREE-rich deposits. Hydrothermal processes can lead to the accumulation of REEs in veins and fractures. Also tropical weathering could forms REE-rich secondary deposits. Major REE deposits include carbonatite-hosted Mountain Pass in California and Bayan Obo in China, which dominate global production (Van Gosen et al., 2017).

Once a rare earth site has been identified, the ore mining techniques used can be open-pit and underground mining, for hard-rock sources, or in-situ leaching for ion-adsorption clay deposits. Once the ore has been extracted, complex chemical methods are used to separate and purify individual elements, making the processing of rare earth elements extremely challenging (Van Gosen et al., 2017).

REEs are vital for numerous applications. Their indispensability for advanced technologies has made them critical to global economies and national security. They are used in precision-guided munitions, in many of our batteries, and in superconductors. Neodymium-iron-boron magnets, which find applications in electric vehicles, wind turbines, and electronics, are acknowledged as the strongest magnets available. Considering the automotive industry, lanthanum and cerium improve petroleum refining and automotive catalytic converters. They are also used in glasses industry, to enhance optical properties and add color to lenses.

With their central role in green and defense technologies, REEs are classified as critical minerals, requiring secure and diversified supply chains.

2.3.3 Copper

Copper (Cu) is one of the most versatile and widely used metals, with a rich history and critical applications across various industries. It is the 29th element of the periodic table and has some important properties such as high electrical conductivity and significant corrosion resistance.

It is commonly found in sulfide and oxide forms. Most famous sulfide ore are chalcopyrite (CuFeS_2), which is also the most abundant source of copper, while considering oxides ores, most famous are malachite ($\text{Cu}_2\text{CO}_3(\text{OH})_2$) and azurite ($\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$). Copper can also be found as a native metal in its metallic form, but is relatively rare.

The primary kind of copper deposits are the porphyry copper deposits. Globally, porphyry deposits account for more than half of copper production, making them the largest source of copper. These deposits can also yield gold (Au), silver (Ag), and other by-products (Wilkinson, 2013). Their economic importance stems from the combination of high tonnage and relatively low-grade ores, making open-pit mining economically viable. Porphyry copper deposits form in intrusion-related geological settings, typically 3–5 km beneath the Earth's surface. They are associated with large igneous systems and to subduction zone systems and are driven by magmatic-hydrothermal processes (Wilkinson, 2013). The world's largest copper mine, in Chile, showcases classic porphyry mineralization with high-grade hypogene and supergene zones.

Copper deposits can produce distinctive gravity and magnetic signals due to their geological characteristics. Especially in porphyry systems, they are often associated with ferrous ores such as chalcopyrite and bornite which have higher densities compared to surrounding rocks. As a result, porphyry copper deposits may produce positive gravity anomalies. At the same time, the presence in porphyry copper systems of magnetic minerals such as magnetite may lead to magnetic anomalies, which vary depending on the extent and type of magnetic mineralization (Wilkinson, 2013).

Copper properties make it an indispensable mineral for our economy, in particular in sectors of electrical and electronics (e.g. production of wires, cables and circuit), in the world of construction, for transportation components (e.g. for electric vehicle) and for industrial machinery. It is also used for coins and alloys production.

Major producers include Chile, Peru, China, the USA, and the Democratic Republic of Congo. It is important to know that copper is a 100% recyclable material, without any loss of quality, contributing to a circular economy. Nevertheless, extensive exploiting can cause land degradation, water pollution, and habitat loss.

Porphyry copper deposits represent a cornerstone of the global mining industry, combining geological complexity with economic and strategic value.

2.3.4 Niobium

Niobium (Nb) belongs to the transition metal and is the 41st element in the periodic table. It plays a crucial role in modern industrial and technological advancements, yet often not recognized. Niobium is a grey metal with a high melting point and remarkable durability. It is nearly always found in conjunction with tantalum (Ta) due to their similar chemical properties. Its exceptional properties, such as resistance to corrosion, ductility, and superconductivity, make it indispensable across various fields, from infrastructure to cutting-edge technology (Schulz et al., 2017).

Niobium's formation and concentration are closely tied to unique geological settings: it is commonly hosted in pyrochlore-rich deposits within carbonatites. Pyrochlore is the most important commercial source of niobium. It is a complex oxide containing niobium. It is predominantly found in carbonatite; however, it is also present in alkaline granites and syenites, typically associated with carbonatite formations (Schulz et al., 2017). Pyrochlore is by far the dominant source of niobium, accounting for the vast majority of global production. Other minerals like columbite and tantalite are important in regions where pyrochlore is absent or less abundant. Secondary production of niobium is also very important, with weathering processes which can create laterite deposits, concentrating niobium at the surface. Brazil, holding approximately 90% of production, extracts niobium mainly from carbonatite weathering residues (Schulz et al., 2017).

Its geophysical characteristics, including specific gravity and magnetic signals influenced by host rock composition, make niobium deposits identifiable in carbonatite-associated anomalies (Schulz et al., 2017).

Extraction methods depend from the deposit type. In a carbonatite-hosted deposits the pyrochlore is mined and processed to produce ferroniobium, a widely used alloy, while in lateritic deposits are often easier and more cost-effective to mine than primary hard-rock sources. This is also why it is the most common practice to collect niobium (Schulz et al., 2017).

Niobium's properties enable a wide range of applications. About 75% of the niobium production is used in high-strength, low-alloy steels. Adding niobium refines grain structures and enhances strength, toughness, and corrosion resistance, crucial for pipelines, buildings, and automotive manufacturing. Another important use is in the development of superalloys, as the niobium alloys withstand extreme temperatures, ideal for jet engines, gas turbines, and space applications. Thanks to his superconductivity it is also essential to build magnets for magnetic resonance imaging machines and large-scale physics experiments. In the exploration geophysics, this characteristic allows it to be an important element in the production of superconducting technologies, such as superconducting gravimeters with very low instrumental drift or SQUID (superconducting quantum interference device) magnetometers.

As the global economy grows and technologies advance, the demand for niobium is expected to increase, particularly in emerging markets. Its role in creating high-performance materials ensures its relevance in both industrial and high-tech applications. With large global reserves, niobium's supply is secure for centuries, though its production is geographically concentrated, creating potential supply risks.

2.3.5 Tungsten

Tungsten (W) has a unique position in the global economy. It is the 74th element of the periodic table and is predominantly found in hard-rock deposits. Its exceptional hardness and resistance to high temperatures make tungsten indispensable in various industrial applications.

Tungsten minerals are associated with different types of deposits. Vein deposits are the most significant contributors to global tungsten production. Found near granitic intrusions, they form when hydrothermal fluids deposit tungsten minerals in fractures of host rocks. These deposits consist of quartz veins rich in wolframite or scheelite, which are the main ores from which tungsten is extracted (Werner et al., 2013). Scheelite (CaWO_4) is a white mineral and contains approximately 60% tungsten by weight, while wolframite ($(\text{Fe}, \text{Mn})\text{WO}_4$) is a black ore containing different quantity of tungsten depending on its iron or manganese content. These two minerals account for the bulk of the world's tungsten production. Often, they were mined together from mixed ore bodies.

Other typical deposits are skarn, developing where granitic magmas intrude carbonate rocks, and primarily associated to scheelite accumulation, and porphyry deposits, associated with large felsic intrusions. tungsten is also possible in evaporitic deposits, although it is not an option currently exploited (Werner et al., 2013).

Due to its high density, tungsten deposits can be identified through anomalies in gravity field, while the presence of associated magnetized minerals can yield detectable magnetic signatures, also if tungsten itself is not magnetic (Werner et al., 2013).

The extraction employs both surface and underground methods, depending on the deposit's depth and economic feasibility. Minerals are then processed into intermediate compounds like ammonium paratungstate and ferrotungsten, or directly into powders and metal for industrial applications (Werner et al., 2013).

Tungsten's importance lies in its unique properties. Principal features are his hardness and high melting point (over 3400°C), it also has a high heat resistance and chemical stability. This make it indispensable in several fields, in particular in the production of cutting and drilling tools, In

the field of national defense and army production, and in the fabrication of high-temperature resistant components, fundamental for aerospace industry.

Tungsten is classified as a critical mineral due to its important applications and limited global supply. China and Russia dominates the global tungsten supply, holding approximately 2/3 of the world's known reserves. With regard to the European territory, historical deposits are found in Austria, Bohemia, Cornwall and Saxony. In fact, the Scheelite mine in Mittersill (Austria) is one of the most important tungsten mines world-wide. The concentration of resources in a few countries underscores tungsten's geopolitical importance. Industrialized nations rely heavily on tungsten for defense and advanced manufacturing, making its supply a matter of strategic interest.

Chapter 3

Potential Fields and Theory Of Inversion

As explained in the previous chapter, Economic Geology includes in its subjects of study also the part of mineral exploration. Interdisciplinarity is critical in this step, and the different geological, geochemical and geophysical knowledge is requested for the identification of new deposits or the reclassification of existing ones. The geophysical aspect is what we have been focusing on. The use of geophysical techniques for the characterization of interesting sites is a widely used methodology in the mineral exploration, testified by numerous works, e.g. Brodic et al. (2024), Denton et al. (2019), Doyle (1990), Melo et al. (2017), Oldenburg et al. (1998), and X. Wei et al. (2023). Specifically, we tackled the challenge using the potential fields techniques, particularly gravity and magnetic fields, as well as through the inversion of the data.

The inversion of potential field measurements has become a well-established method in the geological investigation of the solid Earth (Aster et al., 2018; Gubbins, 2004; Menke, 2018). Potential field measurements mainly refer to gravity and magnetic fields. These fields are called "potential" because they can be mathematically represented using scalar or vector potentials, which encapsulate their behavior and underlying sources. Starting from observations of gravity or magnetic fields at different locations on Earth's surface, our focus is on modeling the distribution of gravity and magnetic sources responsible for the detected anomalies. These methods are popular mainly because of their low cost and the broad coverage they offer, providing valuable information about the Earth's subsurface structure. Gravity method measures minor variations in the Earth's gravity field, caused by differences in sub-surface density. Measurements are performed using gravimeters, which detect minute changes in gravity. Observations with gravimeters could be made on land, on a plane/ship and on satellites, to have a global data coverage. Gravity anomalies suggest the existence of materials with varying densities beneath the Earth's surface and can be employed to deduce geological formations. Magnetic method detects variations in the Earth's magnetic field caused by subsurface materials with relevant magnetic properties. High-precision magnetometers are used to measure these variations. The magnetic characteristics of a material are influenced by its magnetic susceptibility, which controls its ability to be magnetized, as well as any inherent permanent magnetization present. This method is advantageous because it responds more strongly to shallower sources than gravity and can help identify depth and spatial features in the subsurface. For mining purposes, generally the magnetic field gives more detailed information, as deposits often have high and characteristic induced or residual magnetization, which allows detection of mineral accumulation. On the other hand, the gravitational field succeeds in giving a better overall analysis of the area, including from a structural point of view, as well as defining the distribution of the densities, based on which we can predict mineralization in the subsurface. A joint approach of the two allows reliable visualization of the subsurface, as they see different aspects of the same quantity. From a mathematical perspective, interpreting potential fields signals is an ill-posed problem characterized by instability and a lack of uniqueness in solutions. The non-uniqueness issue is particularly complex, as numerous distributions of mass density or magnetic susceptibility produce identical gravitational or magnetic fields. In order

to solve this problem a possibility is to constrain the inversion with other geologic or geophysical observations. Further details about gravity and magnetic inversion will be provided in the subsequent chapter.

3.1 The Inverse Problem

After a series of processing to delete external contributions to the signal (like topography signal) we retrieve anomalies that we are sure were representative of the sub-surface. Inverting these gravity and magnetic anomalies means reconstructing the shapes, i.e. the size and the position, and the density or the magnetic property of the object causing the anomaly. Many inversion theories have been developed over the years to solve the problem of non-uniqueness of potential methods. One of the first and most cited is the one of Li and Oldenburg (1996) for the magnetic field case, which was then implemented in Li and Oldenburg (1998) for the gravity field case. In their approach they discretize the subsurface into a grid of rectangular cells, each with a uniform susceptibility/density value so that relatively complex geologic bodies can be constructed. The solution to their inversion is obtained by minimizing an objective function that combines the data misfit and a model objective function, introducing spatial and depth weighting functions necessary to correct all those aspect that are not acceptable from the point of view of geological reality, but that are correct with mathematical explanation. To minimize these directional derivatives they relied on Tikhonov's regularization methods (Tikhonov, 1943; Tikhonov & Arsenin, 1977). This method adds a regularization term to the cost function, which helps to control unstable solutions reducing the sensitivity to the noise. A different approach, which underlies the methods we will discuss in more detail and which we used for our works, is analyzed in depth by Tarantola (2005), who formulates the foundational ideas that allow inverse problems to be addressed in a probabilistic framework. In this work Tarantola briefly defines the main features to approach the inverse problem in a probabilistic way, emphasizing the importance of incorporating existing knowledge about the model parameters before data observation, and to manage uncertainties in measurements. To solve this, Bayes' theorem is introduced as an optimal tool for transforming the prior distributions into posterior distributions, estimating parameters with associated uncertainties. The Monte Carlo method is then discussed in detail by the author as the best tool for solving the inverse problem when the models are large and complex. Monte Carlo methods involve random sampling techniques to estimate solutions and uncertainties. In essence, utilizing prior information allows us to narrow down the space of all possible solutions, concentrating only on those solutions that are geologically meaningful. Through sampling, we then consider just a subset of these meaningful solutions, enabling us to infer information about the entire space. Starting from a probability distribution, we generate different data points from that, defined as "samples" to return at the theoretical concept, which help us understand its characteristics without having to look at every point. In high-dimensional spaces problems, like those in complex inverse problems, calculating probabilities or finding solutions directly by evaluating every possible point is computationally impossible. Instead, by generating samples that represent the probability distribution, we get an approximation of the distribution's shape and values. Samples allow us to estimate the principal key properties, like the mean or the variance, of the distribution. This allow us also to calculate the uncertainty value of the predictions. Various sampling techniques exist, ranging from basic to advanced. The selection of an appropriate method is primarily influenced by the problem at hand, the extent of the distribution space, and the computational resources at our disposal.

As we have extensively discussed above, inverse problems of the potential fields can have multiple possible solutions. This makes the probabilistic approaches fundamental to address the ambiguity problems. In our work for the inversion of potential fields, we tried two different methods, which we present in the next chapters:

- a Bayesian method, proposed by Sansó and Sampietro (2021)
- a Limited-memory BFGS method, proposed by Moorkamp et al. (2011) and enhanced in Moorkamp (2022) with Mutual Information concept

3.2 Bayesian Joint Inversion

Bayesian inversion method used for the work is based on the principles discussed in Sansó and Sampietro (2021). The authors in the book treated all aspects of the gravity field, starting from Newton's law through the definition of the forward model, by concluding with the inversion modeling. In this last part, the authors first show some main aspects of the inversion of the gravity field, like the modeling of an anomaly in terms of simple subsurface geometries and with a constant density distribution considering mathematically terms the problem of indeterminacy and depth instability of the gravity field. After that they mathematically address the general problem of the inversion using both a deterministic and a probabilistic approach, preferring the latter. Bayes' theorem is a conditional probability theorem which, in its general formula, is used to calculate the probability of an event x occurring, conditionally by an event y , knowing the probabilities of the two events and the conditional probability of y respect to x . In the framework of potential fields inversion, Bayesian approach is applied to manage uncertainties and incorporate prior knowledge about physical and geological features. We assume that unknown parameters x and observations y have associated uncertainty, represented by probability distributions. The goal is to find the posterior probability distribution $f_{X|Y}(x|y)$ updating the prior distributions with new information, given by likelihood of observed data, to obtain a more reliable posterior distribution for the model parameters.

Let x represent the model parameters, like density distributions in a geological structure, and y the observed data, such as gravity anomalies. This is given by:

$$f_{X|Y}(x|y) = \frac{f_{Y|X}(y|x) \cdot f_X(x)}{f_Y(y)}$$

where $f_{Y|X}(y|x)$ is the likelihood function, also indicated with $L(y|x)$, representing the probability of observing y given x , $f_X(x)$ is the prior probability distribution of x , encoding prior knowledge about the parameters (e.g., geological constraints), and $f_Y(y)$ is the evidence or marginal likelihood, which is a normalizing constant ensuring the posterior integrates to 1. By this, the equation of the posterior distribution is generally expressed as proportional to the product of the likelihood and prior:

$$f(x|y) \propto L(y|x)f(x)$$

This equation represents the Bayes theorem in its classical form. In our framework, the prior encodes information on geological constraints. Represent our starting model, derived from geological observation. For example, the prior can specify ranges of density for different layers, enforcing realistic constraints based on geological labels. These constraints are essential for creating solutions that adhere to known geological structures. Assuming a variable to be normal distributed with average μ and variance σ^2 its probability density function is expressed as:

$$f(x) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{(x_i - \mu_i)^2}{2\sigma_i^2}\right)$$

In gravity inversion, the likelihood which represents the connection between the unknowns (density) and the data (gravity anomalies) is obtained using the Newton integral. More in general the likelihood can be described starting from the forward model, which refers to the function that converts the unknowns into observations. Supposing for the sake of simplicity also in this case that the observation error is normally distributed, the likelihood can be expressed as:

$$E(y|x) = \frac{1}{2}(y - A \cdot x)^T C_v^{-1}(y - A \cdot x)$$

where C_v is the covariance matrix of the observational errors, and A is the matrix representing the forward model.

The situation becomes even more complex if instead of a single variable, we would like to model more variables, considering different conditions, like in a joint inversion problem in which we want to estimate the values of density and magnetic susceptibility. In this case we have to consider the fact that the set of parameters to be estimated will no longer consist only of x conditioned by y , but we'll get a couple x_1, x_2 , which in our case will be ρ (the density) and χ (the magnetic susceptibility), conditioned by y_1, y_2 , defined for our example by Δg and ΔB , the gravity anomaly and the total magnetic intensity respectively. In the Bayesian algorithm used in this study, an additional vector of unknowns, denoted by L , is added to the problem. This L serves as a discrete categorical variable, representing a "label" for each volumetric element (voxel) in our model, reflecting the geological characteristics inherent to the voxel itself. This novel variable is utilized to avoid the smoothing effect commonly associated with 3D potential field inversions. Moreover, it enables us to indirectly connect various parameters, such as density and magnetic susceptibility.

After all this consideration, substituting these new parameters in the posterior distribution equation, we'll have:

$$\begin{aligned} P(\rho, \chi, L | \Delta g^o, \Delta B^o) \propto \exp\{ & -(\Delta g^o - A_g \rho)^T C_{\Delta g}^{-1} (\Delta g^o - A_g \rho) - \\ & -(\Delta B^o - A_B \chi)^T C_{\Delta B}^{-1} (\Delta B^o - A_B \chi) - \frac{1}{\sigma_{\rho l}^2} (\rho - \bar{\rho}_l)^T (\rho - \bar{\rho}_l) - \\ & - \frac{1}{\sigma_{\chi l}^2} (\chi - \bar{\chi}_l)^T (\chi - \bar{\chi}_l) - s^2(L, L^o) - q^2(L) \} \end{aligned}$$

Where:

Δg^o and ΔB^o are the vector of observed gravity and magnetic anomalies;

$C_{\Delta g}$ and $C_{\Delta B}$ are the covariances matrix associated;

A_g and A_B are the forward modeling operator which convert ρ and χ in g and B ;

$\rho_l, \chi_l, \sigma_{\rho l}^2$, and $\sigma_{\chi l}^2$ are the expected values and their variability;

s, q are two terms defining the a-priori probability of L . They are defined as "distance" functions and are penalty functions, which measures how much penalty is incurred when assigning a specific label L_i to a voxel V_i , compared to its reference or prior label L_i^0 .

In general term, the penalty functions is expressed as:

$$d_i(L_i, L_i^0) = \begin{cases} 0, & \text{if } L_i = L_i^0 = k, \\ q_{ij}, & \text{if } L_i = j \neq k. \end{cases}$$

if $L_i = L_{0i} = k$ the penalty condition is not applied ($d_i = 0$) and this means that inversion agrees with the prior label, while if $L_i = j \neq k$, the penalty q_{ij} is applied. Penalty value reflects the likelihood of assigning a label j that differs from the prior k . Larger q_{ij} values imply that the assignment $L_i = j$ is less probable, while a smaller q_{ij} increase the likelihood of such an assignment.

The complexity of calculating the posterior, particularly in high-dimensional problems like potential fields inversion, makes it necessary to use sampling methods. To approach this problem, a Gibbs Sampler is used to approximate the posterior distribution by generating samples. With this Markov Chain Monte Carlo method, each parameter is sequentially sampled conditional

on the current values of the other parameters, iteratively approximating the posterior distribution. This approach is efficient for handling large sets of parameters, such as voxel-based density and magnetic distributions in joint inversion models. To identify the global maximum of the posterior distribution, since numerous local maxima are expected, a simulated annealing algorithm is employed. This approach aids in converging toward the maximum posterior estimate by minimizing the energy function linked to the posterior. This stochastic optimization improve the efficiency of the Gibbs Sampler by helping it escape local minima and explore the entire solution space more effectively. This procedure iteratively refines the density, susceptibility, and geological unit labels within each voxel, producing a 3D model that fits the observed gravity and magnetic fields while respecting prior geological knowledge, representing the most reliable model of the area investigated.

3.3 L-BFGS Optimization

Moorkamp et al. (2011) focuses on the framework for a 3-D joint inversion that enables the integration of diverse geophysical data types to enhance subsurface imaging, relying on modularity and efficient large-scale optimization techniques. The framework consists of several interchangeable modules, including components for optimization, data transformation, and forward and gradient calculations. The framework utilizes optimization methods suitable for handling a large number of parameters. Efficiency is achieved through a balance between computational cost and memory usage. Methods like Gauss–Newton and Quasi–Newton are compared for suitability based on problem size and parameter distribution

The Gauss-Newton method is suitable for problems in which parameter sensitivity matrices are sparse. This method is effective but requires significant memory when matrices are dense, while Non-Linear Conjugate Gradient (NLCG) and Limited-memory Broyden – Fletcher – Goldfarb – Shanno (L-BFGS) are preferred due to their low memory needs, with each having trade-offs in computational steps and storage requirement.

This two algorithms are commonly used in large-scale inversion problems. Both methods are similar in the sense that they use information from previous iterations to improve the current model update. The main difference is that NLCG only uses the previous model update and gradient, while L-BFGS uses a number of correction pairs n_{cp} , that can be chosen by the user. NLCG therefore only requires $2M$ extra storage, while L-BFGS requires $2n_{cp}M$ extra storage, with M number of model parameters.

Main advantage is that Quasi–Newton methods only require the derivative ($\nabla\Phi = \delta\Phi/\delta m$) of the objective function (Φ) with respect to the model parameters (m). Parameters m refer to the variable investigated, in this case Density and Susceptibility. L-BFGS method analyzed in this project use information from each iterations to improve the current model update, based on gradient calculation. Given a starting model, we perform several optimization iterations until the value of the objective function, the misfit between observed and synthetic data, reaches a defined threshold.

As for the previous methods, we are going to perform a joint inversion. In this case the objective function is expressed as the sum of all the misfits parameters:

$$\Phi_{joint} = \sum_i \Phi_i$$

that for our basic example are

$$\Phi_{joint} = \Phi_{d,grav} + \Phi_{d,mag} + \Phi_{Reg,\rho} + \Phi_{Reg,\chi}$$

Where $\Phi_{d,grav/mag}$ represents the misfits between synthetic data calculated from the current model and observed data, and $\Phi_{Reg,\rho/\chi}$ is a regularization term which encourages smoothness,

by penalizing abrupt changes in model parameters and balancing between data misfit minimization and realistic structures. In this framework Moorkamp (2021) go to introduce a new concept of “Variation of Information”. Its a method which constructs a one-to-one relationship of a-priori unspecified form between the properties under consideration. Is a theoretical measure of the amount of information contained in variable x about another variable y , based on the Shannon entropy of the solutions terms. To couple the variables investigated within the inversion framework, VI must be minimized. This will result in models where each value x corresponds to a unique value y . To minimize, also VI is insert in the previous objective function, as follow:

$$\Phi(\rho, \chi) = \lambda_1 \Phi_{d, Grav}(\rho) + \lambda_2 \Phi_{d, Mag}(\chi) + \lambda_3 \Phi_{VI}(\rho, \chi) + \lambda_4 \Phi_{Reg, \rho}(\rho) + \lambda_5 \Phi_{Reg, \chi}(\chi)$$

We deconstruct the objective function and analyze the different terms of the equation:

$$\phi_d(\rho) = [g(\rho) - d_{obs}]^T C_d^{-1} [g(\rho) - d_{obs}]$$

$$\phi_d(\chi) = [g(\chi) - d_{obs}]^T C_d^{-1} [g(\chi) - d_{obs}]$$

$g(\rho)$ and $g(\chi)$ is the synthetic data from the forward calculation for the given model, d_{obs} the vector of observed data and C_d the inverse of the data covariance matrix, which adjusts for noise and error in data. This expression quantifies how well the synthetic model $g(m)$ matches the observed data d_{obs} , with greater differences indicating poorer fits. Minimizing this misfit in inversion produces a model that aligns well with observations.

Including covariance matrix in the objective function reduces the influence of observations with large errors and equalizes the influence of data with similar relative errors irrespective of the magnitude of each datum

The regularization terms were included to stabilize, as follow:

$$\phi_{reg}(\rho) = \sum_i \alpha_i (\rho - \rho_0)^T W_i^T C_M^{-1} W_i (\rho - \rho_0) + \beta (\rho - \rho_0)^T C_M^{-1} (\rho - \rho_0)$$

$$\phi_{reg}(\chi) = \sum_i \alpha_i (\chi - \chi_0)^T W_i^T C_M^{-1} W_i (\chi - \chi_0) + \beta (\chi - \chi_0)^T C_M^{-1} (\chi - \chi_0)$$

The matrices W_i are finite difference approximations to the first or second spatial derivative of the model parameters in the respective direction (Farquharson & Oldenburg, 1998), enforcing smoothness or continuity in model variations. Depending on the choice of W_i we seek a model that has a minimum parameter variation between adjacent cells or minimum curvature, respectively. ρ_0 and χ_0 are an a-priori models that use to keep the inversion result close to this reference model. α_i is a weights function and C_M is the covariance matrix of the model.

The objective function of the mutual information is represented as:

$$VI(\rho, \chi) = 2H(\rho, \chi) - H(\rho) - H(\chi)$$

with H , Shannon Entropy, defined as:

$$H(\rho) = - \sum_i p(\rho_i) \log p(\rho_i)$$

$$H(\chi) = - \sum_i p(\chi_i) \log p(\chi_i)$$

To ensure that parameters remain within specified limits, they are transformed in generalized parameters ($\rho = \rho(m)$ and $\chi = \chi(m)$). The inverse problem is solved into this generalized space.

Finally, inversion algorithms require the gradient of the objective function, with respect to the generalized model parameters:

$$\frac{\delta\Phi_{Grav(m)}}{\delta\rho(m)} = \frac{\delta\rho}{\delta\rho(m)} \frac{\delta III}{\delta\rho} \frac{\delta t}{\delta III} \frac{\delta\Phi_{Grav}}{\delta t}$$

Term $\delta\rho/\delta\rho(m)$ relates the changes of the objective function with respect to the physical parameters to the generalized model parameters.

Term $\delta III/\delta\rho$ describes how the refined grid changes when one of the parameters on the inversion grid changes.

$\delta t/\delta III$ is the sensitivity matrix for the gravity (and magnetic) data with respect to the refined grid. We adopt the same solution for each terms in the joint inversion:

$$\frac{\Phi_{Joint}(m)}{\delta m} = \frac{\Phi_{Grav}(m)}{\delta\rho(m)} + \frac{\Phi_{Mag}(m)}{\delta\chi(m)}$$

It is also necessary to add the partial derivatives for the VI, with respect to the model parameters ($\delta VI/\delta\rho$ and $\delta VI/\delta\chi$). This can be performed analytically by calculating the respective derivatives for the Gaussian kernel and applying the chain rule to account for the Entropy calculation.

$$\frac{\delta H(\rho)}{\delta\rho_i} = - \sum_{j=1}^N (1 + \log(p(\xi_j))) \frac{\rho_i - \xi_j}{\sqrt{2\pi M\sigma^2}} \sum_{k=1}^N \exp\left(-\frac{(\rho_i - \xi_j)^2 + (\chi_i - \xi_k)^2}{2\sigma^2}\right)$$

The same as performed for $\delta H(\chi)/\delta\chi_i$. Once the partial derivatives for entropy have been calculated, the derivative for VI can be calculated as a simple linear combination.

$$\Phi_{VI} = a \cdot \frac{\delta H(\rho)}{\delta\rho_i} + b \cdot \frac{\delta H(\chi)}{\delta\chi_i}$$

As explained above, also VI is not calculated on the quantities themselves, but on the generalized model parameters. This has the advantage that the input quantities are dimensionless and have comparable variance.

Therefore the final solution proposed is:

$$\frac{\Phi_{Joint}(m)}{\delta m} = \frac{\Phi_{Grav}(m)}{\delta\rho(m)} + \frac{\Phi_{Mag}(m)}{\delta\chi(m)} + \Phi_{VI}$$

This gradient is used to update the inversion model with the L-BFGS algorithm, until a threshold value of misfit is reached.

Chapter 4

Gravity And Magnetic Inversion Applied To Different Case Studies

4.1 Large Scale Inversion (First Article)

The following article was accepted for publication on 13 November 2023, in *Journal of Geophysical Research: Solid Earth*. It is available at the doi: <https://doi.org/10.1029/2023JB027383>. Supporting Information may be found in the online version of the article. The work was presented in several national (GNGTS 2023) and international (EGU 2023: <https://doi.org/10.5194/egusphere-egu23-14551>, IUGG 2023: <https://doi.org/10.57757/IUGG23-1974>.) congress

A new lithospheric density and magnetic susceptibility model of Iran, starting from high resolution seismic tomography

4.1.1 Keypoints

3D Bayesian joint inversion builds a reliable model of the lithosphere in the Iranian collision belt, useful for rheological calculations.

Most of the magmatic and tectonic features can be followed by density variations in the crust, partly extending to the lower crust.

Jointly with the seismic Vs tomography, rigidity is obtained which explains the inhomogeneous distribution of seismicity in the area.

4.1.2 Abstract

We propose a new model for the crust and upper mantle in Iran by joint inversion of gravity and magnetic fields, constrained with a seismic tomography model. We then calculate shear modulus from the Vs velocities and densities. The crust and mantle tomography model is first converted to a density cube through empirical and petrological velocity-density relations. The starting susceptibility is assigned to a two-layer homogeneous model, above a heat flow derived Curie depth. Considering the uncertainties in the density-velocity relations, and the starting layered susceptibility variation, we refine the model by a constrained inversion of the gravity and magnetic fields with a Bayesian approach, producing the final 3D density and susceptibility model. The area is tectonically active with high seismicity and active faulting which are regulated by the crustal density and rigidity variations. Higher rigidity matches lower seismicity and extended deserts and basins, suggesting the control of their development. The Neo-Tethys suture, extending ~1500 km long, as well as the Paleo-Tethys suture match crustal scale density variations, defining characteristics of the lighter Arabian plate and denser

Eurasian crust. The South Caspian Basin is enigmatic, due to focusing of the seismicity along all its borders, but with relatively low average rigidity, which is contrary to what is observed for Iran, where the reduced rigidity correlates with higher seismicity. The 3D density model will be useful for numerical geodynamic models and obtaining geologic inferences from the crustal scale units.

4.1.3 Plain Language Summary

The inversion of potential fields may produce inconsistent results, since there are always multiple models that resolve the anomalies, and the use of other geophysical datasets is necessary. To resolve the problem, we extract information from a high-resolution seismic tomography. With seismic velocities and defining the different layers of the model, using data available in literature, we realize an a-priori model, on which we perform a Bayesian joint gravity and magnetic inversion, to obtain a final 3D model of the Iranian lithosphere, with a detailed distribution of densities and susceptibilities. With density and velocity values, we also calculate the rigidity of the area. We then compare the models obtained, with geological and tectonic information of the area, observing how density and susceptibility distribution reproduces the position of the magmatic outcrops and the principal tectonic lineaments, indicating the position of the Neo- and Paleo-Tethyan sutures. Also, the rigidity model is consistent with the seismicity distribution of the area.

4.1.4 Introduction

Working with gravity data means adopting an open approach to all other branches of geophysics, considering that 3D inversion of a gravity dataset is an ill-posed problem since multiple solutions can reproduce the anomalies and more than one density model can be associated with the solution. To avoid this inconsistency, a multi-disciplinary approach is required, which combines a purely geological knowledge of the area investigated and different geophysical measurements (e.g. seismic and magnetic methods). Thanks to this combination of disciplines, we are able to reconstruct the crustal and lithosphere structure as reliably as possible.

The primary focus of this work is the study of the characteristics of the lithosphere of Iran through a 3D density model derived from a high-resolution seismic tomography model of the Middle East region (Kaviani et al., 2020). The use of seismic tomography is a technique already implemented for density studies and lithosphere modeling (Kaban et al., 2016; Tadiello & Braitenberg, 2021). Here we selected an area that includes the entire Iranian territory, reaching a depth of 105 km. It is an area of broad scientific interest, and many geophysical studies have been conducted (Arkani-Hamed & Strangway, 1986; Babikoff et al., 2022; Kaviani et al., 2018, 2022; Maggi & Priestley, 2005; McKenzie, 2020; Molinaro, 2004; W. Wei et al., 2019), because of its central position in the collision zone between the Eurasian and Arabian plates. An approach inverting or forward modelling the gravity field, geoid and local isostatic equilibrium considering the density dependence on temperature has been made by Motavalli-Anbaran et al. (2016) and references therein. McKenzie (2020) observes that most part of the Middle East region has a relatively small lithosphere thickness, which reaches maximum values of 70 km. Irandoust et al. (2022a) detect a pattern with low velocity along the Zagros mountains, which indicates the underthrusting of the Arabian plate beneath the Iranian platform.

The extreme structural complexity and the presence of numerous faults makes the area seismically very active. In his quantitative analysis, Raeesi et al. (2017) identified 11 faults in the mature stage of the seismic cycle, located in the northern and eastern parts of Iran. They also report 4 seismically mature regions in southern Iran and 4 additional fault segments potentially active even without a big sign of maturity.

One open question regards the reasons for the extreme inhomogeneity of the spatial distribution of seismicity observed in the region, which we study in terms of correlation with the density structure of the crust. The density together with the seismic velocity is a means to calculate

the elastic rigidity, which in turn is the parameter that together with the bulk modulus controls the strain response to tectonic stress. A further question relates to the directions of faults in Iran which take up well defined homogeneous orientations in tectonic units or between tectonic and geologic blocks, and which must be guided by rheologic inhomogeneities that we find to correlate with the density structure. A third question we address is whether the important sutures which have been defined in Iran can be associated to crustal or lithospheric scale transitions across the sutures, identifying the properties and extents of the original fragments. The sutures demonstrate the amalgamation of lithospheric fragments detached from Gondwana, which were dislocated from the Gondwana margin through the opening and closure of oceanic basins, as the Paleo and Neo-Tethys. The high spatial resolution of the final density model (25 km), achievable particularly for the upper crust compared to the tomographic seismic model, allows to considerably improve understanding of the mentioned problems and acquire new insights.

To exploit gravity and magnetic data we use a joint Bayesian inversion algorithm. This approach needs, as starting point, a-priori information about density and magnetic susceptibility distributions. To build this starting model, we use known empirical and experimental relations (Brocher, 2005) and techniques for the conversion from velocity to density within the crust, while we exploit petrological properties for the upper mantle. The starting susceptibility is a homogeneous layer above the Curie depth. The inversion delivers a final model of the Iranian lithosphere, with the distribution of densities and susceptibilities, which suggests valid geologic and geodynamic interpretations.

4.1.5 Geological setting

The collision zone of Arabia-Eurasia in Iran is part of the Alpine-Himalayan orogenic belt which began forming in late Eocene (Ballato et al., 2011; McQuarrie & van Hinsbergen, 2013) and intensified in Miocene (McQuarrie & van Hinsbergen, 2013). The factors controlling the kinematics of the area have been diverse in time, like the extension of the Mediterranean Sea and the rifting of the Red Sea and the Gulf of Aden, or the different stages of opening and closure of the Paleo- and Neo-Tethys oceans (Irandoost et al., 2022a; R. Zhu et al., 2021). Presently the tectonics is driven by the northward movement of the Arabian plate relative to the Eurasian plate, leading to high rates of seismicity (Raeesi et al., 2017), including destructive events as the Turkey-Syria earthquake of February 2023 (Barbot et al., 2023), or the 2003 Bam earthquake in South East Central Iran (Nadim et al., 2004). Iran has a complex structure, outcome of the amalgamation of blocks of different ages and formed due to different geologic events, including collision of lithospheric plates, and subduction of continental and oceanic lithosphere (Agard et al., 2011; Ballato et al., 2011). The Central Iranian territory (Fig. 4.1.1) is boarded, from a structural point of view, at south-west by the Zagros orogen, at south by the Makran oceanic subduction zone, and north by the Alborz and Kopeh-Dagh orogenic belts, and east by the Sistan Suture zone, which marks the transition to the Afghan Block (Irandoost et al., 2022a). The ongoing convergence between the Eurasian and Arabian plates is estimated from GPS at a present rate of ~ 22 mm/yr, and is accommodated by northwards shortening within the Zagros, Central Iran, Alborz, and relative movement of the South Caspian Basin and movement along strike slip faults of different orientations, according to the region (Vernant et al., 2004). Deformation of the Iranian orogenic belts is presumably guided by variations of crustal rigidity and the presence of rigid blocks, a question which we address in this work. We identify different geological provinces and blocks in the study area (Gharibnejad et al., 2023; Irandoost et al., 2022a; Rabiiee et al., 2019) shown in the Figure 4.1.1. We briefly describe the principal properties of these provinces in the next subsections.

Zagros orogenic belt

The Zagros orogenic belt separates the Iranian domains on the Eurasian plate, from those on the Arabian plate. It is part of the much larger Alpine - Himalayan orogenic system and extends from the northwestern Iranian border to southeastern Iran, from the East Anatolian strike-slip fault to the Oman Line (Alavi, 2007; Mouthereau, 2011). It is divided into three different parallel tectonic zones which are, from the northernmost, the Urumieh-Dokhtar Magmatic Arc (UDMA), the Sanandaj-Sirjan Zone (SSZ), and the Zagros Fold-and-Thrust Belt (ZFTB). UDMA is the most internal part of the orogen. It is a magmatic system composed of both intrusive and extrusive rocks in correspondence with the back-arc area of the Neo-Tethys oceanic lithosphere subduction. The oldest rocks are Early Cretaceous, while the youngest mainly include recent lava flows and pyroclastic layers (Alavi, 2007). The SSZ forms the boundary of the Eurasian plate. It is mainly composed by both sedimentary and metamorphic rock facies, with rocks that were transported in a period from the Paleozoic to the Cenozoic by the thrust system (Alavi, 2007; Mouthereau, 2011). In the SSZ we find the suture line due to the closure of Neo-Tethys ocean, crossing the province from north-west to south-east. Last, the ZFTB is the southern and outermost part of the orogen, and it is underlain by the basement of the northeastern margin of the Arabian plate. It is the part that in the zone accommodates a good percentage of the continental plate movements, with the presence of numerous strike-slip and thrust faults along the belt.

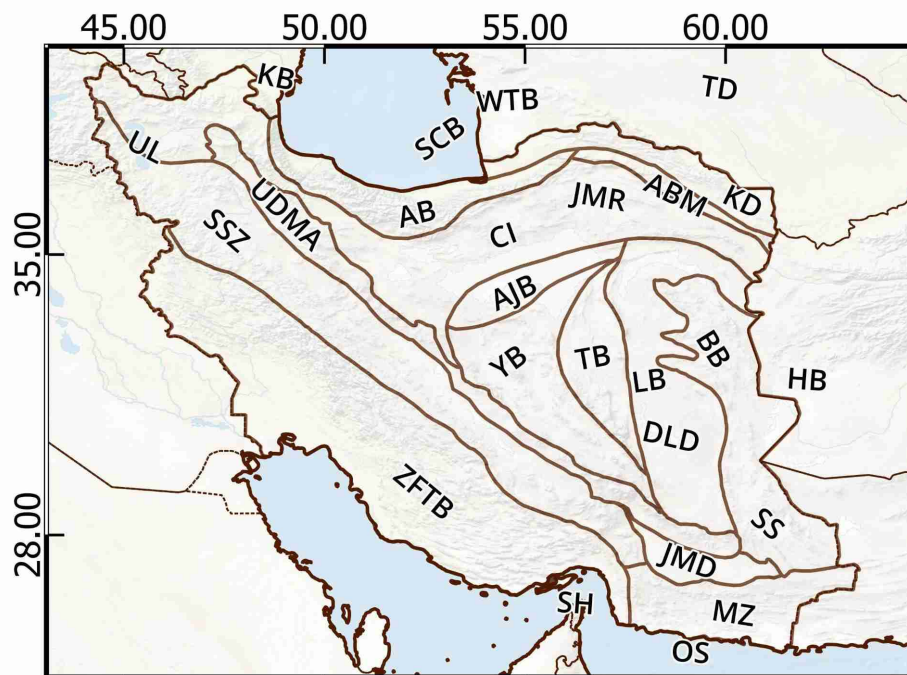


Figure 4.1.1: Geological provinces of Iran and principal blocks, extracted from Rabiee et al. (2019), Gharibnejad et al. (2023) and Irandoust et al. (2022a). AB: Alborz Belt; ABM: Aladagh-Binalud Mountains ; AJB: Anarak-Jandagh Block; BB: Birjand Block; CI: Central Iran; DLD: Dash-e Lut Desert; HB: Helmand Block; JMD: Jaz Murian Depression; JMR: Jaghatai Mountain Range; KB: Kura Basin; KD: Kopeh-Dagh; LB: Lut Block; MZ: Makran Zone; OS: Oman Sea; SCB: South Caspian Basin; SH: Strait of Hormuz; SS: Sistan Suture zone; SSZ: Sanandaj-Sirjan Zone; TB: Tabas Block; TD: Turan Depression; UDMA: Urumieh-Dokhtar Magmatic Arc; UL: Urmia Lake; WTB: West-Turkmenistan Basin; YB: Yazd Block; ZFTB: Zagros Fold-and-Thrust Belt. Outlines of the geologic provinces in brown, national borders: dark brown stippled lines. Shaded topography here and in other figures made with Natural Earth. Free vector and raster map data (<https://www.naturalearthdata.com/>)

Alborz belt

The Alborz belt (AB) is a tectonically active orogen that extends in northern Iran from the Lesser Caucasus southwards and wraps around the southern South Caspian Basin (SCB). According to different studies (Şengör et al., 1988; Stöcklin, 1974) the belt formed through the Cimmerian orogeny which affected parts of Cimmeria separated from Gondwana and collided with the Eurasian plate during the Triassic. The evidence of this collision is the Paleo-Tethys suture which separates the belt from the SCB (Guest et al., 2006), while the presence of Paleocene folds and faults are explained by the accommodation of compressional events occurred during the closure of the Neo-Tethys along the Zagros suture (Guest et al., 2006). In the suture area the presence of pre-Jurassic metamorphosed ophiolites and deep-sea sediments, deformed by intense thrusting and folding, and partially covered by Cenozoic strata has been defined (Alavi, 1996). Main faults are thrusts at the northern and southern external domains of the Alborz range, indicating double vergence, southwards/northwards dipping at the northern/southern domains, respectively. Inside the range vertical left lateral strike slip faults dominate. The strain displacement along the faults is estimated to vary between 2 and 7 mm/yr according to the location and fault mechanism (Ballato et al., 2011; Djamour et al., 2010; Rashidi et al., 2023).

East Central Iran and Sistan suture zone

East Central Iran has been defined as a microcontinent (ECIM), comprised of the Anarak-Jandagh Block (AJB), Yazd Block (YB), Tabas Block (TB), and Lut Block (LB) (Gharibnejad et al., 2023). Towards east the ECIM is separated by the Sistan Suture Zone (SS) from the Afghan Block or microcontinent, also termed Helmand Block (HB) (Irandoost et al., 2022a) (see Figure 4.1.1). The Sistan suture on east Iran formed as an accretionary complex from the closure of the Neo-Tethyan ocean basin, which extended in north to south orientation between the Lut Block and the Afghan microcontinent. The suture extends NS for 700 km and forms the border between Iran and Afghanistan and Pakistan. The suture is post-Cretaceous and includes melanges of ophiolitic rocks emplaced in schistose rocks. Of relevance for the density modeling is the documented presence of high density rocks as gabbros, basalts, and slabs of ultramafic and mafic rocks, and eclogite or amphibolite (Bröcker et al., 2022). The geochronology of the metamorphism and post-metamorphic intrusions, and the age of the protolith gabbro are discussed in Bröcker et al. (2022). Documented ophiolites line the western margin of the Lut Block (Saccani et al., 2010). The center of the Lut Block hosts the Dash-e Lut desert (DLD). Strike slip faulting with highly destructive earthquakes characterizes the eastern and western margins of the Lut Block, generally with strike slip faulting. The Lut Block is described based on geologic observations of faulting as a rigid block, limited to the east by the Nehbandan fault system which overprints the Sistan suture. At the western margin the Lut Block is separated from central Iran by NS or NNW-SSE trending right lateral fault systems (Rashidi et al., 2019). The extremely active seismicity struck with 7 earthquakes with magnitude $M > 6$ in the short time period between 1981 and 2011, which includes the destructive M 6.5 Bam earthquake of 2003 (Rashidi et al., 2019). We shall quantitatively ascertain if the rigidity variation can be shown from the density and seismic models.

Makran subduction zone

The Makran subduction zone (MZ) is a 1000 km long belt bounding the southern border of the Eurasian plate, beyond the southern end of the Zagros belt. In this area the subduction of the Oman oceanic crust occurs. Makran has an W-E trend and is delimited on both sides by two N-S transform fault systems: to the west the Minab Fault (MF), which separates the oceanic subduction from the continental collision between the Arabian and Eurasian plates; to the east the Chaman fault system (CF) (Fig. 4.1.2), which separates the Eurasian and Indian plates, being an important fault continuing northeastwards (Abdollahi et al., 2018). We can

identify five different geological units into which we can divide the belt, each one separated by major thrust zones. These are from the north to the south the North Makran, the Inner Makran, the Outer Makran, the Coastal Makran, and the offshore Makran (see Abdollahi et al. (2018)). Main differences are between the North Makran which preserves remnants of the period before the beginning of the subduction, and the central parts of the belts which have sedimentary layers resulted from the Eocene subduction. The North Makran hosts the Jaz Murian Depression (JMD, see Figure 4.1.1). We report also the presence of a volcanic belt in the northernmost part of Makran area with a SW-NE trend of the three main volcanic centers, which are in order the Bazman, Taftan and Sultan volcanoes (Fig. 4.1.2). These volcanoes are the youngest representation of the arc-related volcanism, still active in Iran (Abdollahi et al., 2018).

Iranian magmatism

Magmatism related to the recent geologic history as well as to the subduction of the Neo-Tethyan ocean lithosphere is present in Iran (Omidiyanfar et al., 2023). Mostly the magmatism is Cenozoic, and we can divide the principal outcrops present into three different magmatic belts: the Urumieh–Dokhtar Magmatic Arc (UDMA), the Alborz Magmatic Belt (AMB), and the Sistan Magmatic Belt (SMB). About UDMA we have already discussed in the previously chapters. It is one of the principal component of the Zagros belt, directed from north-west to south-east, composed by calc-alkaline rocks. For this reason it is interpreted like an Andean-type magmatic arc, following the Neo-Tethyan subduction (Chiu et al., 2013). SMB is a magmatic area in the east of Iran, crossing Lut Block and Sistan Suture zone. Rocks within the SMB include magmatic intrusive rocks from Jurassic and Late Cretaceous, and Late Cretaceous lavas (Chiu et al., 2013), while Cenozoic lavas and rocks form a massive magmatic sequence. Magmatism is not directly related to the Lut-Sistan collision, but could be the result of Eocene-Oligocene asthenospheric upwelling (Pang et al., 2013). The AMB has its origins from the collision of Iranian Block with the Eurasian plate, which continues in the present days with the on-going intra-continental deformation caused by the convergence of the Arabian and Eurasian plates (Castro et al., 2013). It consists mainly in Precambrian to Eocene volcanic successions, intruded by Mesozoic to Cenozoic plutons (Castro et al., 2013). To make final considerations we use the catalogue of the magmatic outcrops from USGS (Pollastro et al., 1997), shown in Figure 4.1.2.

4.1.6 Geophysical data

Regional Velocity tomography model

The 3D shear wave velocity (V_s) model of Kaviani et al. (2020) is the dataset used for calculating the starting crustal density model, obtained from the velocity to density conversion based on given empirical and physical equations, as explained below. The velocity model was obtained from group-velocity dispersion curves analysing continuous seismic ambient noise from 709 broad-band stations, mainly distributed in the Turkish and Iranian territory, and regional earthquakes from 143 permanent broad-band stations of the Saudi National Seismic Network. On the Arabian Peninsula continuous seismic ambient noise records were not available, so here the earthquake records contributed most to improving ray coverage across the area (Kaviani et al., 2020).

Datasets resulting from ambient noise and earthquakes records overlap in the period range 8 – 75 s, in the Saudi Arabia ray paths. To avoid problems due to the proximity of the measurements, all the analogous paths have been grouped and considered like single ones (Kaviani et al., 2020). Group-velocities have been then inverted to obtain a depth-dependent shear wave (V_s) model, performing the inversion for periods between 2 and 150 s. For all the other aspects of the tomography and the detailed information regarding the inversion technique used, we refer to Kaviani et al. (2020). From the tomography velocity model, we select our area of study,

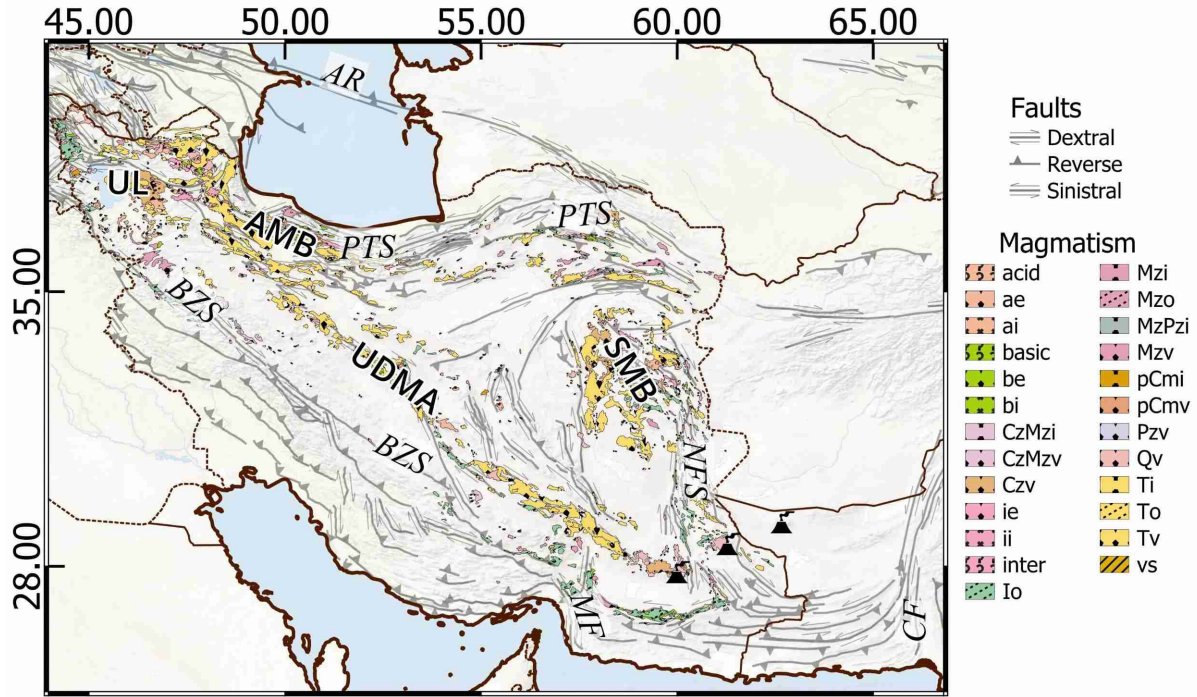


Figure 4.1.2: Iranian magmatism (AMB: Alborz Magmatism Belt; SMB: Sistan Magmatism Belt; UDMA: Urumieh–Dokhtar Magmatic Arc) and principal faults (AR: Aspheron Ridge; BZS: Bitlis–Zagros Suture; CF: Chaman Fault; MF: Minab Fault; NFS: Nehbandan Fault System; PTS: Paleo–Tethys Suture) previously described. With the volcano symbol we indicate the position of the three main volcanoes in the Makran Zone (from south–west to north–east: Bazman Volcano; Taftan Volcano; Sultan Volcano). For the information about the legend relative to the magmatism, we refer to Pollastro et al. (1997). Faults database from Styron and Pagani (2020).

using a bounding box of 25° by 40° N in latitude, and of 44° by 63.4° E in longitude (Fig. 4.1.3). Spatial resolution used for our final model is 0.2° (~ 22 km), while maximum depth reached is 105 km, with a variable vertical resolution that starts from a minimum of 1 km in the first 60 km, then gradually increases to a maximum of 7 km in the deepest part. For details regarding the vertical resolution and the rest of the model, we refer to the “readme” file of the model.

Gravity and magnetic data

The gravity field used to perform the Bayesian inversion of the lithospheric density cube is calculated using the model XGM2019e (Zingerle et al., 2020). It is a global gravity field model developed by the Institute of Astronomical and Physical Geodesy of the Technical University of Munich, and represented in spheroidal harmonics up to maximum degree and order (d/o) of 5399. This high d/o guarantees a nominal final spatial resolution of 2 arc min (~ 4 km). Basically, it is a combined model, composed by the satellite model GOCO06s (which collects data from GOCE and GRACE missions) to cover degree and order up to 300, and by two different ground gravity datasets, a 15 arc min (~ 28 km) and a 1 arc min (~ 2 km) augmentation dataset, to resolve the shorter wavelengths. The first, developed by NGA (US National Geospatial-Intelligence Agency), is for land and ocean gravity observation and is limited to d/o 719; the second one is derived from altimetry and topography observations, and is used for the high-resolution of the model, resolving the band from d/o 719 up to 5399. Consequently in our study we limit the maximum d/o to 719, corresponding to 27 km half-wavelength resolution (Barthelmes, 2013), coherently with the spatial resolution of our 3D volume of 0.2° . Starting from the XGM2019e model we compute the Bouguer anomaly exploiting the rock equivalent topography model dV_ELL_RET2014_plusGRS80 (Rexer et al., 2016). The spherical harmonics

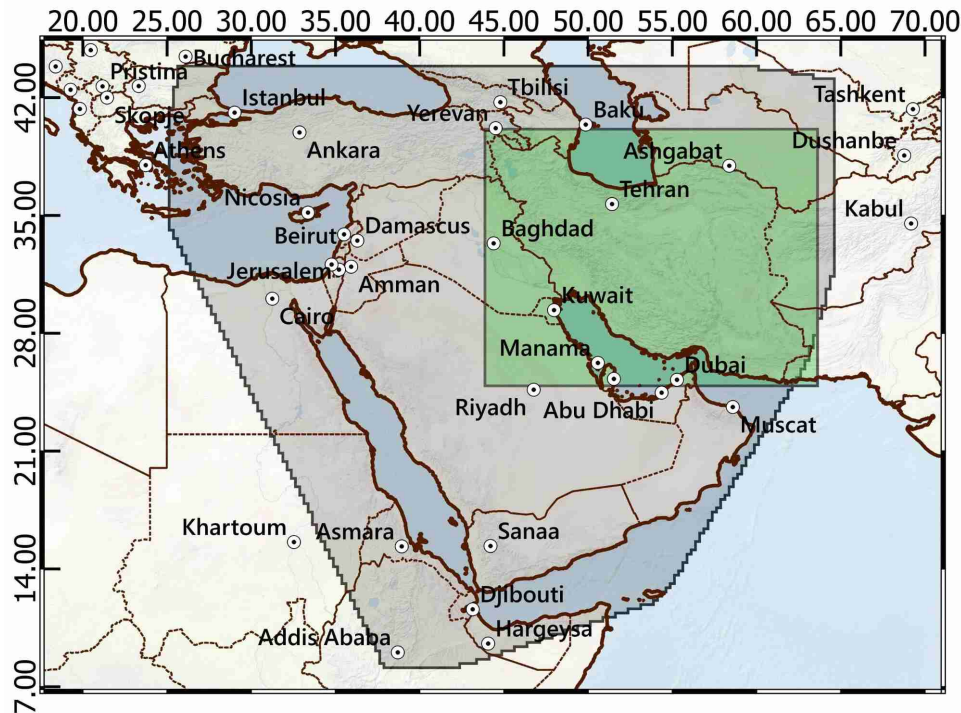


Figure 4.1.3: Map with the area covered by the regional tomography (black area). The green box is the area selected for this work.

coefficients of the models have been retrieved from the ICGEM web server (Ince et al., 2019). The gravity field was calculated at the height of 4000 m above the ellipsoid. The gravitational effect of the deep mantle has been also removed by considering only spherical harmonic degrees larger than 12 accordingly to Tadiello and Braitenberg (2021). Regarding the magnetic field, we use the global model EMAG2v3 (Meyer et al., 2017) as observable, developed by NOAA National Center for Environmental Information. It was realised with the combination of satellite and magnetic observatory data, and airborne and marine magnetic measurements, with a resolution of 2 arc min (~ 4 km), at an altitude of 4 km above the geoid. Differently from previous models this grid is based only on interpolation of observed data, and does not use a-priori information about geologic structure or ocean bottom age. This because it has been observed that in the other global magnetic anomaly grids this inclusion forced artificial linear patterns (Meyer et al., 2017). In Figure 4.1.4 we can see the final maps of the two datasets. For further information about the two models we refer to the cited articles.

Sediment thickness, Curie depth models and magnetic susceptibility distribution

In the inversion methodology we pursue, a division of the starting model into different layers is required, each one with its characteristics and values. Leaving aside for a moment the Moho discontinuity, and focusing inside the crust only, we decide to divide the model into four different layers. These crustal layers are the sedimentary basin and the crystalline crust, divided by the basement depth surface, and the magnetized and non-magnetized crust, separated by the Curie surface. To our best knowledge, an exhaustive and resolute sediment thickness model for the entire Iran is not publicly available to date. We have found localized sediment thickness models for limited areas, but an integration to formulate a comprehensive sediment thickness model was not feasible. We therefore adopt a thickness model defined by seismologic investigations, where a seismologic V_s velocity value of 3.1 km/s was used to define the basement depth variations (Irandoost et al., 2022b). Regarding the depth of the Curie surface, we choose to use the one proposed by Mousavi and Ardestani (2023), who define a 3D surface heat flow

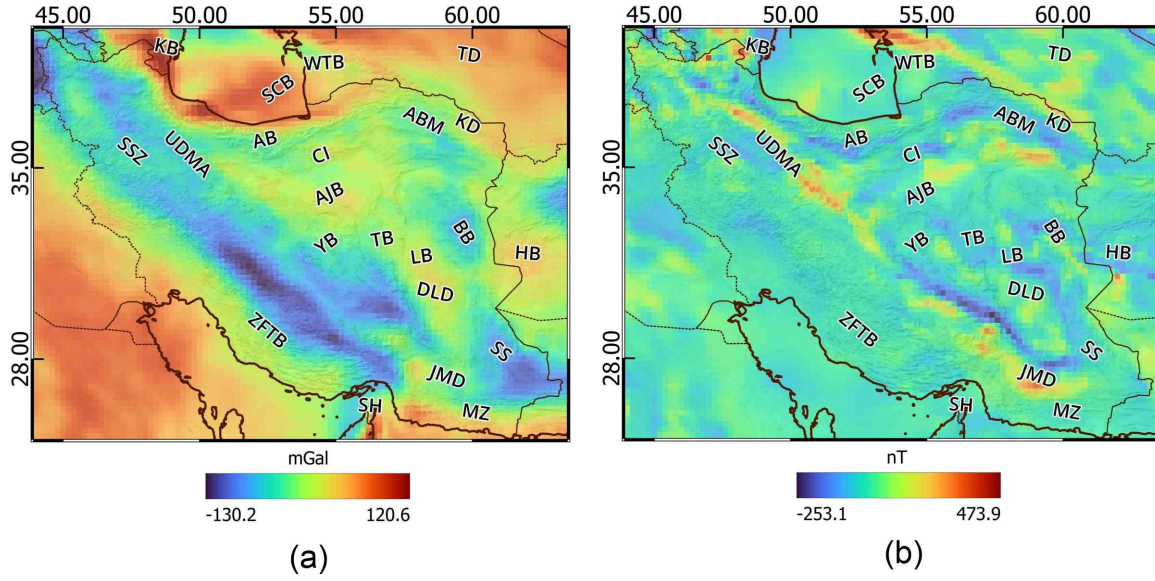


Figure 4.1.4: Bouguer Gravity anomaly reduced for the deep mantle gravity contribution (Rexer et al., 2016; Tadiello & Braitenberg, 2021; Zingerle et al., 2020) (a) and Total Magnetic field anomaly (Meyer et al., 2017) (b) observations for the final inversion. The acronyms are defined in the caption of Figure 4.1.1.

model in Iran, derived and calculated by geophysical and petrological observations, and who then extract the Curie surface corresponding to the depth of the nodes on the isotherm at 580 °C. Figure 4.1.5 shows the maps of the two surfaces used with the relative depths.

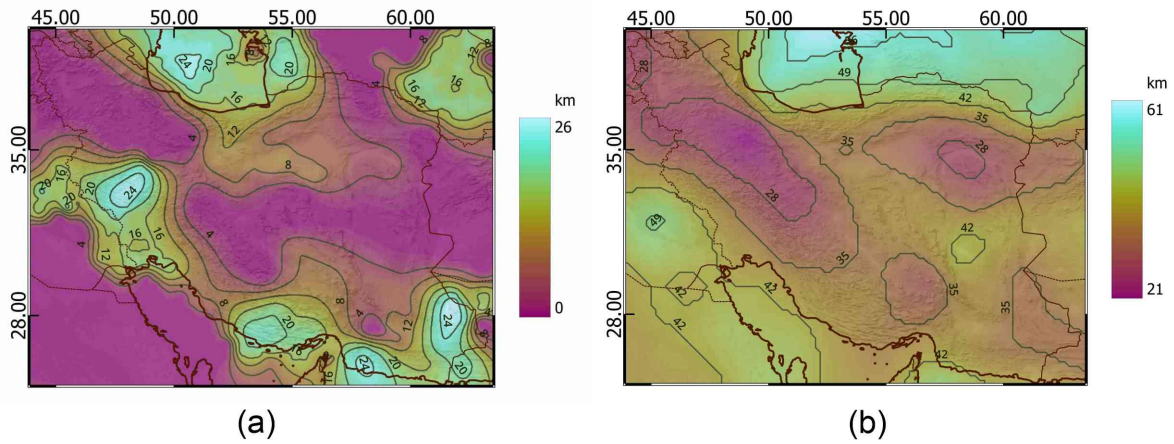


Figure 4.1.5: Depth of base sediment (a) and Curie depth (b) layers used in the realisation of the starting model.

With the magnetized crustal layer, it was necessary to suppose a magnetic susceptibility distribution. In detail, in absence of direct information about the possible magnetic susceptibility of crust and sediments in the area, we consider a constant average value of 0.018 SI for the former (derived from Hemant and Maus (2005)) and of 0.005 SI for the latter (Hunt et al., 1995). Modeling the Moho discontinuity, as will be described in the next chapter, we encountered intersections between the crust-mantle transition layer calculated and the available Curie surface. We decided to add a magnetized layer in the mantle, to which we assigned a starting susceptibility value in the a-priori model of 10^{-5} SI.

4.1.7 Methods

A multidisciplinary approach is adopted to solve the problem of defining the density structure for Iran and surrounding areas. In this section we explain all the processing stages starting from the initial tomographic dataset and arriving to the new model of the Iranian lithosphere. The first step (step 1) is to fill void pixels in the regional velocity model aimed to obtain a regular 3D grid, with which we define a new map for the depth of the Moho (step 2). The calculated Moho is then used to divide the voxels of the velocity cube which are in the crust, from those that are in the mantle. This distinction is used in the third and fourth steps, namely in the velocity to density conversion, which requires different methodologies in crust (step 3) and mantle (step 4). Step 5 begins with the addition of mean susceptibility to the magnetized crust and magnetized mantle layers and continues with the Bayesian 3D inversion from which we obtain the final model of the Iranian lithosphere. To conclude we also use the final inverted model and starting velocity tomography to calculate the shear modulus in the area (Fig. 4.1.6).

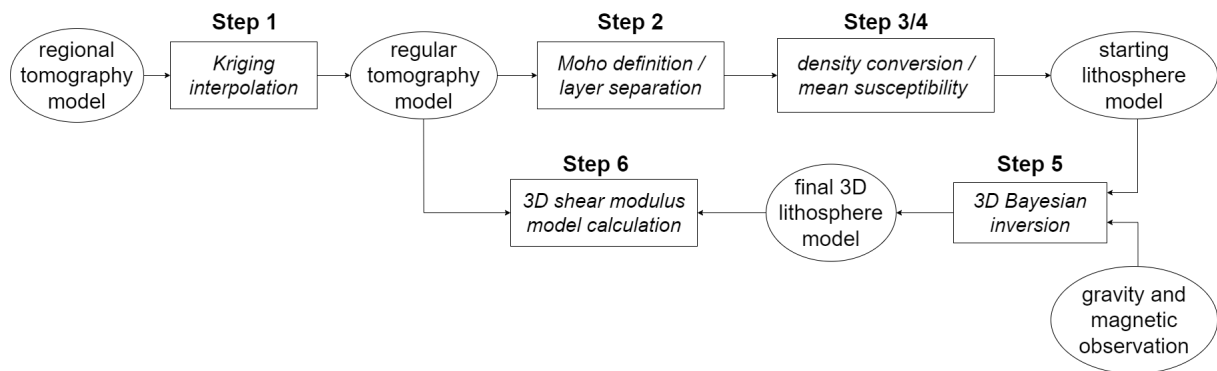


Figure 4.1.6: Flowchart of the processing operations.

Regional tomography interpolation on regular grid through Ordinary Kriging

The first problem faced during the processing is that the Kaviani tomography model (Kaviani et al., 2020) contains cells with no values, which gives the model an irregular shape, difficult to process. To resolve this problem, we operate with a geostatistical approach, interpolating the regional tomography on a regular grid with a resolution of 0.2° applying an Ordinary Kriging technique (Wackernagel, 1995). In detail, a set of bi-dimensional interpolations, one for each height of our model, has been performed. The empirical variograms are modelled with a "Stable" function (Wackernagel, 1995). The result of the interpolation, for one slice, is shown in Figure 4.1.7.

Moho undulation (Gradient Method)

The interpolated velocity cube is analysed to define the depth of the Moho discontinuity. The chosen method studies the vertical gradient of the seismic velocity model (Kaviani et al., 2020; Tadiello & Braitenberg, 2021), seeking the largest vertical velocity gradient in the velocity interval identified as typical for the region above and below the Moho. First, we conduct a velocity analysis using the global tomography of Simmons et al. (2015), where the Moho depth has been published on a grid spacing of 1° , to define the mean shear wave velocity at the Moho transition of the area. This analysis constrains the depth of the Moho to be located in a range of V_s velocities from 3.87 km/s to 4.57 km/s. We therefore consider this range of variability as the set of velocities to be further investigated to define our Moho map. Then, for each node of the area, we define the depth with the maximum vertical velocity gradient, calculated in the range proposed. The depth of the node with maximum gradient is associated to the Moho depth. From this analysis we find an evident similarity between the resulting Moho and the

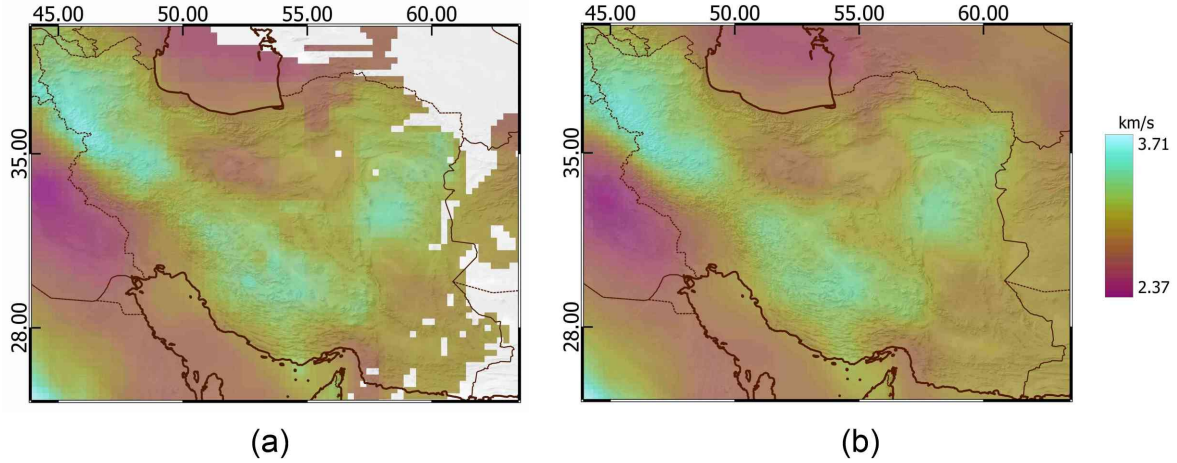


Figure 4.1.7: Example Vs tomography slice (5 km) that illustrates the performance of the Kriging interpolation. On the left the slice from the starting cube (a), on the right the result after the interpolation (b).

Moho proposed by Kaviani et al. (2020), mainly due to the similarity of the techniques used to derive the depth, both based on the velocity vertical gradient (Fig. 4.1.8). We prefer using the recalculated Moho depth as it is consistent with our re-interpolated velocity model.

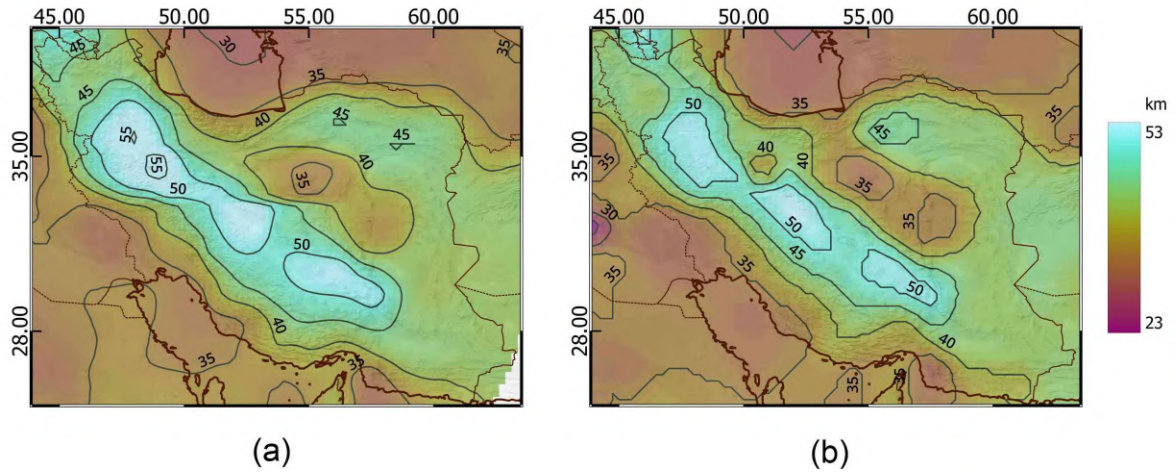


Figure 4.1.8: Moho depth proposed by Kaviani et al. (2020) (a) and recalculated from the tomography model through the maximum gradient method (b).

Vs-velocity to crustal density conversion

The above mentioned Moho depth allows us to separate the velocity cube into two main layers: crust and mantle. This division is necessary for the velocity to density conversion in crust and mantle separately, since the two conversions require different methods. Considering the crust, numerous equations have been proposed, most of which convert density from body waves (V_p). Therefore, it is necessary to first convert V_s from our cube into V_p , using the “Brocher’s regression fit” (Eq. 4.1) proposed by Brocher (2005), valid for V_s between 0 and 4.5 km/s, for crystalline and sedimentary rocks, estimated from boreholes and laboratory data.

$$V_p (km/s) = 0.9409 + 2.0947V_s - 0.8206V_s^2 + 0.2683V_s^3 - 0.0251V_s^4 \quad (4.1)$$

For the density conversion from V_p , we consider the polynomial relation (Eq. 4.2) defined by Brocher (2005), based on the “Nafe-Drake curve” theorized by Ludwig et al. (1970), who empirically found the parameters for the conversion valid for V_p between 1.5 and 8.5 km/s. The result is the following relation, which returns density values in g/cm^3

$$\rho (\text{g/cm}^3) = 1.6612V_p - 0.4721V_p^2 + 0.0671V_p^3 - 0.0043V_p^4 + 0.000106V_p^5 \quad (4.2)$$

We find that the above equation can be suitably reduced to a fourth order polynome, without loss of representativity of the experimental laboratory data reported in Brocher (2005). We repeat Brocher’s best fit on his data using the Least Square method and we investigate the minimum polynomial order explaining the data by means of statistical inference. In detail, we ask ourselves whether, with a significance level of 95%, the hypothesis that each estimated coefficient of the polynomial is different from zero is satisfied (details about this statistic test can be found in Cazzaniga (2008)) (Fig. 4.1.9).

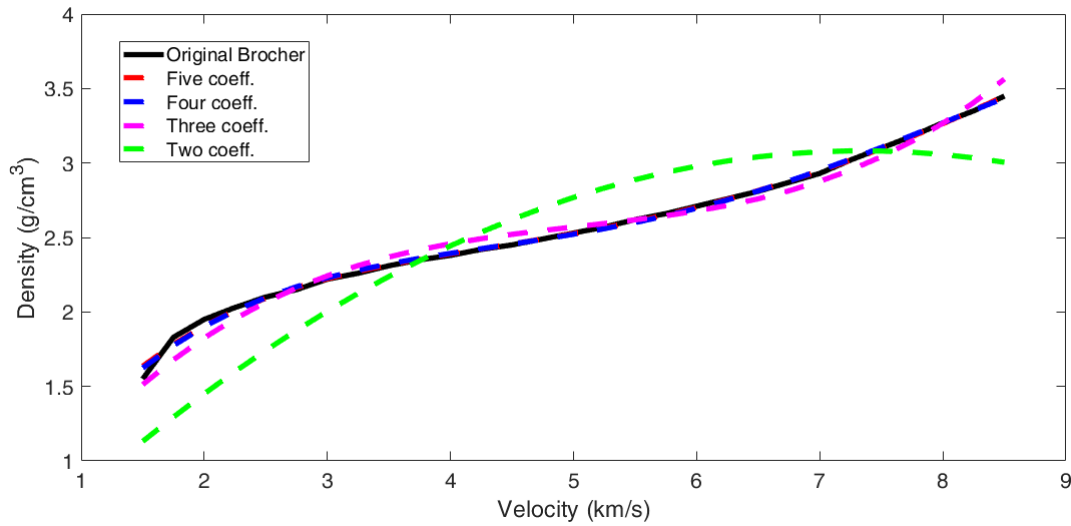


Figure 4.1.9: Test of Brocher’s relation (Brocher, 2005) with different number of polynomial coefficients. We find the best fit parameters, for equations from fifth to second order by computing Fisher test and calculating the acceptance degree of the new equations.

It turns out that, with the above confidence level, the fifth order polynomial and the fourth order one are statistically equivalent. We therefore choose to use the fourth order polynomial, defining a new relation equally valid for the velocity-density conversion.

$$\rho (\text{kg/m}^3) = (1.6026V_p - 0.4164V_p^2 + 0.0493V_p^3 - 0.0020V_p^4) * 1000 \quad (4.3)$$

This last equation (Eq. 4.3) returns density values in kg/m^3 , and is used for all the crustal density conversion steps.

Mantle modeling (Perple_X)

The modeling of the mantle density requires another approach compared to the crustal modeling, due to the fact that the empirical relation of Brocher (2005) and therefore our Eq. 4.3 are limited to crustal velocities and rocks. We compare the mantle velocities from tomography with synthetic upper mantle velocities and densities calculated with the open-source software

Perple_X (Connolly, 2005). Perple_X is a collection of FORTRAN programs used for the calculation of phase equilibrium diagrams minimizing Gibbs free-energy to map the phase relations (Connolly, 2005). The necessary starting point is a specified rock compositional model: for the selected zone, we take it from Tunini et al. (2014) assuming a standard mantle chemical composition expressed according to the NCFMAS system (Na_2O - CaO - FeO - MgO - Al_2O_3 - SiO_2), derived from global studies (Griffin et al., 2009).

Table 4.1.1: Mantle chemical composition used for the modeling

Na_2O	CaO	FeO	MgO	Al_2O_3	SiO_2	Total
0.13	1.90	7.90	41.60	2.00	45.20	98.73

In Table 4.1.1 the percentage of the elements used to build the model are shown. The software requires a few calculation parameters which we describe here. The thermodynamic model refers to Holland and Powell (1998), which is the default, and results in phase equilibria and elastic properties. Further necessary for the processing is the computation setting without saturated fluids or components, and the use of chemical potentials, activities or fugacities as non-independent variables. Pressure and temperature are considered as independent from each other. We calculate the phase diagram in a range between 0.1 GPa to 7 GPa for pressure, and from 500°C to 1300°C of temperature. For the description of the default thermodynamic model and further computational details, we refer to the software documentation. At the end the result is an equilibrium phase diagram, showing the stability fields for different minerals, depending on pressure and temperature. The software is also able to return several thermodynamic parameters, derived from the calculated phase diagram. From it we extract synthetic seismic velocity and density values, related to a specific combination of pressure, temperature, and chemical composition. To derive the densities which we then use in the starting model, we compare the seismic velocities obtained from Perple_X with the velocities in the tomographic model, using pressure values calculated at the given depth. The comparison gives also information on the temperature, since the synthetic velocities are both pressure and temperature dependent. We start calculating the pressure at the Moho depth using the crustal densities previously defined, and then continue for greater depths in the mantle using the synthetic densities. At the end we match mantle velocities calculated by the software with the velocities from the tomography to obtain the calculated mantle densities, relative to the tomographic depths.

Lithosphere model (Bayesian Inversion)

Since the geometries as well as the density and susceptibility distributions of our 3D volume show large uncertainty due to the different hypotheses and approximations presented above, we exploited potential field data to improve our initial model. As outlined at the beginning of Section 4.1.7, the result of the previous steps together with the data reported in Section 4.1.6 are used to create an initial three dimensional geological model, characterised by several layers (namely sediments, magnetised and non-magnetised crust, magnetised and non-magnetised mantle) each one with its own density and magnetic susceptibility distribution. For all these quantities we also define ranges of variability by means of a careful analysis of the available literature on the area (Irandoost et al., 2022b; Kaviani et al., 2020; Mousavi & Ardestani, 2023; Mousavi & Ebbing, 2018) and considering the uncertainties in the starting seismic velocity model and in the conversion to density: density and susceptibility range of variability used have values of $\pm 30 \text{ kg/m}^3$ and $\pm 0.005 \text{ SI}$ for the sediments layer, $\pm 50 \text{ kg/m}^3$ and $\pm 0.018 \text{ SI}$ for crust layer, and $\pm 20 \text{ kg/m}^3$ and $\pm 10^{-5} \text{ SI}$ for the mantle layer, while considering the surfaces variability, we adopt values of $\pm 12.4 \text{ km}$ for the basement, $\pm 8 \text{ km}$ for the Curie, and $\pm 15 \text{ km}$ for the Moho depths. We use the joint Bayesian inversion described in Sampietro et al. (2022) and Sansó and Sampietro (2021) to modify this initial model in such a way that its gravity and

magnetic responses fit the observed potential fields, but always preserving the original intrinsic characteristics of the model. In other words, the algorithm, which has already been tested in several synthetic and real case studies such as Capponi et al. (2022), Sampietro and Capponi (2023), and Sampietro et al. (2023), modifies at the same time the initial geometries and the distribution of density and susceptibility values, within the confidence intervals of the a-priori model to fit the observed gravity and magnetic anomaly data. For a more detailed description about the Bayesian inversion algorithms, we refer to the supplement materials and to the above references.

Shear modulus calculation

The inversion produces the final model of the lithosphere in Iran, with density and susceptibility values. These final cubes, joined to the starting tomography, allow to calculate the elastic shear modulus, and therefore investigate the rheology of the area. The equation relating shear wave velocity and density values, allows the calculation of the shear modulus as follows:

$$\mu = V_s^2 \rho \quad (4.4)$$

We express the shear modulus by the product of the square of the shear wave velocity tomographic model and the final density model (Eq. 4.4). With this simple equation we are able to obtain a 3D model of the lithosphere rigidity.

4.1.8 Results

We now show the inversion results, starting to quantify the reliability of the final model with the residual maps. In Figure 4.1.10 the residuals after the Bayesian inversion are plotted, calculated from the differences between the gravity and magnetic fields used as observations, and the gravity and magnetic fields generated by the final model. Considering the two maps, our final model fits gravity data with a standard deviation of ~ 7 mGal and the magnetic data with ~ 15 nT. Almost all anomalies are resolved by the model, even if some localized anomalous high-residual patterns remain. These can be explained by the presence of density and susceptibility superficial bodies (in the first 10 km), not defined in the a-priori model and therefore undetectable from our inversion. To verify this condition, we perform some tests starting from the obtained final model trying to invert only the first 10 km, in order to define what the amount of density and susceptibility variations would be required to explain the Bayesian residuals. This estimate is to be considered in general terms only, as a detailed inversion of these upper structures would require having more constraining data. This second simplified inversion solves all the residuals (reducing their standard deviation to less than 1 mGal and 4 nT for the gravity and magnetic field respectively) identifying the presence of different superficial bodies. These density variations reach up to ~ 150 - 200 kg/m³ in localized extreme spots. The same condition is valid for the magnetic residual, almost entirely solved by the presence of two isolated magnetized bodies (~ 0.04 - 0.06 SI). Maps of the estimated density and susceptibility distributions are reported in the Supplementary materials.

With this kind of inversion we also obtain a datacube with the uncertainties of the final models. We give below the accuracy calculated for each layers: for the density model, uncertainties have a maximum value of 19 kg/m³ for the sediments layer, 29 kg/m³ for the crust layer, and 14 kg/m³ for the mantle layer, while considering the susceptibility inverted model, uncertainties reach maximum value of 0.0015 SI for the magnetised sediments layer and 0.006 SI for the magnetised crust. Maximum uncertainty values for the density model are concentrated in the South-West Caspian Sea area and in the Amu-Darya Basin (ADB), while in the susceptibility model uncertainties are more distributed within the Iranian plateau, with higher values in the East Central Iran microcontinent (ECIM) and in the Sanandaj-Sirjan Zone (SSZ). From

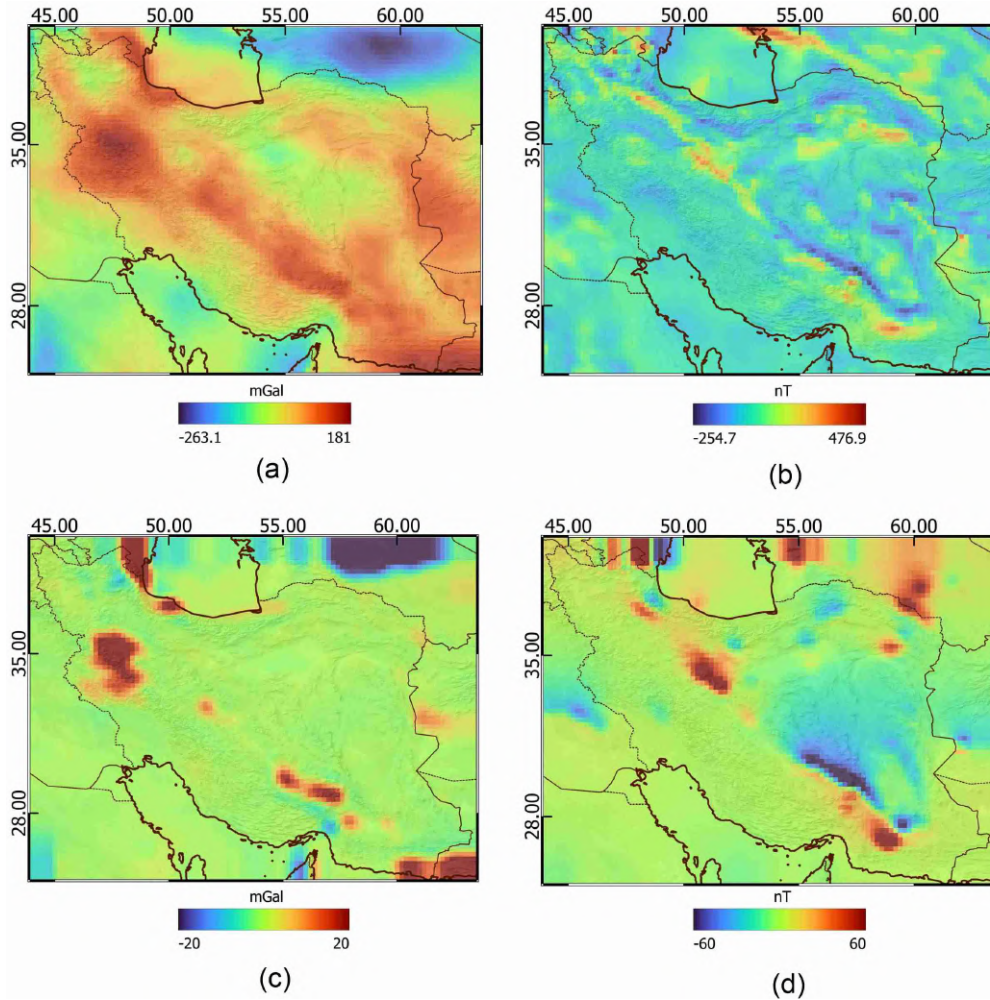


Figure 4.1.10: Gravity (a) and magnetic (b) residuals before the inversion, and gravity (c) and magnetic (d) residuals after the inversion. The maps represent the differences between the original observation and the forward calculated fields of the starting model (a,b) and the final model (c,d).

the resulting inverted model we extract the new interfaces between the modelled geological horizons: the inversion is allowed to modify the input layer in the bounds dictated by the uncertainty of the layer depth, expressed in Section 4.1.7 (Lithosphere model). In the final model, the position of the sediment basins is quite changed, making some corrections on the depths, which are generally less deep (Fig. 4.1.11.a). The South Caspian Basin (SCB) results collectively shallower and linked in a more continuous basin, with reduced depths extending southwards, and connecting eastwards to the West Turkmenistan Basin (WTB) and westwards to the Kura Basin (KB). The Amu-Darya Basin (ADB) became deeper and occupies a larger area of the Turkmenistan Depression (TD), while considering the Persian Gulf, we have an important reduction of the depth along the entire area. The Mesopotamian Foredeep Basin (MFB) passed from the 26 km in the original model to a maximum of 15 km, and its depocenter is shifted southwards compared to the original, while in the Makran area (MZ), the basins present in the starting model almost disappear, even if we can identify two small depocenters (Bandar Abbas Basin (BAB) and Hamun-Mashkel Basin (HMB)). The Moho, marking the interface between lower crust and upper mantle, has systematically shallower depth along the entire Zagros belt, which seems to have a more superficial crustal root, while the rest of the area basically is uplifted, even if main features were conserved (Fig. 4.1.11.b). Finally, considering the Curie depth surface, in the final model it is basically flattened, with the deeper nodes being uplifted and the more superficial parts of the model being lowered (Fig. 4.1.11.c). Also in this case we can retrieve the

same features between initial and final model, with the entire Zagros belt (ZFTB, SSZ, UDMA) and part of the East Central Iran microcontinent (ECIM) that have a superficial Curie depth surface, which becomes deeper under the South Caspian Basin (SCB) and in Turkmenistan (TD). A shallow Curie depth for the thick crust below Zagros is expected due to a greater radiogenic heat production of the thick crust, compared to a thinner crust. The thick crust has a greater thickness of radiogenic heat producing rocks, leading to higher crustal temperatures and a steeper temperature gradient with depth, compared to a thinner crust. The consequence is a shallowing of the temperature isothermal surfaces, and therefore also a shallowing of the Curie depth. The Curie depth is tied to the crustal temperatures, with a shallower Curie depth for higher temperatures.

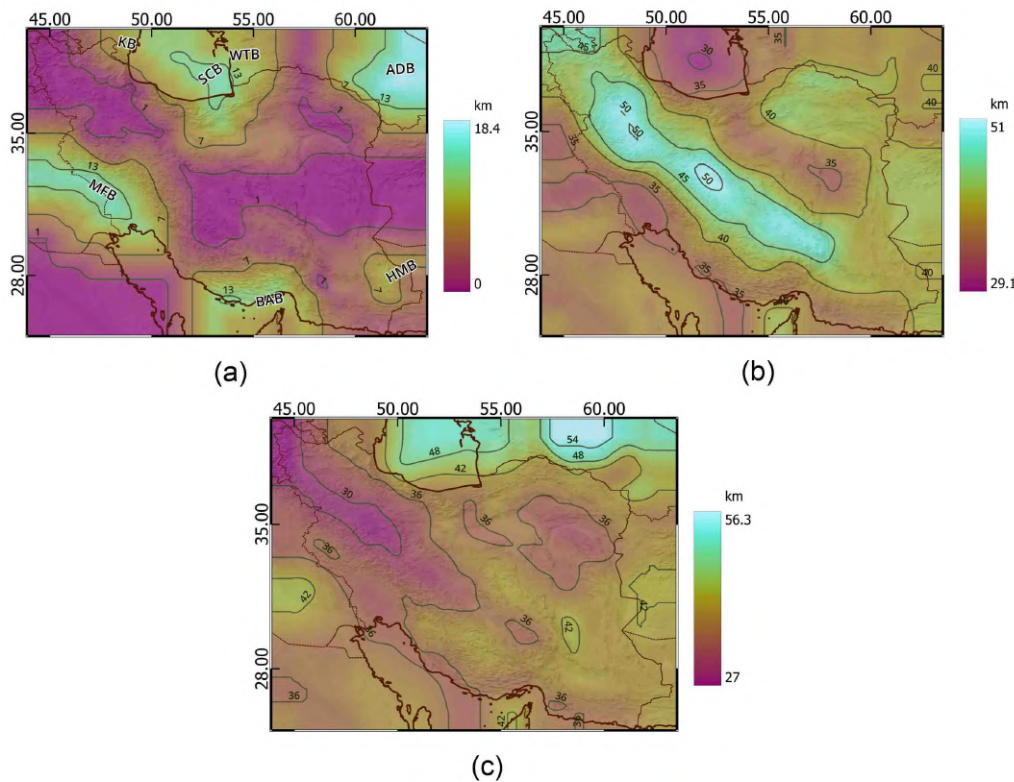


Figure 4.1.11: New layers extracted from the inversion. (a) is referred to the depth of the sedimentary basins (ADB: Amu-Darya Basin; BAB: Bandar Abbas Basin; SCB: South Caspian Basin; HMB: Hamun-Mashkel Basin; KB: Kura Basin; MFB: Mesopotamian Foredeep Basin; WTB: West Turkmenistan Basin), (b) is the final Moho discontinuity, and (c) is the Curie depth surface.

General description of the inverted density model

We describe the inverted density model, which defines the 3D density distributions of the sediment, crust, and mantle layers, illustrating density maps at different heights between 10 and 70 km (Fig. 4.1.12). Starting at 10 km, we can see the presence of the sedimentary basins (the Amu-Darya Basin (ADB) on the Turan Platform, the South Caspian Basin (SCB), the Mesopotamian Foredeep Basin (MFB) and the Bandar Abbas Basin (BAB)), with lower values in Central Iran, and also the sedimentary rocks making up the Zagros orogenic belt, the salt deposits in Southern Zagros, and the Jaz Murian Depression (JMD). High density trends are detected along the Sanandaj Sirjan Zone (SSZ) and the Urumieh–Dokhtar Magmatic Arc (UDMA), in the Yazd Block and in the Helmand Block. More localized increased density areas are found northwest of the South Caspian Basin (SCB), in the northwestern part of the Paleo-Tethyan suture. A last increased density is found in the southern part of the Lut Block (LB), in the Dash-e Lut desert (DLD). At 20 km depth the pattern changes, and the areas with increased density are

less extensive, while the low dense area along the Zagros Fold and Thrust belt (ZFTB) and the East Central Iran microplate (ECIM) are more noticeable. In Central Iran (CI) we find two high density spots, in the Qom area south of Teheran, and south of the Jaghatai Mountain Range (JMR), separated by a low density area. Other high density trends are found at the northern extreme of the Paleo-Tethys suture following the suture southeastwards along the Alborz (AB), and from north-west to south-east boarding the Urumieh-Dokhtar Magmatic Arc (UDMA) and the Sanandaj Sirjan Zone (SSZ), until the Jaz Murian Depression (JMD). Even the high in the southern Lut Block (LB) persists in the deepest layers, while around it the Sistan Suture zone (SS) has a lower density.

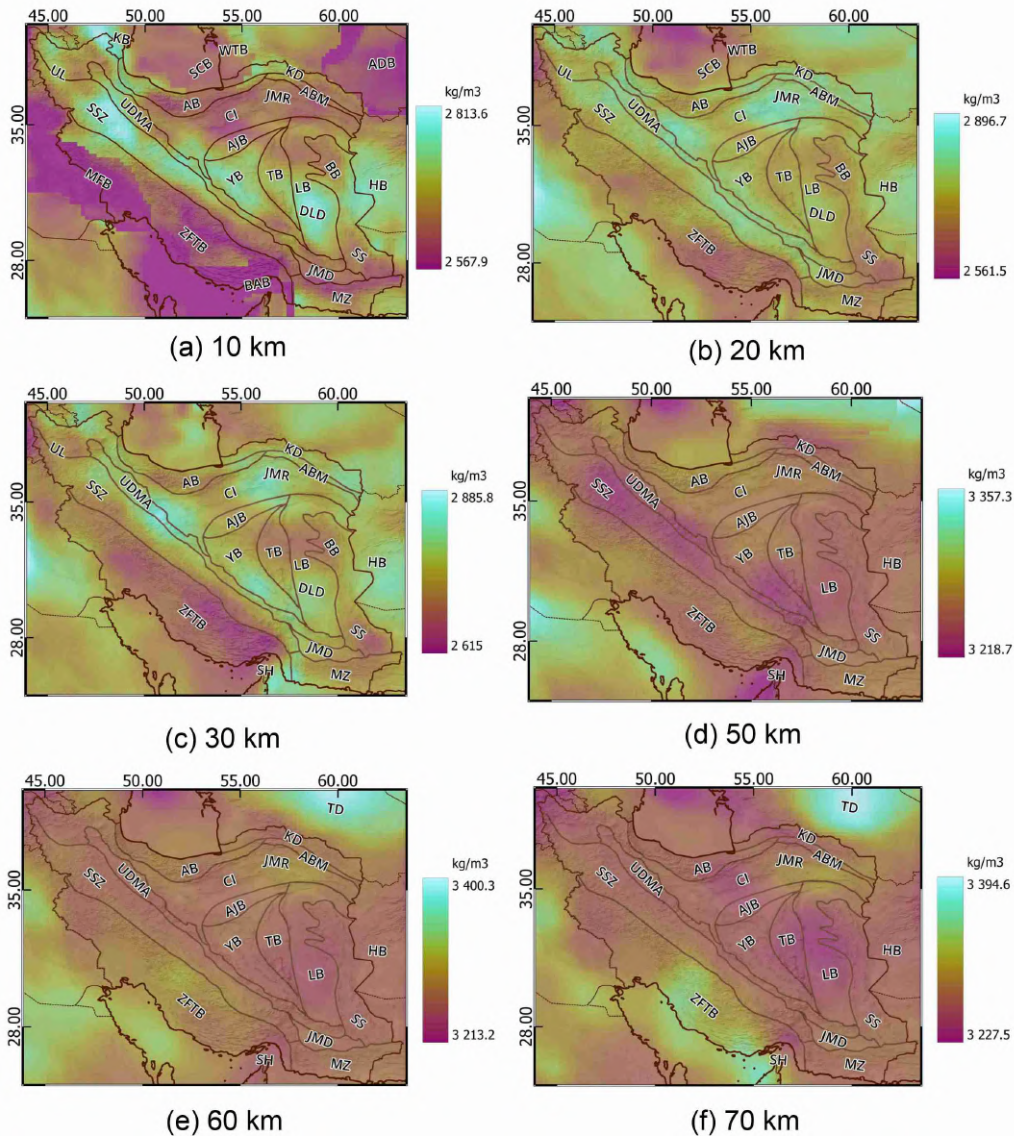


Figure 4.1.12: Slices at different depths representative of the final density model. Geological provinces and blocks are also indicated with their acronyms. For references and acronyms explanation see Figure 4.1.1.

At 30 km, high density values in the eastern South Caspian Basin (SCB) start to appear, due to the fact that we are approaching the mantle in that area at this depth, and a new localized high density body ($\sim 2850 \text{ kg/m}^3$) is also found in the Straits of Hormuz (SH), marking the transition between the southern end of the continental collision of the Arabian Plate to the oceanic subduction of the Makran area. The rest of Iran remains quite consistent with the superficial slice, with the low density along the Zagros Fold and Thrust Belt (ZFTB) and Alborz

(AB), and the high density area in Central Iran (CI) and Yazd Block (YB). The Dasht-e Lut desert (DLD) high density is still visible, with the exception of the reduced density in the Birijand Block (BB), connecting to the Sistan Suture zone (SS), and an area protruding westwards to the Tabas Block (TB). The Afghan Block (HB) extends the high density down to 30 km depth, defining a separate crust compared to the Sistan suture (SS). At 50 km depth we are entirely in the mantle, and the density values range between 3200 and 3350 kg/m³. By qualitatively analysing the density distribution, we observe a trend reversal along the Zagros belt, where the previously higher density areas along the Sanandaj Sirjan Zone (SSZ) and the Urumieh-Dokhtar Magmatic Arc (UDMA) become lower density than the Zagros Fold-and-Thrust belt (ZFTB). A low density anomaly, as opposed to the upper layer, is visible also in the Strait of Hormuz (SH), while the rest of Iran becomes quite homogeneous. Higher density areas are located in the southeastern part of the South Caspian Basin (SCB), in northern Turkmenistan (TD), and in the western Persian Gulf. At 60 km depth the density is more homogeneous over the entire Iran, with lower density bodies in the Lut Block (LB) and in the Strait of Hormuz (SH), and an extended higher density area in Turkmenistan (TD) and in the Persian Gulf. These features are reinforced at 70 km depth, with the high density of the Persian gulf that invades the Zagros Fold-and-Thrust Belt (ZFTB), and the studied area acquires greater inhomogeneity: the Central Iran province (CI) is separated into two opposing blocks, one less dense west of Teheran and one more dense south of the Aladagh-Binalud mountains (ABM) and Lut Block (LB) and Tabas Block (TB) become less dense in comparison to the rest of the East Central Iran microplate (ECIM). The only contrast to the previous mantle slice is in the Strait of Hormuz (SH), where we have an inversion compared to the lower densities of the upper layer.

The inverted density model in relation to the geologic and tectonic structures

We make some considerations regarding the density volume generated and described in the previous section, relating it to the known geological and tectonic aspects in the area. In particular, for this analysis we focus on the first 20-30 km of the model and considering the average density of the crustal layer. Average crustal density is calculated considering the density column for each node in the grid, using only the density values related to the voxels in the crystalline crust layer. Firstly, we consider the higher-density anomalies in the average crust, and compare them with the position of the magmatic bodies previously presented, extracted from the USGS catalogue (Pollastro et al., 1997).

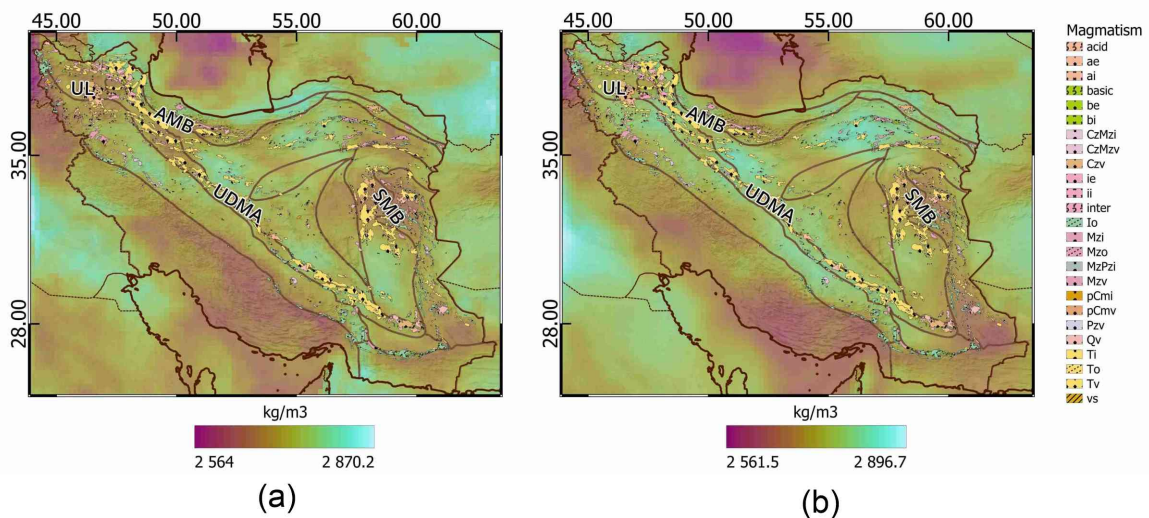


Figure 4.1.13: Average crustal density (a) and density slice at 20 km depth (b) with superposed the distribution of the magmatic outcrops. The greater part of the high density trends follows the position of the magmatic lineaments. The acronyms are defined in Figure 4.1.2.

We can see that some trends have very similar shapes, even if they do not correlate perfectly. Regarding the mean crustal density (Fig. 4.1.13.a), the high density lineaments of the Alborz area (AB) correspond to the presence of Tertiary magmatic bodies, and some high density patterns are also detectable along the Urumieh-Dokhtar Magmatic Arc (UDMA), although these do not correspond in an optimal way with the map of magmatic outcrops. The situation changes if we consider the mid-crustal slice at 20 km (Fig. 4.1.13.b). Here we can appreciate how all the magmatic features correspond to high values in density, in particular along the Urumieh-Dokhtar Magmatic Arc (UDMA) and Alborz area (AB), where before some similarities were already visible, now the two maps are perfectly related. In this 20-km slice, additional high positive anomalies are visible also in the Jaghatai Mountain Range (JMR) south of Kopeh-Dagh (KD) which correlates with Tertiary and Mesozoic magmatic bodies, and in the Lake Urmia (UL) volcanic area, in north-western Iran, which is affected by Cenozoic magmatism. The only anomaly which persists in both average values and in the 20 km layer is in the Sistan Suture zone (SS), where the magmatism in the area seems to correlate with low density values compared to other areas. Turning to more tectonic aspects, considering again the average crustal density, we observe that high-density lineaments which stand out from the surrounding areas, almost overlap with the locations proposed by literature for the Paleo- and the Neo-Tethys suture lines (Irandoost et al., 2022a; Wan et al., 2021). We therefore try to draw a density-derived suture, calculating the horizontal gradient of the average crustal density and then following the anomalous lineaments. Our suture lines are proposed in Figure 4.1.15, based on the gradient shown in Figure 4.1.14.

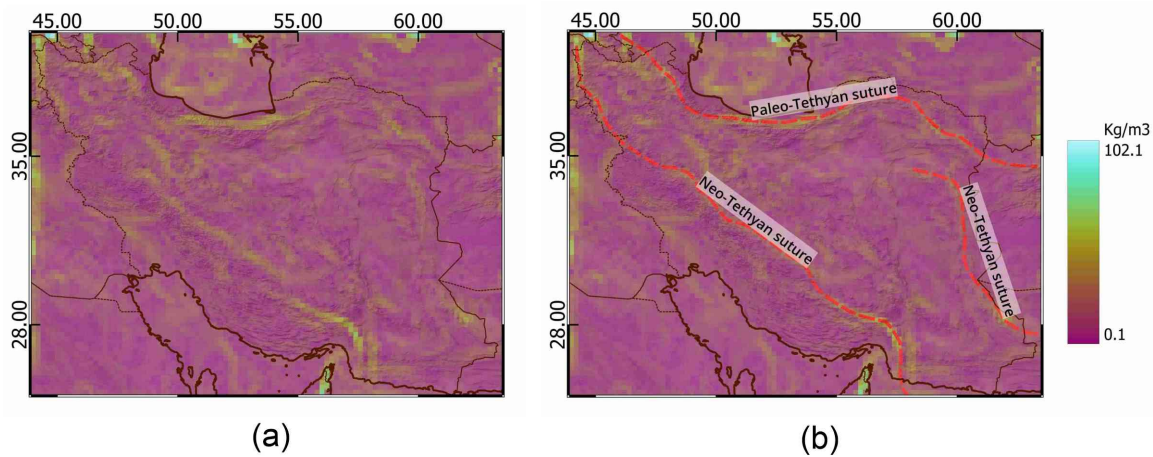


Figure 4.1.14: Density gradient (a) calculated from the final model, used to track the position of the Paleo- and Neo-Tethyan sutures (b).

In particular our Paleo-Tethys suture follows the Kopeh-Dag (KD), Alborz (AB), and then proceeds to the northwest following the Caucasus, while the Neo-Tethys suture extends from the north-western Iranian border along the Zagros belt until the Minab fault (MF, see Figure 4.1.2), after then it moves south toward Makran subduction (MZ). The Paleo-Tethys position seems giving a high-density trend following all the northern border of Iran, while for the Neo-Tethys, it marks the separation between an high-density area northeast of the suture and a low-density area in the opposite part. We also note from the gradient the position of another suture along the Sistan Suture Zone (SS) marking the differences between the lower densities in the Iranian plate and the higher densities in the Afghan plate, which according to Bröcker et al. (2022) we associate to the Neo-Tethyan suture, that after continuing parallel to the Makran Zone, crosses Iran again, along the Sistan Suture Zone. Focusing on the eastern Iran, differences in density can be identified, reflecting the tectonic lineaments between the Lut Block (LB) and the Sistan Suture zone (SS). In particular an high density body is found in the southern part of the Lut Block (LB), corresponding to the Dash-e Lut Desert (DLD) surrounded by lower density zones,

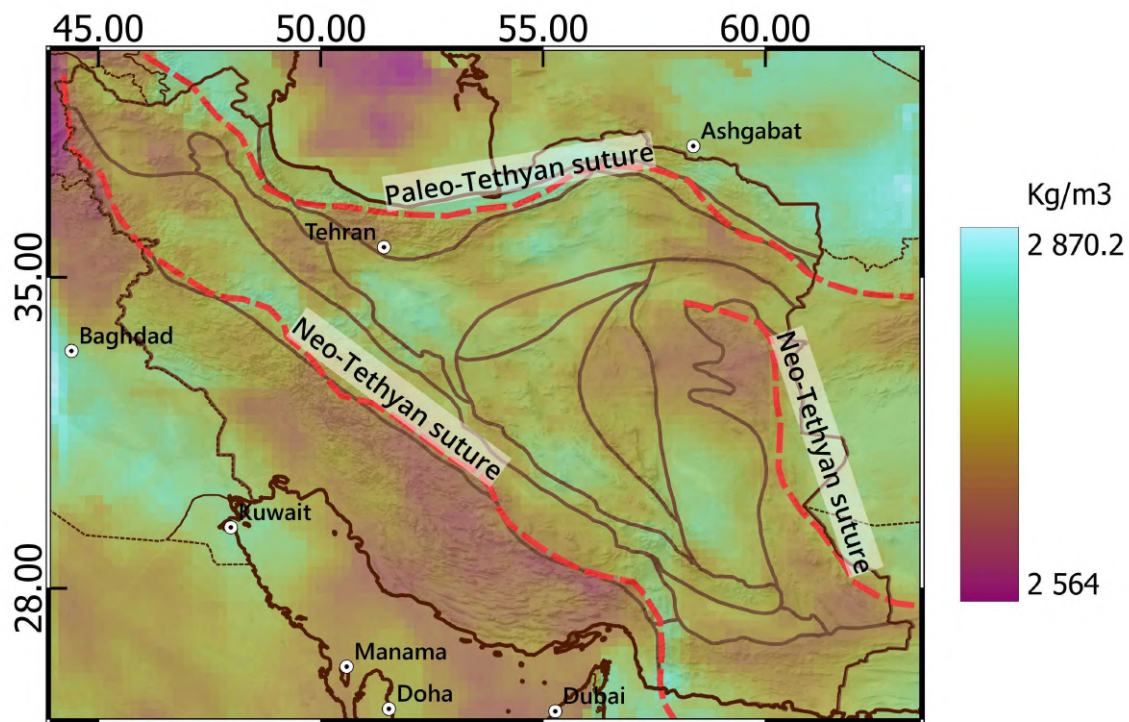


Figure 4.1.15: Average crustal density and position of the three founded sutures, derived from the final model.

which follow up with the lineaments of the Sistan suture zone (SS). In Figure 4.1.16 it is clearly visible that the strike-slip faults limiting the western and eastern Lut Block mark the separation between the higher density nucleus of the Lut Block and the lower density zones. The lower density body in the Birjand Block (BB) seems to rotate around the central dense body of the Lut Block (LBDB), rotation of the block that is known in literature (Rashidi et al., 2022), and that is also explainable observing the orientation and movement of the strike-slip faults in the area. Our model suggests the presence of a crustal dense and stable body in the Lut Block, which acted as block that guides the crustal movement to the east and west of it in response to the compressive stresses present due to the Makran subduction. The principal compressive stress orientation along the right-lateral strike slip fault system along the western margin of the Lut Block is estimated to be N15E (Rashidi et al., 2019).

Description and consideration of the mean crustal susceptibility

We now describe the map with the average crustal susceptibility resulted from the inversion (Fig. 4.1.17). Like the average crustal density, average crustal susceptibility is calculated averaging the column of the susceptibilities for each node from the inverted model, only considering the values included in the magnetized crustal layer. The inversion detected a series of magnetized bodies within the crustal layer, in particular in certain areas along the Sanandaj-Sirjan Zone (SSZ) and the Urumieh-Dokhtar Magmatic Arc (UDMA), and in the western part of the Makran accretionary prism (MZ). Areas with considerable magnetization are detected also in the Kopeh-Dagh (KD), in the eastern part of the South Caspian Basin (SCB), in the West-Turkmenistan Basin (WTB) and in East Central Iran microplate (ECIM), in particular in the northern part of the Lut Block (LB). The entire Central Iran seems to have no magnetization as well as the Zagros fold-and-thrust belt (ZFTB). Also the dense crustal body in the Lut Block, found and described in the previous chapters, appears without a significant magnetization. Comparing with the magmatic outcrops catalogue also used for the considerations regarding

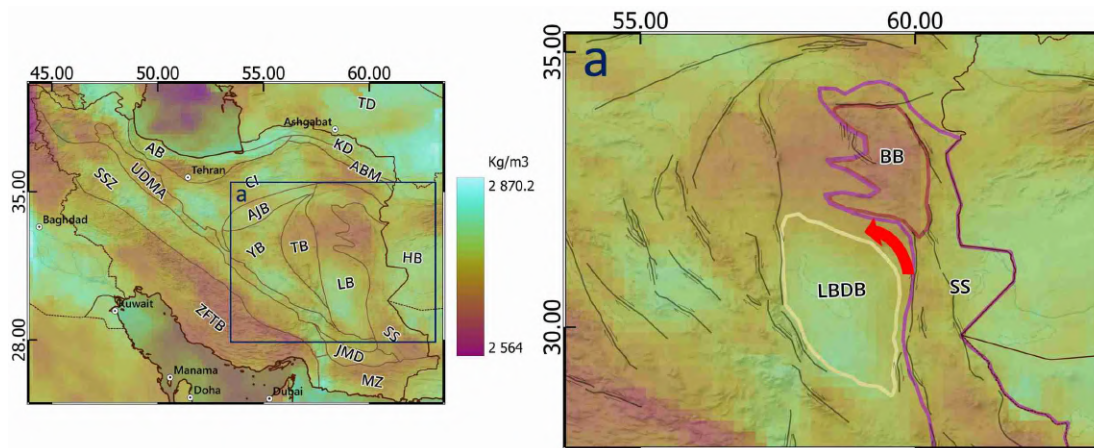


Figure 4.1.16: Focus on the Central East Iran zone, comprising the Lut Block (LB) and the Sistan Suture zone (SS). The Sistan Suture Zone, in particular the less dense area of the Birjand Block, wraps around the central high-density body of the Lut Block (LBDB).

the density model, we partly observe a correlation between magmatic bodies and magnetization. In general the southern UDMA seems to not have relevant magnetization, like the magmatic belt along the Sistan suture, even if also in these apparently unrelated areas it is possible to observe some small correlated spots. Considering the northern part of the Urumieh-Dokhtar Magmatic Arc (UDMA), we found an important link between the position of the outcrops and high magnetization, in particular on the border with the Azerbaijan, in the Urmia Lake volcanic area, as also in a central segment of the Sanandaj-Sirjan Zone (SSZ). In the west of Makran Zone (MZ), a magnetized area could be associated to the presence of lineaments of ophiolitic outcrops, on the border with the Jaz Murian Depression (JMD). Also the Alborz magmatic belt gives some small areas with high magnetic trends in accordance with the presence of outcrops. In summary, most of the magmatic presence is evidenced by the magnetic anomalies in the area, but there are many high anomalies (Kopeh-Dagh (KD), South Caspian Basin (SCB) and West-Turkmenistan Basin (WTB), Eastern Central Iran ECIM) that are not explained by a plain presence of rocks outcropping at the surface.

General description of the shear modulus model

We analyse the shear modulus model starting from the top, investigating the same slices described above for the density model. Starting with a qualitative analysis, in the superficial layer corresponding to 10 km (Fig. 4.1.18.a), we notice the area to be basically divided into two distinct parallel trends: a more rigid band from north-west to south-east, along the Sanandaj-Sirjan zone (SSZ) and crossing the Yazd Block (YB), Tabas Block (TB), culminating in the southern Lut Block (DLD), and a parallel more ductile band, along the Zagros Fold-and-Thrust belt (ZFTB) and Makran zone (MZ). The Afghan Block (HB) and Turkmenistan (TD) are also more rigid, exception for the Amu-Darya Basin (ADB). Comparing with the location of the epicentres of the earthquake for the years 1905 to 2021, with magnitude greater 4.5 taken from the U.S. Geological Survey (2021), we observe that the position of superficial earthquakes matches often the more ductile superficial zones. The rigid band corresponds to an aseismic area and sets the boundary between the highly seismic Zagros Fold-and-Thrust belt (ZFTB) and an intermediate seismic area to the north in Central Iran (CI), along the Kopeh Dagh (KD) and northern Afghanistan, which follows the tectonic lineaments of the zone and where also superficial earthquakes occur.

Proceeding to the depth of 20 km (Fig. 4.1.18.b), the low rigidity anomaly moves toward north-east, maintaining the same parallel orientation to the Zagros, but being more aligned with the

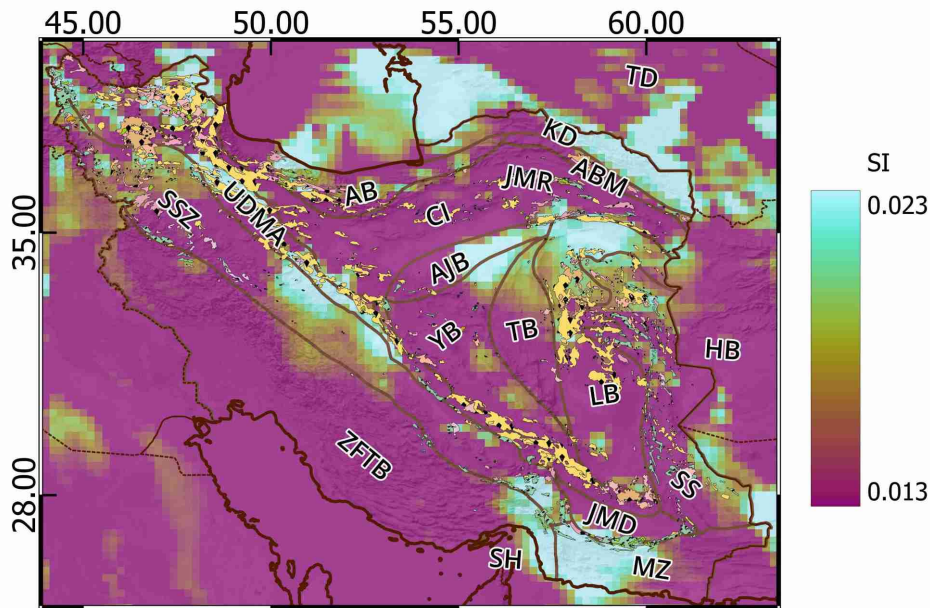


Figure 4.1.17: Average crustal susceptibility with geological provinces and magmatic outcrops. It is difficult to identify correlations between magmatic outcrops and high crustal susceptibility.

central axis of the Zagros Fold-and-Thrust belt (ZFTB). Also the earthquakes in this case perfectly match with the low rigidity area. The rest of Iran becomes more homogeneous, and most of the rigidity anomalies previously presented are reduced, while Central Iran (CI) becomes more rigid, in particular south of Tehran, in the Qom area, and south of Jaghatai Mountain Range (JMR). To the East of the Jaz Murian Depression (JMD), located in the forearc of the Makran subduction, the area becomes more ductile, merging northwards into the Sistan Suture zone (SS). The South Caspian Basin (SCB) also becomes a very ductile area, even if no earthquakes match with the zone. At 30 km (Fig. 4.1.18.c), the major part of the anomalies in the previous slice are preserved, and become more marked. The minor band along the Zagros and Makran foreland basin is interrupted by an anomalous very rigid spot in the Strait of Hormuz (SH). The Sistan Suture Zone (SS) shows increasingly marked differences in rigidity compared to the surrounding areas, with the ductile body that from the Birjand Block (BB) crosses the Eastern Central Iran (ECIM) to the Tabas Block (TB), while an high rigidity zone starts to appear in the Yazd Block (YB). High rigidity anomalies are still visible in Central Iran (CI), south of Tehran and south of Jaghatai Mountain Range (JMR). Entering into the mantle, at 50 km (Fig. 4.1.18.d), we observe that the low rigidity anomaly continues its displacement towards north-east, causing a sort of reversion from the crustal trend, since the area along the Sanandaj-Sirjan Zone (SSZ) and the Urumieh-Dokhtar Magmatic arc (UDMA) that previously was the most rigid, now becomes the only ductile part in the area. The remainder of Iran is quite homogeneous. Considering the entire model, this low rigidity anomaly seems to form a ramp in a northeastern direction extending towards increasing depths. Considering the average crustal shear modulus, the seismicity in general correlates with the regions of reduced rigidity (Fig. 4.1.18.e), with the low rigidity perfectly matching with the faulting, and with the location of the superficial earthquakes, with depths from 0 to 30 km, and covering the interval from 1905 to 2021. In particular this correlation is important along the Zagros-Fold and Thrust Belt (ZFTB), the Sistan suture (SS), and in the Eastern Central Iran (ECIM). The South Caspian Basin (SCB) does not show this correlation with the earthquakes location, because it has values of reduced rigidity, but the seismicity follows its border, and divides the southern from the northern Caspian Basin through the seismicity of the Aspheiron ridge (AR). The map of the final average crustal shear modulus is more coherent compared to the initial shear modulus

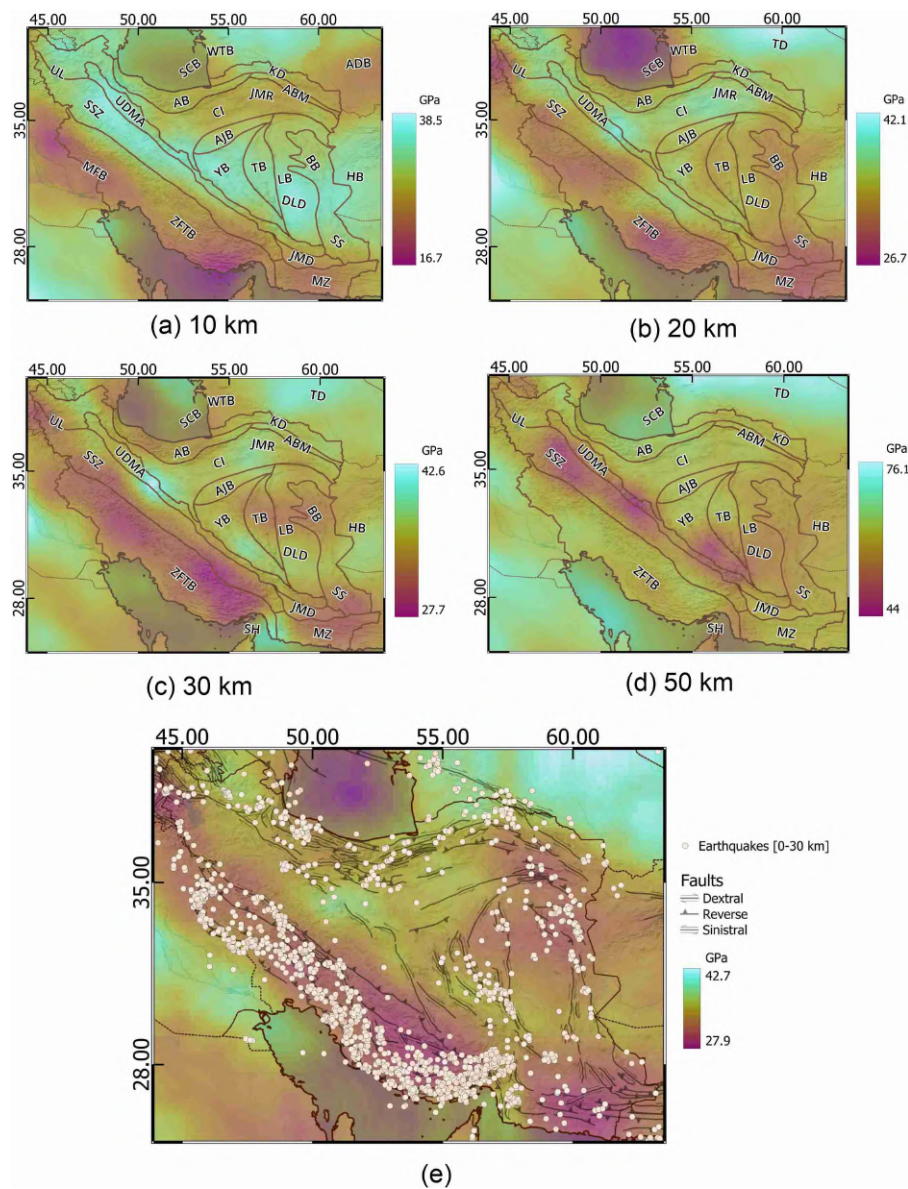


Figure 4.1.18: Shear modulus model at different depth slices. Geological provinces are also indicated (a-d). (e) crustal average shear modulus model and the position of the superficial earthquakes, from 0 to 30 km hypocenter depth.

shown in the Supplementary.

4.1.9 Discussion

To our knowledge this work proposes the first well defined high resolution 3D density model of the entire Iran, for crust and lithospheric mantle down to a depth of 105 km. The results are based on one of the most recent 3D seismic tomographic model publicly available, and therefore should guarantee the maximum resolution that today is possible to be achieved in the public domain (Kaviani et al., 2020). A more recent seismic tomography has been published after we had started the inversion processing, but the 3D tomographic model is not available (Irandoost et al., 2022a).

The inversion of the gravity field in the Caspian and Alborz has been reported by Motavalli-Anbaran et al. (2013) and along profiles crossing our area in Motavalli-Anbaran et al. (2011). The method uses gravity, geoid and topography to constrain a forward modelling or a Bayesian inversion which aims to define Moho depth, lithosphere-asthenosphere boundary (LAB), and

average crustal density. A thermal modeling through solving the steady state heat transport equation constrained by gravity, geoid, isostatic equilibrium condition and heat flow values has been made along a north-south profile extending from the Makran to the Turan platform. The density of the mantle lithosphere is temperature dependent and controls the modelled geoid (Entezar-Saadat et al., 2017). The approach is different to ours, because the reduction in ambiguity of the inversion is achieved by fixing a-priori parameters as the LAB temperature, the assumption of linear variation with depth of lithosphere density, and the assumption of an average density for the crustal column including sediments, mid and lower crust. A further constrain is the local Airy-type isostatic compensation of topography through the underlying density model. Although the methods and assumptions are different, many features are common, like the thickening of the Moho below the Sanandaj-Sirjan Zone (SSZ) to over 50 km, the shallower Moho around 40 km over the Turan platform, the Central Iran (CI) with a shallower Moho compared to the Zagros around 40 km, and the shallow Moho below the South Caspian Basin (SCB). Our average crustal density is consistent with Motavalli-Anbaran et al. (2013), apart from some local deviations.

Due to the rock-physical relation connecting seismic velocity and density, it is expected that the higher velocities in the tomographic model will correspond to higher density, an observation which our model allows to quantify, bringing a further insight to the Iran lithosphere. The higher spatial resolution of the density and magnetic model compared to the seismic model is given by the higher resolution with which the fields are available, and through which particularly for small scale and upper crust features the density model brings a refinement of the tomographic model. This brings to a clearer match of geological structures defined by age, geodynamic evolution, inheritance of rock formation, with the density and susceptibility variations, especially in the upper crustal layers. The Bitlis-Zagros suture (BTS) marks the transition between the Arabian and Eurasian plates, and therefore is expected to produce a major variation in rock properties. The suture marks a density boundary over the entire crustal thickness, with systematically lower density in the Zagros Fold-and-Thrust Belt (ZFTB) down to the Moho depth to 40-50 km (up to 200 kg/m³ density difference), and an inversion of the sign of the difference in the mantle down to 80 km (40-50 kg/m³), a depth after which another inversion occurs, with the Arabian lithosphere that returns less dense than the Iranian lithosphere (30-40 kg/m³) down to the bottom of the model. The suture marks also a difference in the crustal rigidity, with systematically lower rigidity in Zagros to the SW of the suture, and higher rigidity to the NE of it. This rigidity discontinuity shifts towards the Urumieh-Dokhtar Magmatic Arc (UDMA) for increasing depths, up to the Moho (Zagros rigidity 17 GPa at 10 km to 27 GPa at 30 km, Sanandaj-Sirjan Zone (SSZ) and Urumieh-Dokhtar Magmatic Arc (UDMA) 38 GPa at 10 km, to 42 GPa at 30 km). Below the Moho the rigidity matching the suture is limited to a narrow band below the Sanandaj-Sirjan Zone (SSZ) and Urumieh-Dokhtar Magmatic Arc (UDMA), with values that are systematically higher below the Zagros and the Central Iran (CI). This systematic difference is not visible in the magnetic susceptibility variation. The higher rigidity of Central Iran (CI) could be the cause of the lower occurrence rate of significant earthquakes, which rather are found in the lower rigidity crust. The Zagros has a very high density of earthquakes, up to the higher rigidity margin, but only in the northern half of Zagros, the southern half having epicenters limited to the external (southwestern) parts of the Thrust and Fold belt, whereas the areas closer to the suture have low seismicity. One reason of the absence in this deformable zone could be the presence of the Late Precambrian Hormuz salt layer overlying the basement (Jahani et al., 2009), seen even in satellite images through the folding that salt diapirs generate, and which could favour deformation along detachments. The East Central Iran (ECIM) which is an amalgamation of four blocks, shows density and rigidity variations which cross the blocks, and differentiates rather than the blocks, subunits of the blocks. The Sistan Magmatic Belt (SMB), shared between the north Sistan Suture zone (SS) and north Lut Block (LB), is systematically less dense over the entire crustal column, compared to the remainder of the mentioned blocks. Below the Moho the density values are homogeneous,

and units composing the East Central microplate do not show up. The rigidity variations are similar, with the Sistan Magmatic Belt (SMB) of the microplate being less rigid in the crust. The layer below the Moho is differentiated, as the southern Yazd Block (YB) is less rigid. We find that the higher crustal rigidity controls the development of large basins as opposed to topographic ranges, a rule we find valid for large flat desert areas as the Turkmenistan Depression, the Central Iran Dasht-e Kavir, the Dasht-e Lut (DLD), and the Hamun Jaz Murian. This observation is valid when considering the rigidity values below 10 km down to the Moho. The Rigidity at 10 km has only broader features, and does not show this correlation with the flat topography development.

Considering the susceptibility variations in the crust resulting from the inversion, the areas with most intense magnetized bodies, are identified in the Makran Zone (MZ), in the north-western part of the Urumieh-Dokhtar Magmatic Arc (UDMA), and in the north of East Central Iran (ECIM). It is difficult to match our results with two previously published susceptibility models, due to the different approaches used to explain the magnetic anomalies with the susceptibilities. One approach is to define the average susceptibility over the crustal thickness through spectral methods (Teknik et al., 2020), which inherently will give a different result compared to ours. In fact, our model constrains the magnetization to be above a thermally defined Curie depth. A shallow Curie depth requires a reduced value of the susceptibility to explain the anomaly, since the magnetized layer has a smaller volume, respect to a deeper Curie depth. This is a reason for differences in our results with the model of Mousavi and Ebbing (2018), due to some significant differences in the a-priori Curie depth. For example in the Makran Zone (MZ) the Curie depth of Mousavi and Ardestani (2023) is about 30 to 35 km, whereas Mousavi and Ebbing (2018) has a deeper value of over 50 km. The much deeper Curie depth leads to a lower value of susceptibility. Another difference between the conceptual setup of our model and the one of Mousavi and Ebbing (2018), are the depths for which the susceptibility is allowed to vary. In our case, the susceptibility is inverted from the surface to the Curie depth. In the final model of Mousavi and Ebbing (2018) the susceptibility is inverted between base sediments and a constant boundary at 20 km depth, with constant low susceptibility value below 20 km down to the Curie depth (0.01 SI). This may be the reason for which our values are on average smaller compared with those found in Mousavi and Ebbing (2018), because our magnetized layer is generally thicker than 20 km. In detail, the area of the Makran Zone (MZ) results more magnetized than the Jaz Murian Depression (JMD), trend that appears reversed in the cited models. However, we note that all three models perfectly border the position of the ophiolites present in the Makran Zone (MZ). Another similar situation occurs in East Central Iran (ECIM) where our model detects an increased magnetization bordering the position of magmatic bodies, anomaly that in Teknik et al. (2020) and Mousavi and Ebbing (2018) is extended in Central Iran (CI), incorporating the Jaz Murian Depression (JMR). For the remainder, the anomalies identified by the inversion are quite consistent with the above two models, in particular along most of the Urumieh-Dokhtar Magmatic Arc (UDMA) and in the Urmia Lake (UL). In general, where the Curie depths are comparable, as in the Urumieh-Dokhtar Magmatic Arc (UDMA), the susceptibility values are also comparable.

4.1.10 Conclusion

The target of this work is to realise a model of the lithosphere in Iran performing a gravity and magnetic joint Bayesian inversion, in order to study the different density and susceptibility distributions and bind them to different geological and tectonic aspects. We also wanted to calculate, starting from previous results, a shear modulus model to investigate the rheological aspects of the area. To realise the model we start from an available regional tomography model and through a series of processing steps that led to the formation of an a-priori model, including the identification of the different layers and a first transformation from velocity to density using empirical relation, the inversion delivers a reliable and interpretable model. Thanks to this

model we are able to make some tectonic and geological considerations about the lithosphere of Iran. In particular:

- the density distribution in the upper crust reflects for most areas the trend of magmatic lineaments;
- position of Neo- and Paleo-Tethyan sutures can be detected through the density model, as it generates a strong and measurable gradient signal over the entire crustal thickness;
- the faulting system in the Sistan Suture zone (SS) and the rotation of the Birjand Block (BB) are enhanced by the presence of a dense and rigid body within the Lut Block, around which the faulting and orientation of structural lineament occur;
- the rigidity model shows a more ductile zone under the Zagros, moving northeastward with increasing depth, in which most shallow earthquakes occur.
- the calculated density and susceptibility cube are an innovative data product which are published alongside the paper, and find various applications, including starting rate calculation, if a stress field is given as input. The Curie depth model based on the magnetic inversion is an input for new thermal calculations.

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Authors Contribution

GM prepared the datacube used for the inversion and prepared the final figures. CB proposed and coordinated the research and is the scientific responsible of the above two projects at the University of Trieste. GM and CB worked on data retrieval, preparing the GIS database, fulfilled the discussions throughout the work. DS and MC dealt with the gravity and magnetic data inversion and with the Bayesian method development. All authors contributed to the manuscript preparation and interpretation of results.

Open Research

The Data Cube containing the results of the inversion is available through the publicly accessible repository Zenodo at <https://doi.org/10.5281/zenodo.8096623>.

Data: Starting seismic tomography is freely available at http://ds.iris.edu/ds/products/emc-midd_east_crust_1/ (Kaviani et al., 2020) (last access June 2023).

The Bouguer anomaly is calculated from the International Centre for Global Earth Models (ICGEM) provided by International Association of Geodesy and German Research Centre for Geosciences (<http://icgem.gfz-potsdam.de/home>) (Ince et al., 2019) (last access June 2023).

The magnetic model can be found on https://www.ncei.noaa.gov/access/metadata/landing-page/bin/iso?id=gov.noaa.ngdc.mgg.geophysical_models:EMAG2_V3 (Meyer et al., 2017) (last access June 2023).

List of earthquakes is obtained by USGS service from <https://earthquake.usgs.gov/earthquakes/search/> (U.S. Geological Survey, 2021) (last access June 2023).

Active faults database is available at the link <https://github.com/GEMScienceTools/gem-global-active-faults> (Styron & Pagani, 2020) (last access June 2023).

Software: To model the starting mantle densities we used the software Perple_X available at <https://www.perplex.ethz.ch/> (Connolly, 2005)

4.2 Medium Scale Inversion (Second Article)

The following work was presented at different national (GNGTS 2024) and international (PDAC 2024, AGU 2024) congresses.

Gravity and Magnetic datasets inversion of the Cornubian Batholith (South-West UK), using Variation of Information

4.2.1 Abstract

Cornwall Peninsula is an extended region in the southwest of Great Britain, which is characterized by the presence of an early Permian granitic body, the Cornubian Batholith, as a result of the Variscan orogeny. It is composed of six major plutons, intruded into a metasedimentary matrix of Devonian and Carboniferous rocks. The batholith has a rich mining history dating back to the prehistoric period, with ore fields associated with different stages of its emplacement. Active mines, primarily focused on kaolin extraction, also show potential for the production of tin, lithium, and tungsten, as well as the exploitation of geothermal energy. This makes the area attractive from an economic point of view. We propose a new and enhanced 3D model of the Cornubian Batholith, derived from a joint inversion of gravity and magnetic datasets. The inversion was performed through a technique that takes advantage of the concept of Variation of Information. This technique allows to define a direct connection during the inversion between the variable investigated, in this case gravity and magnetic signals sources. Principal goal of the work is to highlight not only the body's edges, but also the distribution of density and susceptibility along the investigated area, with the idea of identifying the areas more interesting for specific mineralization.

4.2.2 Introduction

The Cornubian Batholith is a large early Permian granitic body in the south-west peninsula in Great Britain and is the post-collisional result of the Variscan orogeny. It is placed on the peninsula extending in west-southwest direction off-shore and is composed by six S-type granite plutons, intruded during the early Permian, outcropping and cutting a metasedimentary matrix of Devonian and Carboniferous rocks (Chappell & Hine, 2006) (Fig. 4.2.1). The on-land plutons have been individually studied and it has been observed that each one has a distinctive mineralogy (Simons et al., 2016). Variscan orogeny has been the main guide to the formation of structures present in the area, defining the faulting, the folding, and low grade metamorphism (Fig. 4.2.2). The end of Variscan convergence, and the following beginning of the regional extension, led to crustal partial melting and emplacement of the batholith, occurred during the early Permian (Simons et al., 2016). The Cornubian Batholith has an important mining history, since from Prehistoric period. Mining activity was always carried on in the area, in particular for Tin and Copper. The ore fields were imposed in three distinct stages referred to as pre-, syn-, and post-batholith stages, in relation to the emplacement of the Cornubian Batholith (Willis-Richards & Jackson, 1989). Most of the mineralization took part simultaneously with the formation of the batholith, while the remaining mineralization occurred with the thermal and tectonic evolution of the region (Willis-Richards & Jackson, 1989). Active mines are still present and are operative. The main activity in the area involves kaolin extraction, but several studies have shown its potential regarding critical raw materials extraction, in particular for Lithium and Tungsten production (Romer & Kroner, 2016; Simons et al., 2017), and also for the exploitation of geothermal energy (Beamish & Busby, 2016; Reinecker et al., 2021).

The concept of Variation of Information we used for this inversion is a method that recently was introduced in the field of the geophysical data inversions (Lösing et al., 2022; Lowe et al., 2024; Moorkamp, 2022; Njinju et al., 2023). We use it to invert the gravity and magnetic fields

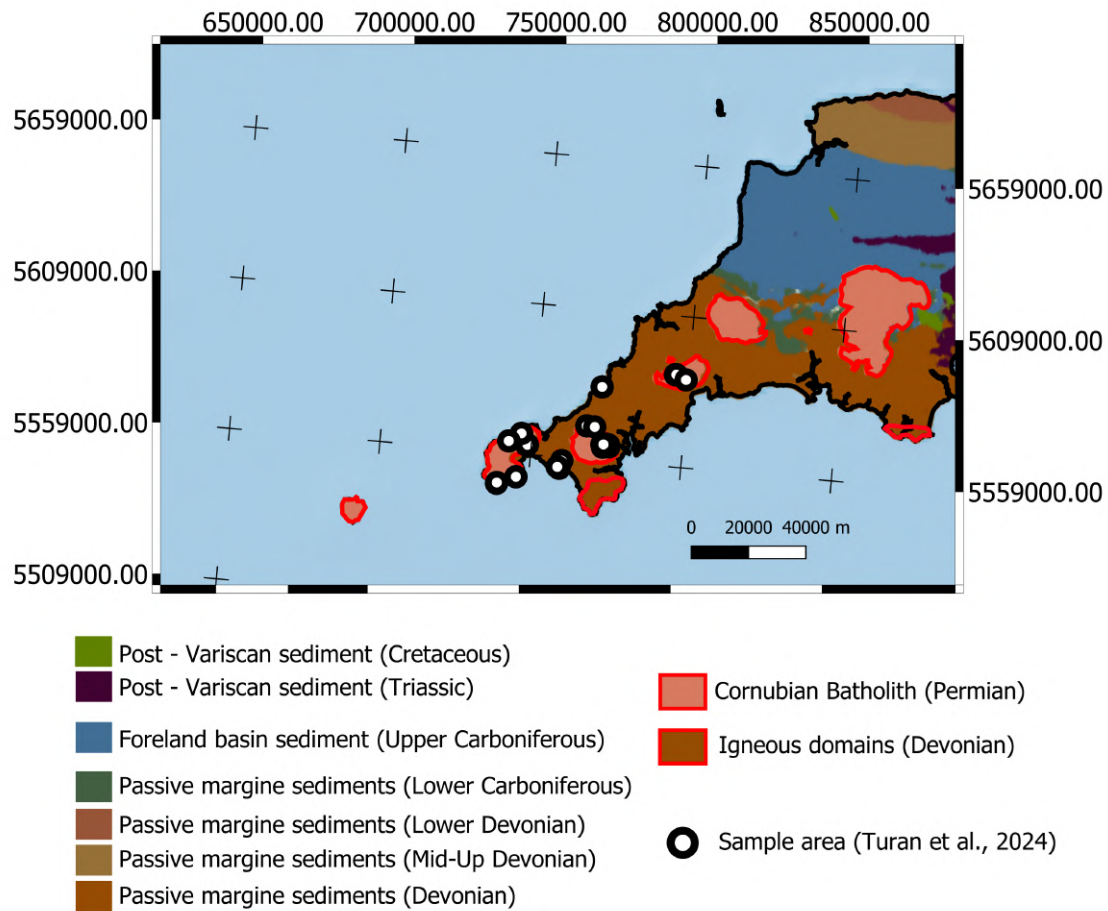


Figure 4.2.1: Geology of the Cornwall peninsula. Modified from Kirkwood et al. (2016).

in the south-west of Great Britain. Geophysical studies in the area have been carried out in the past, and recently the area has returned to great interest, thanks to its potential in mineral extraction. First seismic and gravity survey interpretation was carried out by Edwards (1984), suggesting the continuity of the batholith beyond the Land's End and the existence of thrusts southeast of the Cornubian body. The analysis on a crustal seismic experiment conducted in 1979, by Brooks et al. (1984), indicates the presence of a sub-horizontal reflector at depth of 8 km inside the batholith and another reflector between 10 and 15 km coincident with the base of the granite. A first modern gravity modeling of the Cornubian Batholith was conducted by Taylor (2007), in which the author propose the exposed plutons are tabular intrusions with a near-vertical roots. It was an innovative study on the shape of the Batholith, that first diverged from the previous studies performed on the body. Recently, a more regional solutions (Baykiev et al., 2018; Beamish et al., 2021) led to a lithospheric model of the entire Great Britain, respectively derived by a gravity analysis including a surface elevation model and magnetic data, and a magnetic 3D inversion. A very recent model of the Cornubian Batholith has been realized by Watts et al. (2024), in which the isostatic nature of plutons has been highlighted. In the papers the authors calculated that the lack of mass due to the density difference between the granite and the sedimentary matrix beneath the batholith is similar to the mass excess due to topography. They also propose that the volume and mass of the batholithic body are respectively at 76367 km^3 and $2.022 \times 10^{17} \text{ kg}$. What we add with our work is a 3D model derived from a joint magnetic and gravity inversion, to which information from petrological studies was added, what allowed to isolate the body. With our inversion we enhanced the knowledge of the densities distribution inside the body and adding information about the density and the

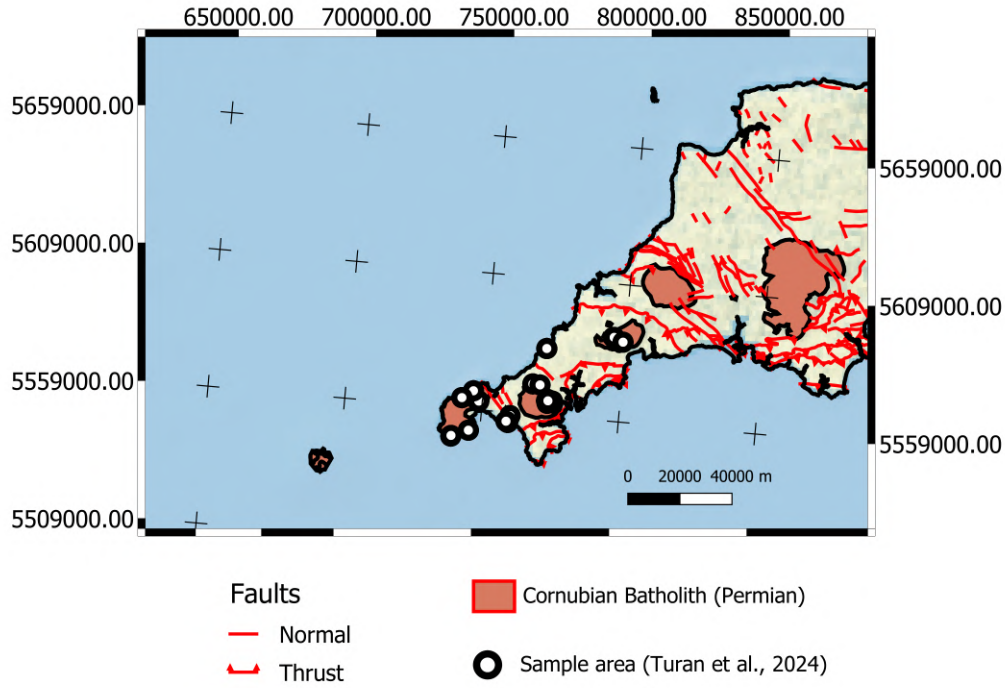


Figure 4.2.2: Tectonic sketch of the Cornwall peninsula. Faults catalogue is downloaded from the British Geological Survey online database.

susceptibility of the sedimentary matrix which cover the area.

4.2.3 Data

The investigated area extends from 7° W to 2° W in longitude and from 49.5° N to 51.5° N in latitude, with a spatial resolution of 2000 m in both directions. Maximum depth reached by the model is ~ 50 km, even if the inversion is performed only until the Moho depth for the density solutions and the Curie layer for the magnetic solutions. Resolution in depth is variable, since it start from 500 m between the first two nodes, then on each following node it increases of the 1.1% respect to the previous resolution, so as to have superficial layers more resolute than middle crust layers. This because we are basically interested in greater detail just for the first kilometers of the model, so we decrease the detail in depth to reduce the amount of data and the size of the final model, as well as calculation time.

Moho and Curie Depth

As explained above, the inversion requires Moho and Curie depth layers to be defined, that go into the input parameters. They basically set a threshold in depth for the final model resulting from the inversions: Moho depth is the bottom limit for the density model, since we are interested only in the crustal density values, while Curie depth is the bottom limit for the magnetic model, since below Curie depth we don't have magnetized material in the Earth. Curie depth is taken from the work of Baykiev et al. (2018), which propose a regional Curie surface for the entire British Isles based on geophysical and petrological observation. We use the regional density model resulted from Baykiev et al. (2018) to define also a map of the Moho depth, analyzing the vertical density gradient for each node of the model, and mapping the maximum density leap. The two layers used to define the investigation depth are shown in Figure 4.2.3.

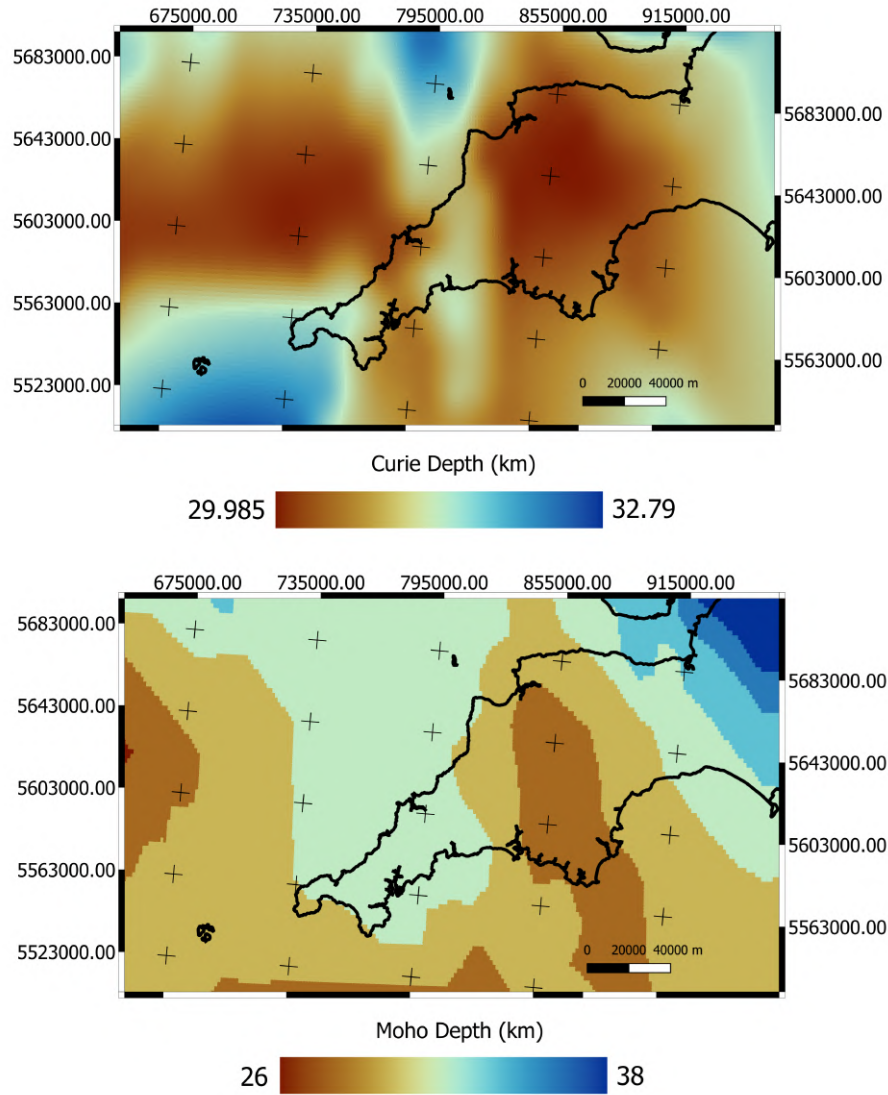


Figure 4.2.3: Above, the map of the Curie layer, taken from Baykiev et al. (2018). Below, the map of the Moho discontinuity, calculated from the density model of Baykiev et al. (2018) analyzing the vertical density gradient.

Gravity data

Original gravity data used to perform the inversion are derived from land measurements conducted on the entire British onshore. The dataset is part of the national archive and consists of the union of different surveys mainly conducted by the British Geological Survey. Measurements cover only the land territory, but the area investigated includes the offshore territory as well. To complete the area, we fill the starting datasets with the global marine gravity anomaly model SDUST2021GRA (C. Zhu et al., 2022). The entire dataset collected is then gridded for the selected area, with a spacing of 0.02° (~ 2 km). An important negative signal, which reaches a minimum of ~ -30 mGal in its most negative part, crosses the entire peninsula from north-east to south-west, defining the presence of a low-density body (Taylor, 2007). To isolate the gravity signal due to the crustal bodies, we reduce the observed signal removing the field generated by the mantle. To do this, we start from a real density model of Great Britain (Baykiev et al., 2018), from which first of all we isolate the mantle densities from the crustal densities, setting the crust density to 0 kg/m^3 , and then we remove a calculated reference model. The reference model is divided into crust and mantle layer, based on the mean Moho depth of the area. Density in the crustal layer is set to 0 kg/m^3 , while for the mantle layer we calculate a mean density

for each depth, to obtain a vertical gradient of density, which increases with depth. To consider the oscillation of the Moho discontinuity, we create two buffer layers: one in the crust, from the reference Moho to the more superficial depth of the real Moho, with a constant density relative to the density in the crust close the Moho; and one in the mantle, from the reference Moho to the deepest depth of the real Moho, with a constant density relative to the density in the crust immediately after passing the Moho (Fig. 4.2.4).

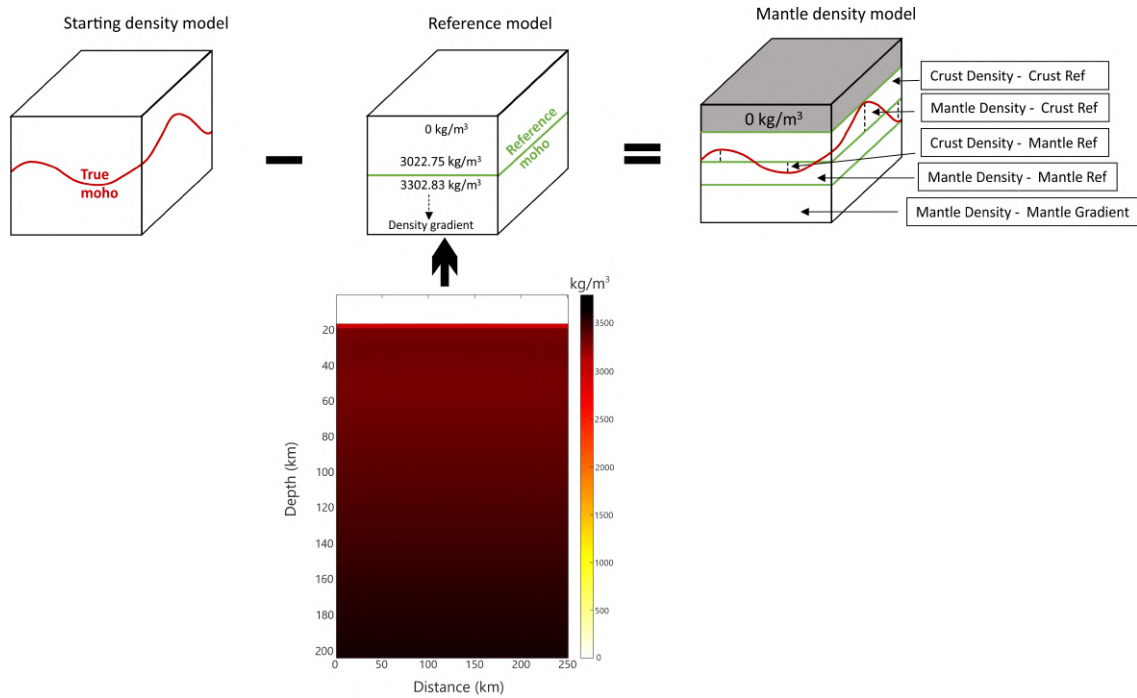


Figure 4.2.4: Sketch explaining the construction of the mantle model, used to calculate the gravity field generated only by the mantle, which was then subtracted from the original gravity signal to obtain the crustal gravity signal. The figure explains how the different layers in the mantle model were created: Starting density model is the density model of Baykiev et al. (2018); Reference model is the built model with density values beginning from the crust-mantle transition (3022.75 kg/m³ is the average density value of the last crustal layer, 3302.83 kg/m³ is the average density value of the first mantle layer); Mantle density model is the model derived from the difference of the previous two models. Crust Ref is relative to the average value of the last crustal layer, Mantle Ref is relative to the average value of the first mantle layer

We subtract this reference model from the real density model, to obtain a mantle density variation model. In the end we perform a forward modeling to calculate the signal generated by the mantle (Fig. 4.2.5). We subtract this signal from our original gravity dataset, and we obtain the crustal gravity signal. Inverting this signal means considering that anomalies are caused only by crustal bodies, which we want to define (Fig. 4.2.6).

Magnetic data

The magnetic dataset used for the inversion derive from an airborne magnetic survey conducted in the area between the years 1957, 1958, and 1961 by the Hunting Geology and Geophysics Ltd and by the Canadian Aeroservices Ltd, overseen by the British Geological Survey (Smith & Royles, 1989). Measured data are then corrected for a local variant of IGRF1990 to obtain the anomalies. Areas which are not covered by the survey were integrated with the WDMAM 2.0 (Lesur et al., 2016) global model, to fill the dataset and obtain a regular input model. As for the gravity datasets, magnetic data was then gridded for the area selected, with the same spacing (0.02°). The south of the peninsula presents a small negative magnetization, while in opposition the north presents a small positive magnetization. A strong dipole is to be

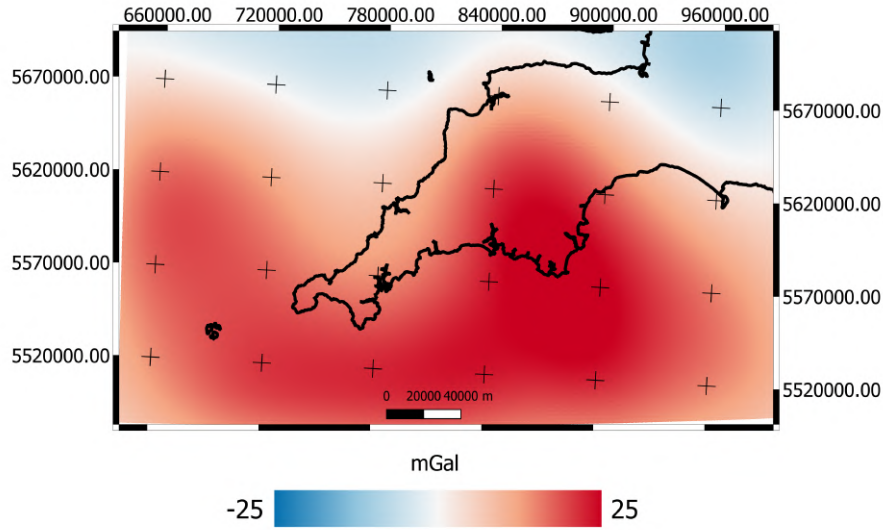


Figure 4.2.5: Gravity signal resulting from the mantle model. This field is removed from the starting data to obtain a residual gravity field indicative only of the crust.

reported, edging the negative gravity anomaly observed from the gravity measurements (Fig. 4.2.6). For all the information about how the survey was conducted, we refer to Smith and Royles (1989).

4.2.4 Methods

Joint Inversion of Gravity and Magnetic data

Joint inversion of gravity and magnetic data is performed using the open-source tool JIF3D (Moorkamp et al., 2011). JIF3D is a 3D inversion framework designed for integrating various geophysical datasets, including gravity and magnetic fields. It employs a limited-memory Broyden – Fletcher – Goldfarb – Shanno (L-BFGS) optimization method, as described in Avdeev and Avdeeva (2009). The methodology, explained in Moorkamp et al. (2011), was then enhanced in Moorkamp (2022) with the inclusion of the mutual information concept. L-BFGS is a Quasi – Newton method which only requires the derivative ($\nabla\phi = \delta\phi/\delta m$) of the objective function (ϕ), respect to the model parameters (m). Therefore, the method uses information from each iteration to update the current model, basing on the gradient calculations expressed (Moorkamp et al., 2011). Starting from an initial model, we perform several iterations until the values of the objective functions, the misfits between observed and synthetic data, reaches a defined threshold. For this inversion we introduce the concept of “Variation of Information” (VI) exploited for geophysical joint inversion by Moorkamp (2021) and Moorkamp (2022). VI is a method conceptually linked to mutual information (MI), which quantifies the shared information between two variables, constructing a one-to-one relationship between the properties under consideration. A low VI value suggests a dependency between the variables, while a high VI value indicates that knowledge of one variable provides little insight into the other. To couple the variables investigated within the inversion framework, VI is minimized. This will result in models where, if possible, each value x corresponds to a unique value y . To minimize the VI, we must include it in the objective function, as follows:

$$\Phi(\rho, \chi) = \lambda_1 \Phi_{d, Grav}(\rho) + \lambda_2 \Phi_{d, Mag}(\chi) + \lambda_3 \Phi_{VI}(\rho, \chi) + \lambda_4 \Phi_{reg, \rho}(\rho) + \lambda_5 \Phi_{reg, \chi}(\chi)$$

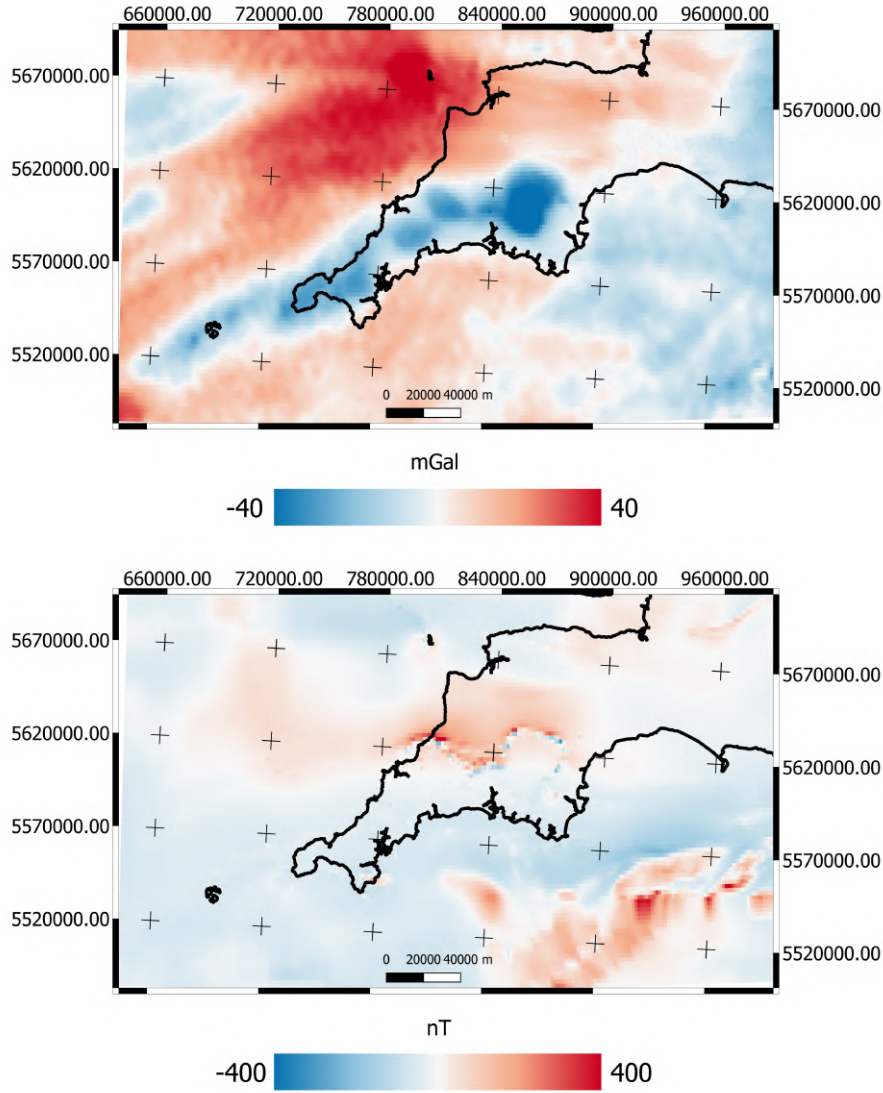


Figure 4.2.6: Gravity (above) and magnetic (below) final field used as input for the inversion.

where $\Phi_{d,Grav}$ and $\Phi_{d,Mag}$ represent the misfit between the observed and inverted gravity and magnetic data, $\Phi_{reg,\rho}$ and $\Phi_{reg,\chi}$ are the regularization terms for density and susceptibility distributions, and Φ_{VI} is the coupling term associated to the variation of information between density and susceptibility retrieved during the iterations. The terms λ represent weighting factors. For more specific information about the mathematical solution of the JIF3D framework, we refer to the article of Moorkamp et al. (2011) and Moorkamp (2022).

Inversion setup

The final model is built by a volume discretized in voxels, with dimension $134 \times 202 \times 25$, for a total of 676700 voxels. Horizontal resolution is set at 2 km, in accordance with the resolution of the gravity and magnetic datasets. Vertical resolution instead is variable with depth. As explained above, inversion occurred up to the Moho discontinuity for the density results, and up to the Curie depth for the susceptibility results, because under the Curie depth rocks lose their magnetization. We perform two different inversions for the same workflow. First, we invert starting with an empty model, where each voxel have values of 0 kg/m^3 in density and 0 SI in susceptibility. Then, we use the results of the first inversion as input for a second inversion. Differences between the two inversions are in the definition of the objective function: for the first inversion we use a high value of coupling and a major regularization. This to enforce

the role of the VI and find similarity between the gravity and magnetic datasets, increasing also the smoothness of the results, because we are inverting on a starting empty model. In the second inversion we minimize the importance of the VI and the degree of smoothness, because in this case we are already inverting on a real model, so we have only the interest that the inversion best fits the two fields. First inversion processed until the limit set in the input definition (80 iterations), while the second inversion stopped after 4 iterations. The exact values of the coupling and regularization, shown in Table 4.2.1, were selected after a series of trials. In the Table are also listed all the technical specifics used for the two inversions.

Table 4.2.1: Input parameters for the two different inversions

	RUN 1	RUN 2
Coupling	30000	10000
Regularization dens/sus	10/10	1/1
Iteration	80	4
Error grav/mag	1 mGal/10 nT	1 mGal/10 nT
Min/max Density	$\pm 250 \text{ kg/m}^3$	$\pm 250 \text{ kg/m}^3$
Min/max Susceptibility	$\pm 0.5 \text{ SI}$	$\pm 0.5 \text{ SI}$
Magnetic field strength	47097 nT	47097 nT
Inclination/Declination	1.1577 rad/0.1788 rad	1.1577 rad/0.1788 rad

Isolation of the body

After the inversion, we obtain as result a cube with density and susceptibility values for the area. To isolate the batholith and obtain the shape of the body we want to investigate, we conduct a numerical analysis basing on the density retrieved. Firstly, we need to retrieve the real density of our model, because we inverted for gravity anomalies and obtain values which express a variation from a background model. To solve this problem, we use the regional model of Baykiev et al. (2018). We properly scale the regional solution, and we add it to the result of the inversion, in order to obtain a model derived from the inversion with real density values. On this model, represented of real ground density values under the Cornwall Peninsula, we conduct an analysis to automatically isolate the shape of the batholith. We refer to a recent petrophysical study conducted on real samples of the Cornubian Batholith (Turan et al., 2024) to select minimum, maximum, and medium density values derived from the samples analysis, which are respectively 2603 kg/m^3 , 2796 kg/m^3 and 2658 kg/m^3 , and which are associated with the top, the bottom and the middle depth of the batholith, assuming that density increases with the depth. With these density values retrieved from the sample analysis we can now conduct a comparison with the densities obtained in our model. Firstly, we note that the maximum density accepted for the batholith, associated with the bottom of the batholith, is observed at a maximum depth of $\sim 18 \text{ km}$, which is so considered the maximum depth reached by the Batholith. This depth is reached in correspondence with the Dartmoor Pluton, which is also the largest of the outcropping plutons. Then, with the other values, we calculate a function which links samples density (Tab. 4.2.2) with the depths of the model. With this function we want to calculate a different density value for each depth in the model, which we assume to be the maximum density accepted for the batholith, at the associated depth. Subtracting from the model all the pixels with a higher density respect to the maximum density accepted, at the representative depth, we are able to isolate the shape of the granitic body.

Table 4.2.2: Depth and respective densities retrieved from Turan et al. (2024) and used to calculate the densities for our layers

Density (kg/m^3)	Depth (m)
2603	200
2658	8966
2796	17676

4.2.5 Results and Discussions

We show now the results of the inversion in the S-W United Kingdom. In Figure 4.2.7.A we see the progress of the Root Mean Square (RMS) values for magnetic and gravity with the iterations. We observe an advancement of the magnetic field curve which is unstable, with approximately-regular spikes. This is the effect of the Variation of Information algorithm, which tends to create mutually similar models in the framework of the joint inversion.

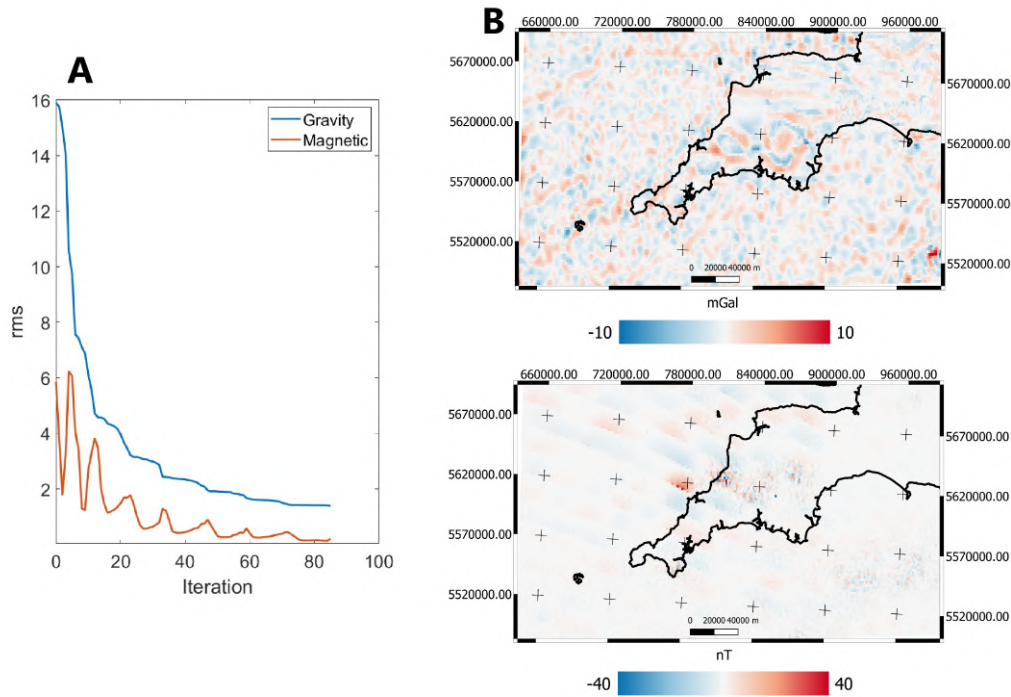


Figure 4.2.7: (A) Gravity and magnetic variation of the RMS with the iteration of the inversion. (B) Gravity (above) and magnetic (below) maps of the residual, obtained subtracting the calculated field from the starting field.

In Figure 4.2.7.B we show the residual field after the inversion, measured by subtracting the model resulting after the inversion from the original model used as input for the inversion. As observed from the maps, all the signal was explained almost perfectly by our density distribution, although there is a salt-and-pepper effect on the gravity map and a striated effect on the magnetic field map, due to the inversion, that we are not able to explain, but that are irrelevant being of low values. Relying on these maps, the model fits gravity data with a standard deviation of ~ 2.2 mGal and the magnetic data with ~ 1.4 nT.

Gravity measurements are relative, so we do not know the absolute value of density within the Earth from regional gravity data. For this reason the program used for the inversion is scripted to invert for gravity anomalies. So after the processing described in the previous section, we obtain as result a cube with density anomalies in the area. Consequently, we also obtain a

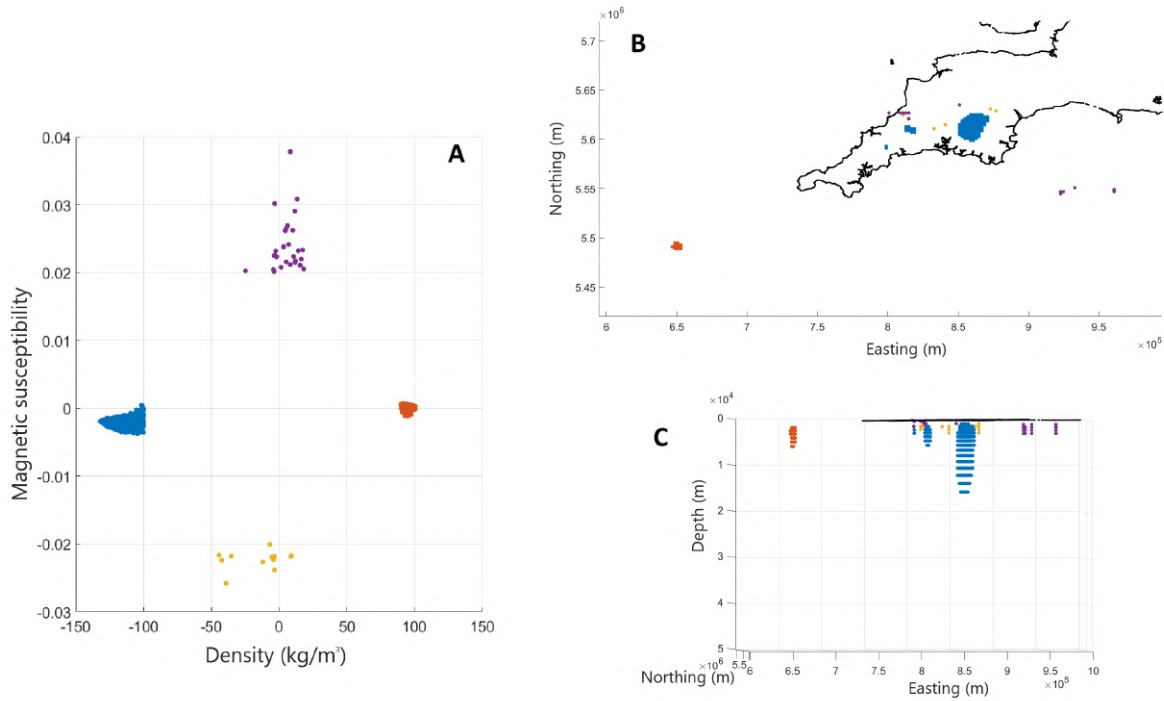


Figure 4.2.8: Different scatter plots of the most anomalous density (blue and orange) and susceptibility (violet and yellow) values resulting from the inversion. (A) Cross-plot between density and susceptibility. (B) Location of the anomalous values on the Cornwall peninsula map. (C) Depth extension of the retrieved anomalous voxels.

cube with the susceptibility values related to the magnetic field. We conduct a preliminary rapid analysis based on these anomaly values. We first realize a scatter-plot where we show the most anomalous values for density ($< -100 \text{ kg/m}^3$ and $> 90 \text{ kg/m}^3$) and for susceptibility ($< -0.02 \text{ SI}$ and $> 0.02 \text{ SI}$) and we display the position of these voxels on the map (Fig. 4.2.8). As expected, we note that most of the anomalous voxels are related with a negative densities, which dominates the peninsula due to the presence of the Batholith. We chose to investigate for this analysis only the least dense voxels in the area setting a threshold of -100 kg/m^3 . Most of these anomalous voxels are located under the Dartmoor Pluton, up to $\sim 15 \text{ km}$. We can say that the root of the Dartmoor represents the least dense area of the Batholith. Dartmoor is also the area with the highest topography, so the deeper and less dense root of the Pluton provides the isostatic balance of the area. Also a small section in the superficial part of the Bodmin Moor pluton presents a set of anomalous values, concentrated between 2 and 6 kilometers of depth. Turning to the positive densities instead, for which the threshold was set to $+90 \text{ kg/m}^3$, we report the presence of a strong off-shore anomaly in line with the direction of the Batholith, positioned to a depth between 2 and 6 kilometers, which should be better investigated. Susceptibility, on the other hand, is not very relevant in the area. However, we report the presence of some superficial voxels with a positive anomaly in susceptibility, at north of the Bodmin Moor pluton, which could be associated with accumulations of magnetic materials. To our knowledge, this model represents one of the most recent and detailed models for the Cornubian Batholith. The work could be considered similar to the very recent work proposed by Watts et al. (2024), but actually our work is different in that we integrate results of our inversion with a regional density model (Baykiev et al., 2018), and use them to define the distribution of the real Batholith densities, while Watts et al. (2024) considers a constant density for the Batholith. After calculating real density values through the use of the regional density model of Baykiev et al. (2018), and through the isolation method described above, we construct our model for the complete granite Batholith, defining the shape and the maximum depths of the body. The complete model is shown in Figure 4.2.9.

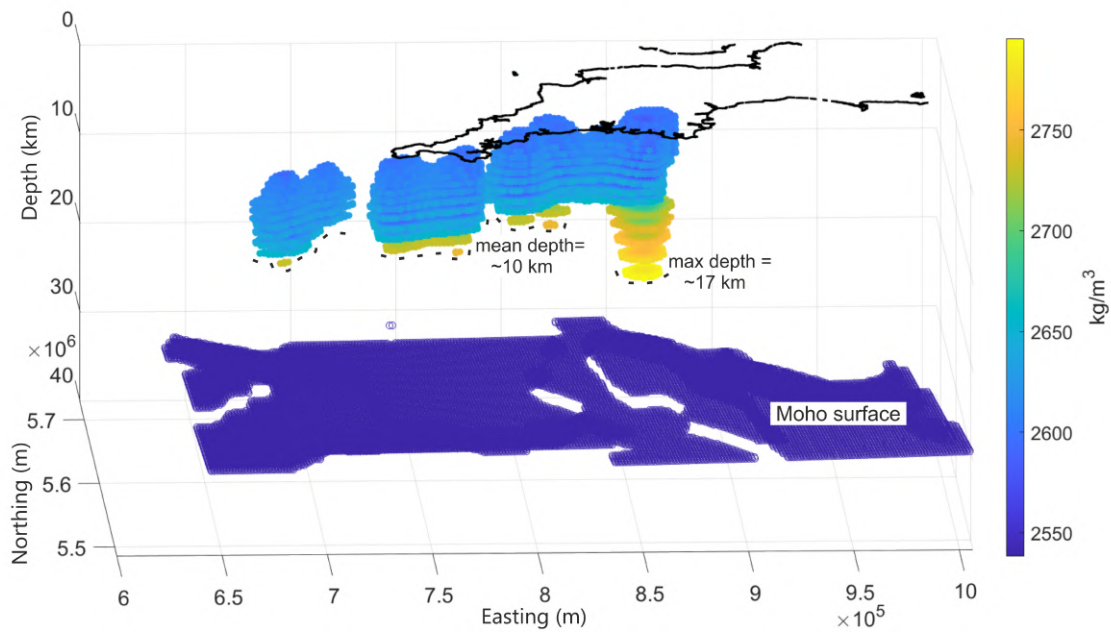


Figure 4.2.9: 3D reconstruction of the Cornubian Batholith, with its density distribution. The model was isolated by crossing the real density data from the inverted cube with the petrological information, using voxels with densities comparable to those of the Batholith samples. We instantly note the separation of the off-shore body. Maximum and mean depth are indicated. With the plot of the Moho surface we want to highlight the position of the Batholith within the crust.

The batholith extends in a northwest-southeast direction across the peninsula, from a latitude/longitude of approximately $50.7^\circ \text{ N}/3.7^\circ \text{ W}$ to $49.75^\circ \text{ N}/6.7^\circ \text{ W}$. The final shape of our model is very similar to that of Watts et al. (2024). It reaches its maximum depth at $\sim 17 \text{ km}$, beneath the Dartmoor Pluton, while in the rest of the body it has an average depth around 10 km . The Dartmoor Pluton corresponds also to the area with the highest topography, associated to the deepest root of the model. The same situation was noted in their model by Watts et al. (2024), and this suggests a connection between topography and roots of the Batholith in which the low-density of the granites operates as a compensation for the surface topography.

We can also see how the body is not continuous as expected but we can essentially divide the on-shore part from the off-shore part. This depended on the methodology used to isolate the body. According to our model, there are no rocks in that area that have physical characteristics comparable to Cornubian granites. For this reason we propose this model with two separated bodies. The Cornwall peninsula is an area that has been affected by intense tectonic activity posterior to the intrusion of the Batholith, from the post-Variscan activity to the recent Atlantic rifting (Shail & Wilkinson, 1994; Ziegler, 1987), that may have caused its rupture.

Considering also the distinct off-shore body as to be part of the complex, we estimate the total volume of the Cornubian Batholith, measuring volumes of the individual voxels and summing them together. The obtained value for the volume of the Cornubian Batholith is 35462 km^3 . Using these volumes and the real densities obtained from the inversion we can also calculate the total mass of the body, which we estimated to be $9.31 \times 10^{16} \text{ kg}$. These estimates include only the subsurface part of the body and not the plutons emerging at the surface. The values of the volume of the body are very similar to the ones proposed by Williamson et al. (2010), based on the model of Taylor (2007), while is considerably lower than the value calculated by Watts et al. (2024), which estimates a volume for the Batholith of 76367 km^3 . Whereas, if we consider the total body mass, our calculations yield a result lower than Watts et al. (2024) result, but the values are comparable.

We now analyze the final density cube, which defines the density distribution in the crust, observing some relevant slices at different depths (Fig. 4.2.10).

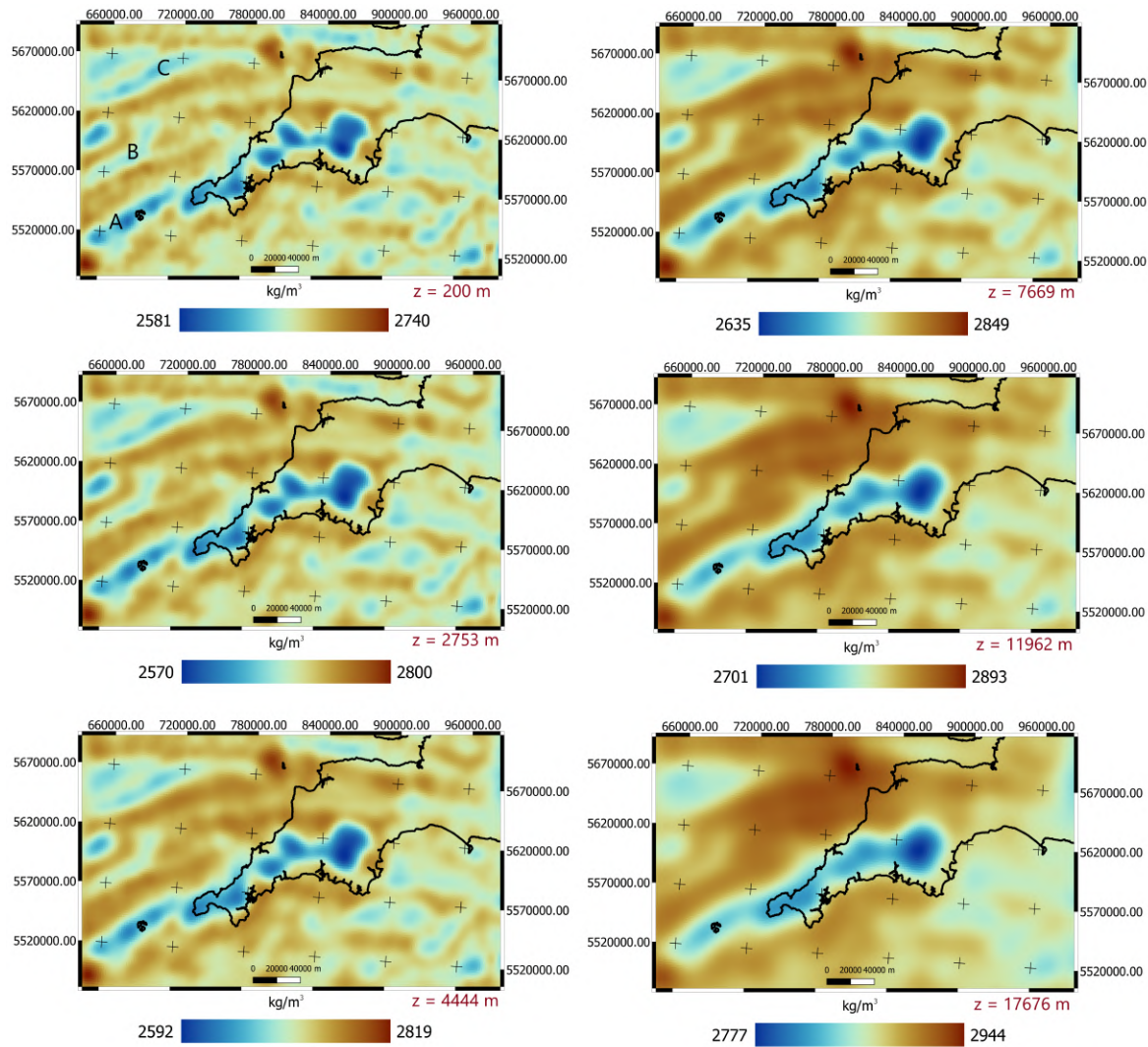


Figure 4.2.10: Slices at different depths representative of the final density model.

Starting from the more superficial slice, to a depth of 200 m, we immediately notice the positions of the granitic plutons, which are highlighted by the lowest density areas on-shore. The sedimentary matrix in which the plutons intruded has a higher density than the batholithic body, although in the northern part of the peninsula it has alternating areas of lower and higher density, which can be traced to different types of sediments. Considering the off-shore part instead, we notice three major low-density lineaments, indicated with the letter A, B and C on the Figure 4.2.10, in the slice relative to $z = 200$. From the southern to northern, this lineaments represent:

- a section of the Cornubian Batholith, separated from the on-shore Batholith (A).
- a second granite body, smaller than the previous one, known as the Haigh Frass Granite (B).
- a third unknown body crossing through the entire area from east to west, interrupted by a denser anomaly near the Lundy island (C).

Lundy is a island in the north of Cornwall peninsula with a volcanic origin tied to deep-seated magmatic activity during the early Paleogene period, associated with the opening of the North Atlantic Ocean when the Eurasian and North American tectonic plates were separating.

Southeast of the off-shore section of the Batholith, we notice a small dense body, which interrupts the batholith, as in the third off-shore lineament described just above, which was related to an island with volcanic origin. Due to the fact that we are at the borders of the area of interest, we are unable to better observe the sources of the anomaly.

Same patterns can also be observed in the other superficial slices, as noted in the ones at 2753 m and 4444 m depths, where even the off-shore lineaments are distinguishable.

The situation changes when we go deeper. At 7669 m we still distinguish lineaments in the sedimentary matrix, although they begin to become homogeneous with the rest of the material, while the off-shore lineaments start to become more feeble and to take a not-well defined shape, not indicative of a particular geological body. Finally, starting from the depth of 11962 m and continuing in depth, the situation becomes almost uniform throughout the area, leaving clearly identifiable the lower density in the Dartmoor and the higher density in the Lundy island.

Turning instead to the analysis of the magnetic susceptibility cube (Fig. 4.2.11), we immediately see that this is almost homogeneous and with nearly zero value over most of the area analyzed. The largely visible high susceptibility values, found in the southern and southeastern area of the map, are not to be considered, as they are most likely errors due to the interpolation of the measured database taken from the British Geological Survey, used as a starting point for all the processing, with the global magnetic field database which we use to fill the voids.

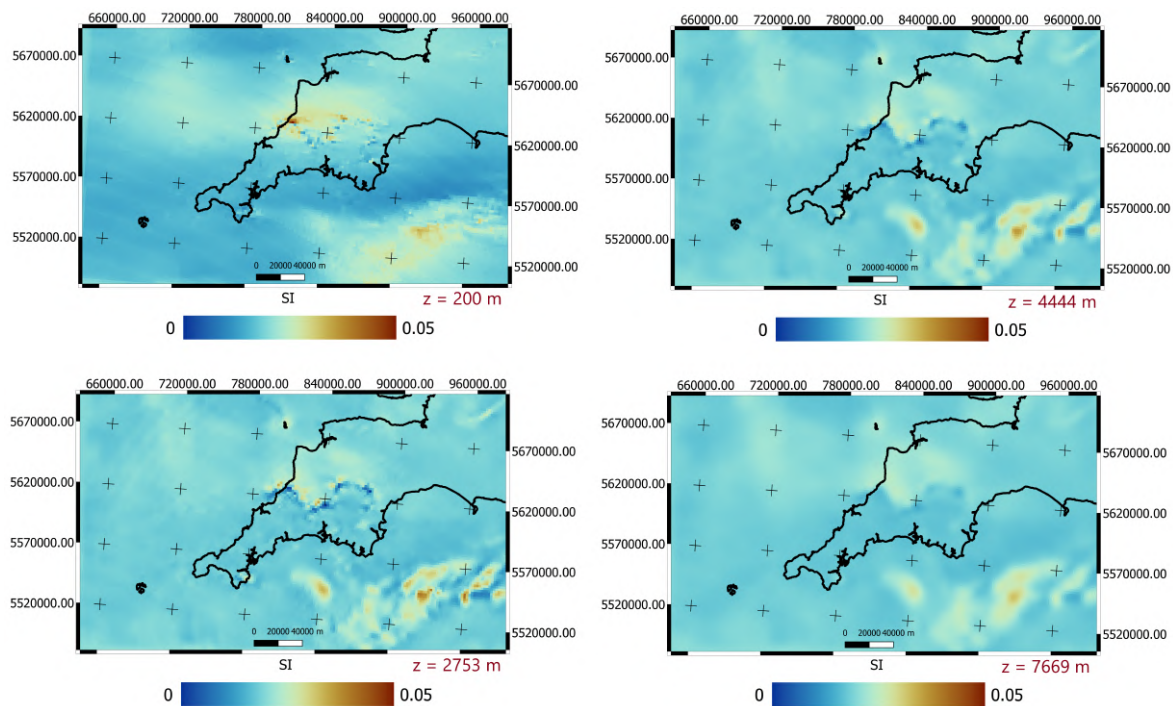


Figure 4.2.11: Slices at different depths representative of the final susceptibility model

Let's consider for a more detailed analysis only that area with higher susceptibility that is visible in the center of the peninsula and extends along a band, in the most superficial slice, while it appears northward edging the Batholith in the slice of the depth at 2753 m. Reached the depth of 2753 m we also note the presence of a small magnetization in the Lizard Complex, southwest of the peninsula, which is the only igneous body that also seems to have a magnetization. The complex is not well known for mining, even if our geophysical results seems to indicate the presence of denser and magnetized materials. Going more in-depth, already from the slice at 4444 m depth, the magnetic field appears to become completely uniform and no susceptibility anomaly is detectable.

Let's now go on to analyze the results of our inversion according to what is the geology in the area. First, we check what is the position of the known superficial igneous bodies with respect

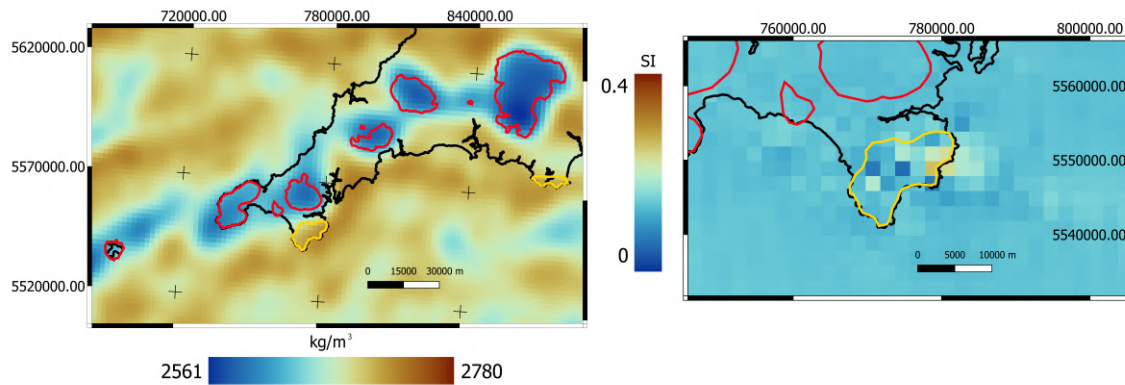


Figure 4.2.12: On the left, density distribution map relative to a depth of 1355 m. With the polygon are indicated the position of the igneous bodies outcropping the area: red contour is for the Cornubian Batholith pluton, yellow contour is for Lizard and Start Complex. On the right, a focus for the susceptibility layer on the Lizard Complex, at a depth of 1355 m. We notice a magnetized part in the eastern part of the Complex.

to our found density anomalies (Fig. 4.2.12). We observe that, as expected, the position of the granitic plutons of the Cornubian Batholith present in the peninsula correspond to the density minima of the area, while for the other two igneous outcrops, the Lizard Complex and the Start Complex, they fall perfectly in denser areas bounded by low-density bands. In particular, the Lizard Complex is another significant geological site present in the area due to its well-preserved ophiolite sequence, which represents a section of ancient oceanic crust and upper mantle uplifted onto continental crust. Analyzing it also considering the susceptibility map, we observe the presence of a magnetized area within the igneous body, a trait that the other complexes in the area do not present.

The results of our inversion are analyzed in relation to the mining presence in the area. We have already extensively mentioned that the area has an important mining history. This is highlighted by the Figure 4.2.13, where the mining hazard catalog for the area is shown. Catalog for mining hazard of the area is taken from British Geological Survey (2021). The dataset identifies the likelihood of past non-coal mining at any particular location.

We note from the map how the western end of the peninsula is the richest and most interesting area in terms of mining. The area overlaps with the low density anomaly retrieved from the inversion. We can consider the mining presence in the area strictly related to the presence of the Batholith. Setting aside the presence of the Batholith, and the associated mineralization, we observe on the map other small spots with great mining potential. Comparing it with the susceptibility map, we report the presence of two high potential mining spots, at north of the Cornwall peninsula and south of the Lizard area, corresponding to two high-magnetization zones. Comparing with the catalog of mines (active and historical) in the area, we observe that the two areas have a not-well known mining history, and would probably be worth investigating more deeply.

We make final considerations on our inverted model by comparing the density anomalies with the different sedimentary coverages in the area.

Observing Figure 4.2.14, we note how different types of sediments give different signals in density. The figure shows the carboniferous sedimentary cover of the area, so the two lithologies, represented with different colors, are coeval. Lithology indicated as 1 in Figure 4.2.14, edging the negative anomaly representative of the Batholith, presents a higher density than the rest of the sedimentary cover, and is representative of the Crackington Formation, a classical flysch sequence of Carboniferous sandstones and grey shales with dark blue-grey mudstones, while lithology indicated as 2 in Figure 4.2.14 is associated with a lower density than the rest of the sediments, and is referred to in cartography as the Bideford Formation. Difference in density

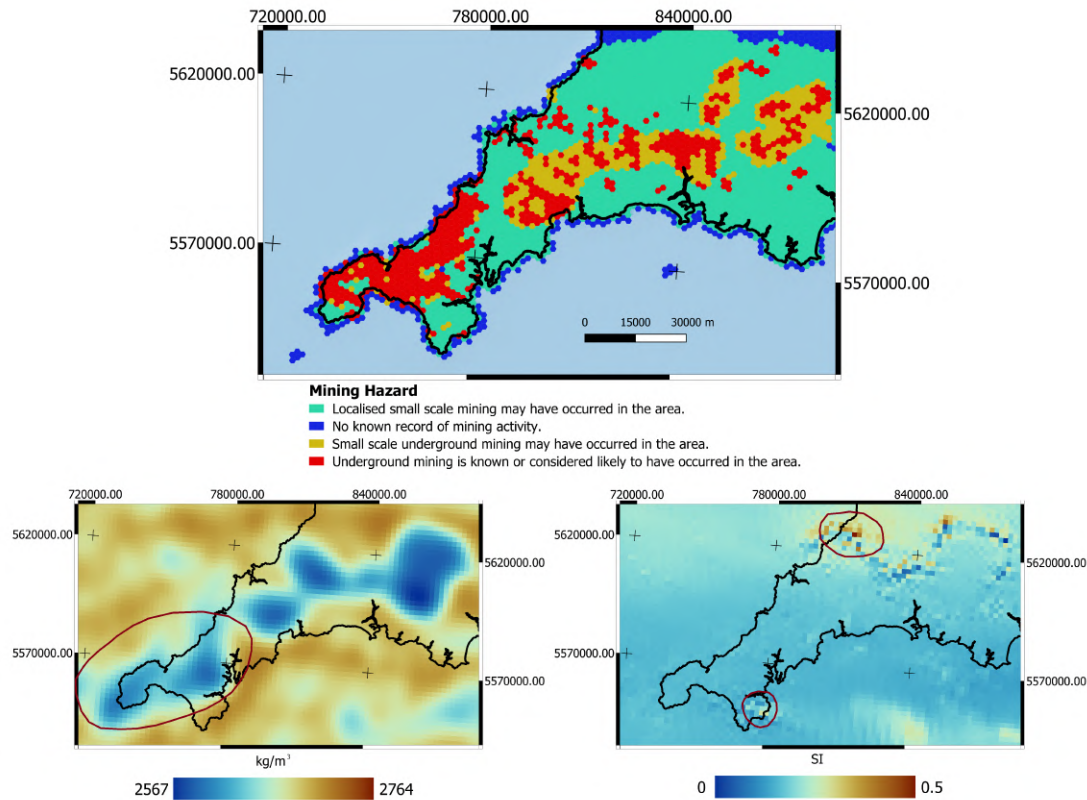


Figure 4.2.13: Thematic map of the mining hazard in the Cornwall Peninsula (Survey, 2021). Map highlights the likelihood that mining may have occurred in the area. In the two maps below, which are indicative of the surface distribution of density (left) and susceptibility (right), are marked with red circles the most interesting areas, where we observe more correspondence between the thematic map and the inversion results.

is defined by the different amount of sandstones in the two formations.

The same considerations can be made for the North Devonian Basin, shown in Figure 4.2.15. Also in this case, the differences in the density retrieved from the inversion are given by differences in the lithologies. Lithology marked in the Figure 4.2.15 with number 2, located in the least dense area, is known as Hangman Sandstone Formation, and is the first to be deposited, in the Lower Devonian. Whereas, lithology marked with number 1 in Figure 4.2.15 is more recent, formed between Middle and Upper Devonian, and indicate a series of different mudstone formations, denser than the previous (Whittaker & Leveridge, 2011).

4.2.6 Conclusion

Target of this work was the production of a crustal model of the Cornwall Peninsula, through a joint gravity and magnetic inversion, with the aim to isolate the granitic body known as Cornubian Batholith, which characterizes the area and produces a strong negative anomaly in gravity field along the entire peninsula. The idea was to define the main characteristics of the body, and the density and magnetic susceptibility distributions in the area, to find a connection with geology and mining occurrence. In the end, we are able to make some considerations:

- the use of a regional density model, joint with our inversion results, give us realistic densities for the batholith;
- off-shore part of the batholith results as a separated body;

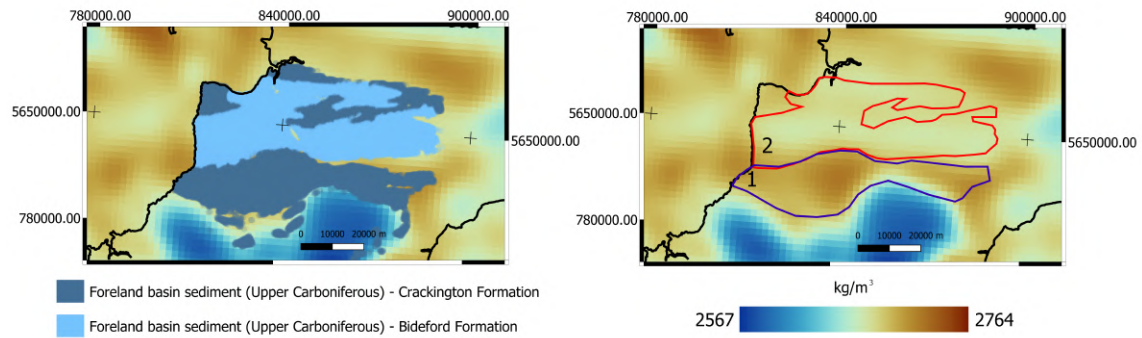


Figure 4.2.14: Map of the densities distribution in the area with overlays of the geological map of the sedimentary cover. In this figure Carboniferous foreland basin sediments are shown: number one, with dark blue in the map on the left, is relative to the Crackington Formation; number two, with light blue in the map on the left, is relative to the Bideford Formation.

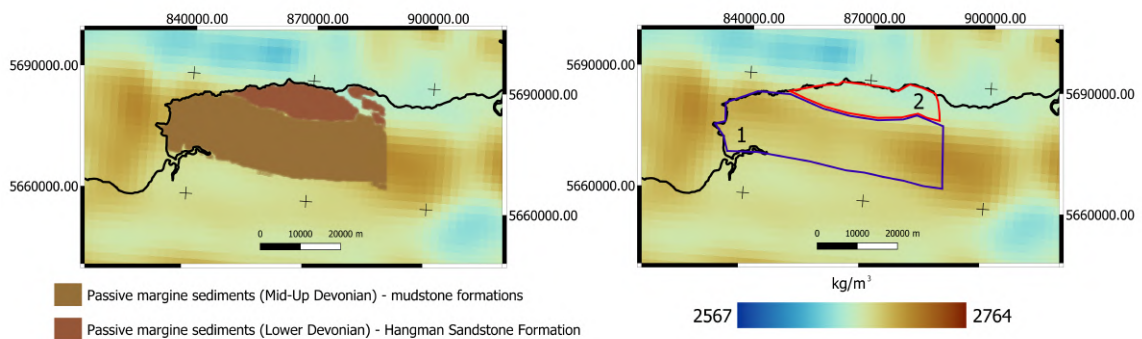


Figure 4.2.15: Map of the densities distribution in the area with overlays of the geological map of the sedimentary cover. In this figure sediments of the North Devon Basin are shown: number one, with light brown in the map on the left, is relative to the Middle to Upper Devonian sediments; number two, brown in the map on the left, is relative to the Lower Devonian sediments.

- terrain plutons are connected to each other. Topography anticorrelates with the depths of the pluton, with the maximum depth of ~ 17 km reached under the Dartmoor pluton. This suggests isostatic behavior of the Batholith;
- the density distribution perfectly reflects the positions of the granitic outcrops. Superficial densities seem to be indicative of different compositions of the sedimentary cover in the north of the Cornwall;
- magnetization does not seem to give a global relevant signals in the area;
- by comparing the results with the Mining Hazard map, we confirm that most of the mineralization is due to the presence of Batholith. We also identify two spots with a relevant magnetic signal that corresponds to potential mining areas, but with few known active or historical mines.

4.3 Small Scale Inversion (Third Article)

The following article was accepted for publication on 4 October 2022, in the journal *Geosciences*. It is available at the doi: <https://doi.org/10.3390/geosciences12100382>. Supporting Information may be found in the online version of the article.

3D Bayesian Inversion of Potential Fields: The Quebec Oka Carbonatite Complex Case Study.

4.3.1 Abstract

Potential fields methods, based on the exploitation of gravity and magnetic fields, are among the most important methods to recover fundamental information on the Earth crust structure at global, regional and local scales. The bottleneck for this kind of geophysical methods is often represented by the development of *ad-hoc* techniques to fully exploit the available data. In fact, each different technique, can observe the effect of a single property of the subsurface and when we want to estimate this property from the observed field (the so-called inverse problem), several problems such as non-uniqueness and instability arise. A possible solution to these problems consists in jointly inverting, in a consistent way, different observed fields possibly incorporating also all the available geological constraints. In the current work, we present an innovative Bayesian algorithm aimed at performing a full 3D joint inversion of gravity and magnetic fields constrained by geological *a-priori* qualitative information. The algorithm is tested on a real-case scenario, namely a local study to estimate a complete 3D model of the Oka carbonatite complex. This complex is a composite pluton in Quebec (Canada), important for mining operations related to critical raw materials such as Niobium and other rare earths. This example shows the reliability of the developed inversion algorithm and gives hints on the fundamental role that potential fields can play in mining activities.

4.3.2 Introduction

The inversion of potential fields, namely gravity and magnetic, is commonly used to infer specific characteristics of the Earth lithosphere. In particular, gravity inversion consists in the determination of the mass density distribution producing a given gravitational signal. Magnetic inversion instead can be exploited to model the magnetic susceptibility distribution that generates a certain anomalous magnetic signal. From the mathematical point of view the inversion is an ill-posed problem presenting two main issues (Sampietro & Sanso, 2012; Sansó & Sampietro, 2021; Sansò et al., 2018): the solution of the inverse problem is not-unique (there are many different density/magnetic susceptibility distributions generating the same response) and unstable (a small difference in the observed signals can lead to a significantly different distribution of the sought property).

Different solutions have been developed in order to solve the gravity and magnetic inverse problems. Among others, we recall here the classical algorithm from Li and Oldenburg. Published in 1996 (Li & Oldenburg, 1996) for magnetic and in 1998 (Li & Oldenburg, 1998) for gravity data, it is a full 3D algorithm to solve the linear inverse problem of estimating the magnetic susceptibility or the density distribution in a given region. In the Li-Oldenburg algorithm, the non-uniqueness of the solution is mitigated by minimising, together with the residuals with respect to the observed gravitational field, also the directional derivatives of the density volume in a Tikhonov fashion (Tikhonov, 1963). Li and Oldenburg also introduced a weighting function in order to prevent the concentration of the density variations close to the surface (minimum energy solution). The strong point of the method is that it represents a 3D inversion scheme but it has also several cons: the choice of minimising the directional derivatives leads to smooth solutions (erasing the sharp discontinuities between different lithological units) and

moreover, the depth weighting function has to be determined in an empirical way (Li & Oldenburg, 1998). For both these aspects, within the years, many contributions tried to improve this algorithm both regarding the mass concentration and the criteria to choose the weighting function (see for instance Portniaguine (1999) and the references therein).

When considering the joint gravity and magnetic inversion, the link between mass density and magnetic susceptibility has to be added into the modelling. This is a hard task usually carried out in different ways: either evaluating possible cross-correlations between the two quantities (see e.g. Fregoso and Gallardo (2009) and references therein) or by establishing empirical relationships between two or more physical parameters (these are the so-called petrophysical methods (Zhang & Wang, 2019)) or through the introduction of geological constraints. A review of pro and cons of the first two methods is reported in Zhang and Wang (2019), while in the following we will focus on the last methodology. With this respect, we recall here the pioneering works of Menichetti and Guillen (1983) where the authors used the generalised inverse method to estimate the shape of causative bodies, in a 2.5-D model (i.e. supposing the model parameters to be constant in one of the planar directions), fixing densities and susceptibilities. In a later work (Serpa & Cook, 1984) the authors used a similar approach to invert for densities, susceptibilities and the vertices of 2.5-D bodies. Zeyen and Pous (1993) instead developed a first algorithm for 3D joint inversion and the authors used geological constraints to reduce the space of the solutions and the steepest descent algorithm to find the result minimising residuals with respect to the observed fields and which is close to the *a-priori* model. In 2006, Bosch et al. (2006) formalised the joint inverse problem in statistical terms by means of Bayes theorem. In their work the authors used a Monte Carlo inversion method to estimate 3D model parameters computing their posterior probabilities. The main disadvantage of this methodology is that it requires the complete *a-posteriori* probability thus *de-facto* allowing the inversion of simplified small problems only. Following the approach described in Bosch et al. (2006) several other methodologies have been developed (Frey et al., 2021; Pollack et al., 2021): however the reported examples are usually limited to extremely simplified models and to the study of very localised anomalies.

In the present work, the 3D Bayesian gravity only inversion algorithm, presented in Rossi (2017), Marchetti et al. (2019) and Sansó and Sampietro (2021) and tested in several synthetic and real case scenarios (Capponi et al., 2022; Sampietro & Capponi, 2021a, 2021b), is extended to allow also for magnetic only or joint gravity and magnetic inversions. In Section 4.3.3 the new elements introduced in the inversion algorithm are presented, while in Section 4.3.4 the joint inversion is applied to a real case study on the Oka carbonatite complex (Quebec, Canada). Finally, Section 4.3.5 summarises the major conclusions and principal results.

4.3.3 Bayesian Inversion of Potential Fields Algorithm

The most challenging aspect of the proposed inversion regards the possibility to estimate, at the same time, the 3D density and magnetic susceptibility distributions and the geometrical shapes of main geological units in the given region, the latter defined by means of a discrete variable (that we will call "label"). Therefore, we have to deal in the inversion with both continuous (density and susceptibility distributions) and discrete unknowns. The Bayesian approach, allowing the connection of the different quantities by means of statistical inference (Mosegaard & Tarantola, 1995), seems to be the most appropriate technique to solve the problem. In our proposed method the studied volume is divided in a set of volumetric elements (voxels): we will suppose to work in planar approximation dividing the volume in right rectangular prisms. However the proposed method can easily be adapted in case of a spherical approximation with voxels made by tesseroids. For each voxel V_i , with index $i = 1, 2, \dots, N$, we define three unknown parameters, namely its density ρ_i , its magnetic susceptibility χ_i and its label L_i . This last variable is used for assigning to V_i a certain geological unit, chosen from an *a-priori* set (e.g. water, sediment, salt, crust, etc.). As mentioned before, ρ_i and χ_i are continuous variables, while

L_i is a discrete one among the M integers denoting the various materials present in the studied volume. We will call $\mathbf{x}$ the set of all the unknown parameters, namely $\mathbf{x} = \{\rho_i, \chi_i, L_i\} i = 1 \dots N$. We suppose that information on $\mathbf{x}$ are in general available from different sources: in fact, studying a certain area, a geologist generally builds up a complex model considering many different information, at different scales and with different levels of confidence. Typical sources can be: regional studies, regional maps, scientific publications, seismic images (2D profiles or 3D volumes), seismic velocities (2D-3D, reflection-refraction), well-logs, etc. A compilation of all this information can be summarised in terms of an *a-priori* 3D structural model. Moreover, in agreement with geologists, it is possible to introduce information on the level of uncertainty about this initial model that can be used to build an *a-priori* probability function $P(\mathbf{x})$ for the unknown parameters $\mathbf{x}$. Note that, if no *a-priori* information is available we can always rely on global models for the major layers (i.e. basement and Moho) or even suppose just one label on the whole cube supposing a certain range of variability for both density and susceptibility. Once $P(\mathbf{x})$ is set, we can exploit the Bayes theorem in its classical form (Bayes, 1763):

$$P(\mathbf{x}|\mathbf{y}) \propto \mathcal{L}(\mathbf{y}|\mathbf{x}) P(\mathbf{x}) \quad (4.5)$$

to get the posterior distribution $P(\mathbf{x}|\mathbf{y})$ of $\mathbf{x}$, given the observations $\mathbf{y}$. In Eq. 4.5 $\mathcal{L}$ represents the likelihood, i.e. the probability of observing $\mathbf{y}$ given $\mathbf{x}$, or in other words the compatibility of the evidence with the given hypothesis.

In the following subsections we will formalise $P(\mathbf{x})$ and $\mathcal{L}(\mathbf{y}|\mathbf{x})$ for the proposed inverse problem, we will compute $P(\mathbf{x}|\mathbf{y})$ and finally we will present a solution to find the set $\mathbf{x}$ maximising the posterior distribution.

The prior probability

As stated above, the prior probability density function $P(\mathbf{x})$, namely $P(\mathbf{x}) = P(L_1, \rho_1, \chi_1; L_2, \rho_2, \chi_2; \dots; L_N, \rho_N, \chi_N)$, should represent the prior knowledge about our 3D volume. The simplest way to formalise $P(\mathbf{x})$, is to decompose the whole probability density function into different factors according to the rule of conditioned probability:

$$P(\mathbf{x}) = \prod_{i=1}^N P(\rho_i, \chi_i | L_i) P(\mathbf{L}) = \prod_{i=1}^N P(\rho_i, \chi_i | L_i) P(L_1, L_2, \dots, L_N). \quad (4.6)$$

Even more, we suppose that ρ_i and χ_i are statistically independent, so that Eq. 4.6 is further simplified in:

$$P(\mathbf{x}) = \prod_{i=1}^N P(\rho_i | L_i) P(\chi_i | L_i) P(L_1, L_2, \dots, L_N) \quad (4.7)$$

meaning that, once a label $L_i = \ell$ has been chosen for the voxel V_i , the corresponding density and susceptibility follows the laws $P(\rho_i | L_i = \ell)$ and $P(\chi_i | L_i = \ell)$, which in our case are truncated normal distributions:

$$\begin{aligned} P(\rho_i | L_i = \ell) &\propto \mathcal{N}(\bar{\rho}(L_i), \sigma_\rho^2(L_i)) \delta_{[\bar{\rho}(L_i) | 3\sigma_\rho^2(L_i)]}(\rho_i) \propto \\ &\propto \exp \left[-\frac{1}{2\sigma_\rho^2(L_i)} (\rho - \bar{\rho}(L_i))^2 \right] \delta_{[\bar{\rho}(L_i) | 3\sigma_\rho^2(L_i)]}(\rho_i) \end{aligned} \quad (4.8)$$

where the characteristic function $\delta_{[\bar{\rho}(L_i) | 3\sigma_\rho^2(L_i)]}(\rho_i)$ truncates the distribution between $\bar{\rho}(L_i) - 3\sigma_\rho^2(L_i)$ and $\bar{\rho}(L_i) + 3\sigma_\rho^2(L_i)$. An analogous term is written for $P(\chi_i | L_i = \ell)$.

In Eq. 4.8 the mean $\bar{\rho}(L_i)$ and the variance $\sigma_\rho^2(L_i)$ represent the expected density of V_i and its variability for the label ℓ . Basically they are the link between label and density, and are given in terms of geological *a-priori* information. Similarly for the expected magnetic susceptibility

$\bar{\chi}(L_i)$ and its variability $\sigma_{\chi}^2(L_i)$. Note also that the relation between χ_i and ρ_i is introduced by L_i .

The independence between ρ_i and χ_i introduced in Eq. 4.7 basically means that it is not expected that there is a relation between density and magnetic susceptibility inside a specific geological unit. We did not find prove of such a relation in literature. The correlation between density and susceptibility, is useful instead when geological units are not explicitly modelled in the inversion (as in Fregoso and Gallardo (2009) and Zhang and Wang (2019)). In this case in fact variations in density can be reflected in variations in susceptibility since they are implicitly subtended by a variation in the material.

As for $P(\mathbf{L}) \equiv P(L_1, L_2, \dots, L_N)$, we assume to have a Gibbs distribution (Azencott, 1988):

$$P(\mathbf{L}) = e^{-\mathcal{E}(\mathbf{L})} \quad (4.9)$$

where the energy $\mathcal{E}(\mathbf{L})$ depends on the values ℓ_i^o provided by the *a-priori* geological model for each label L_i and from cliques (Geman & Geman, 1984) of order two expressing the fact that the value of L_i is more likely to be equal to the value of the labels of the nearest neighbour voxels according to the following rules:

$$P(L_i = \ell | \mathbf{L}_{\Delta_i}) \propto \exp \left\{ -\gamma s^2(L_i, \ell_i^o) - \lambda \sum_{j \in \Delta_i} q^2(L_i, L_j) \right\} \quad (4.10)$$

where γ, λ are parameters to be empirically tuned and, considering the voxel $V_j \in \Delta_i$, Δ_i the neighbourhood of the voxel V_i ,

$$s^2(L_i, \ell_i^o) = s_i^2 = \begin{cases} 0 & \text{if } L_i = \ell_i^o \\ \alpha_i & \text{if } L_i \neq \ell_i^o \end{cases} \quad (4.11)$$

$$q^2(L_i, L_j) = q_{ij}^2 = \begin{cases} a_i & \text{if } L_i = L_j \\ a_{ij} & \text{if } L_i \neq L_j \end{cases} \quad (4.12)$$

defined by the cliques of order two, as mentioned above.

The likelihood

The likelihood distribution is defined by assuming that the observation noise is normally distributed. We define the vector of gravity anomalies observations $\Delta \mathbf{g}^o$, its noise covariance matrix $\mathbf{C}_{\Delta \mathbf{g}}$, the forward modelling operator from densities to gravity anomalies $\mathbf{A}_g$ and the vector $\boldsymbol{\rho}$ composed by the set of densities ρ_i . In a similar way we also define the vector of total magnetic intensity anomalies observation $\Delta \mathbf{B}^o$, its noise covariance matrix $\mathbf{C}_{\Delta \mathbf{B}}$, the forward modelling operator from magnetic susceptibility to total magnetic field intensity $\mathbf{A}_B$ and the vector $\boldsymbol{\chi}$ composed by the set of susceptibilities χ_i . Thanks to the assumptions of statistical independence between the uncertainties of gravity and magnetic methods, the joint likelihood can be modelled again as the product of the likelihood of each geophysical method, thus obtaining:

$$\mathcal{L}(\Delta \mathbf{g}^o, \Delta \mathbf{B}^o | \boldsymbol{\rho}, \boldsymbol{\chi}) \propto \exp \left\{ -(\Delta \mathbf{g}^o - \mathbf{A}_g \boldsymbol{\rho})^T \mathbf{C}_{\Delta \mathbf{g}}^{-1} (\Delta \mathbf{g}^o - \mathbf{A}_g \boldsymbol{\rho}) - (\Delta \mathbf{B}^o - \mathbf{A}_B \boldsymbol{\chi})^T \mathbf{C}_{\Delta \mathbf{B}}^{-1} (\Delta \mathbf{B}^o - \mathbf{A}_B \boldsymbol{\chi}) \right\} \quad (4.13)$$

The posterior probability

The posterior distribution is computed by means of Eq. 4.5, Eq. 4.8, Eq. 4.10 and Eq. 4.13:

$$\begin{aligned}
P(\rho, \chi, \mathbf{L} | \Delta \mathbf{g}^o, \Delta \mathbf{B}^o) \propto \exp \{ & -(\Delta \mathbf{g}^o - \mathbf{A}_g \rho)^T \mathbf{C}_{\Delta g}^{-1} (\Delta \mathbf{g}^o - \mathbf{A}_g \rho) - (\Delta \mathbf{B}^o - \mathbf{A}_B \chi)^T \mathbf{C}_{\Delta B}^{-1} (\Delta \mathbf{B}^o - \\
& - \mathbf{A}_B \chi) - \frac{1}{\sigma_{\rho_\ell}^2} (\rho - \bar{\rho}_\ell)^2 - \frac{1}{\sigma_{\chi_\ell}^2} (\chi - \bar{\chi}_\ell)^2 - \gamma \sum_{i=1}^N s^2(L_i, \ell_i^o) - \\
& - \lambda \sum_{i=1}^N \sum_{j \in \Delta_i} q^2(L_i, L_j) \} \cdot \delta_{[\bar{\rho}_\ell | 3\sigma_{\rho_\ell}^2]}(\rho) \delta_{[\bar{\chi}_\ell | 3\sigma_{\chi_\ell}^2]}(\chi)
\end{aligned} \quad (4.14)$$

where we used the subscript ℓ to indicate the dependency of the variable from L_i . Eq. 4.14 is highly non-linear, non convex and contains a huge number of unknowns, so it is particularly difficult to be sampled or even plotted. Due to these factors, the chosen solution is to find the set of parameters ρ_i , χ_i and L_i maximising the posterior distribution. We observe that, modelling the whole volume with just a unique label, in absence of prior information, is equivalent to removing Eq. 4.9 from Eq. 4.14 thus obtaining the new posterior function:

$$\begin{aligned}
P(\rho, \chi, \mathbf{L} | \Delta \mathbf{g}^o, \Delta \mathbf{B}^o) \propto \exp \{ & -(\Delta \mathbf{g}^o - \mathbf{A}_g \rho)^T \mathbf{C}_{\Delta g}^{-1} (\Delta \mathbf{g}^o - \mathbf{A}_g \rho) - (\Delta \mathbf{B}^o - \mathbf{A}_B \chi)^T \mathbf{C}_{\Delta B}^{-1} (\Delta \mathbf{B}^o - \\
& - \mathbf{A}_B \chi) - \frac{1}{\sigma_{\rho_\ell}^2} (\rho - \bar{\rho}_\ell)^2 - \frac{1}{\sigma_{\chi_\ell}^2} (\chi - \bar{\chi}_\ell)^2 \} \delta_{[\bar{\rho}_\ell | 3\sigma_{\rho_\ell}^2]}(\rho) \delta_{[\bar{\chi}_\ell | 3\sigma_{\chi_\ell}^2]}(\chi).
\end{aligned} \quad (4.15)$$

The maximisation of Eq. 4.15 has the form of a regularised Least Squares Adjustment and gives a solution comparable to that obtained by classical Li-Oldenburg algorithms (Sansó & Sampietro, 2021).

To close this section we want to mention that several other qualitative geological constraints can be added in the inversion (both in a deterministic or probabilistic way). Just to give few examples, we can force an increasing density with depth or we can impose contacts between different geological horizons or the presence of a layered volume, etc. depending on the different case studied.

Maximum a-posteriori by Monte Carlo methods

In the previous sections we retrieved the expression for the posterior probability (Eq. 4.14), and due to its characteristics we chose to find only the set of unknown parameters $\mathbf{x}$ which maximise it. This will be done by means of a simulated annealing algorithm (SA) combined with a Gibbs sampler (Rossi, 2017). In fact the SA provides a mechanism to escape local minima thus finding the global optimum *a-posteriori* (Nikolaev & Jacobson, 2010), while the Gibbs sampler allows to simplify the sampling of the joint distribution (Geman & Geman, 1984). To find the Maximum *a-posteriori* (MAP), we start by defining the target function ε as the opposite of the logarithm of the posterior distribution:

$$\varepsilon(\rho, \chi, \mathbf{L} | \Delta \mathbf{g}^o, \Delta \mathbf{B}^o) = -\log [P(\rho, \chi, \mathbf{L} | \Delta \mathbf{g}^o, \Delta \mathbf{B}^o)] \quad (4.16)$$

as a consequence, the MAP problem is translated into a minimization one, suitable for the simulated annealing. The probability density function P_T to be sampled in the simulated annealing procedure is:

$$P_T(\rho, \chi, \mathbf{L} | \Delta \mathbf{g}^o, \Delta \mathbf{B}^o) = \frac{1}{C_T} \exp \left\{ \frac{1}{T} \varepsilon(\rho, \chi, \mathbf{L} | \Delta \mathbf{g}^o, \Delta \mathbf{B}^o) \right\} \quad (4.17)$$

where C_T is a normalisation constant, and T is the simulating annealing temperature. In order to sample $P_T(\rho, \chi, \mathbf{L} | \Delta \mathbf{g}^o, \Delta \mathbf{B}^o)$ the Gibbs sampler is introduced. The advantage of the Gibbs sampler is that it allows sampling a multidimensional random variables by drawing samples

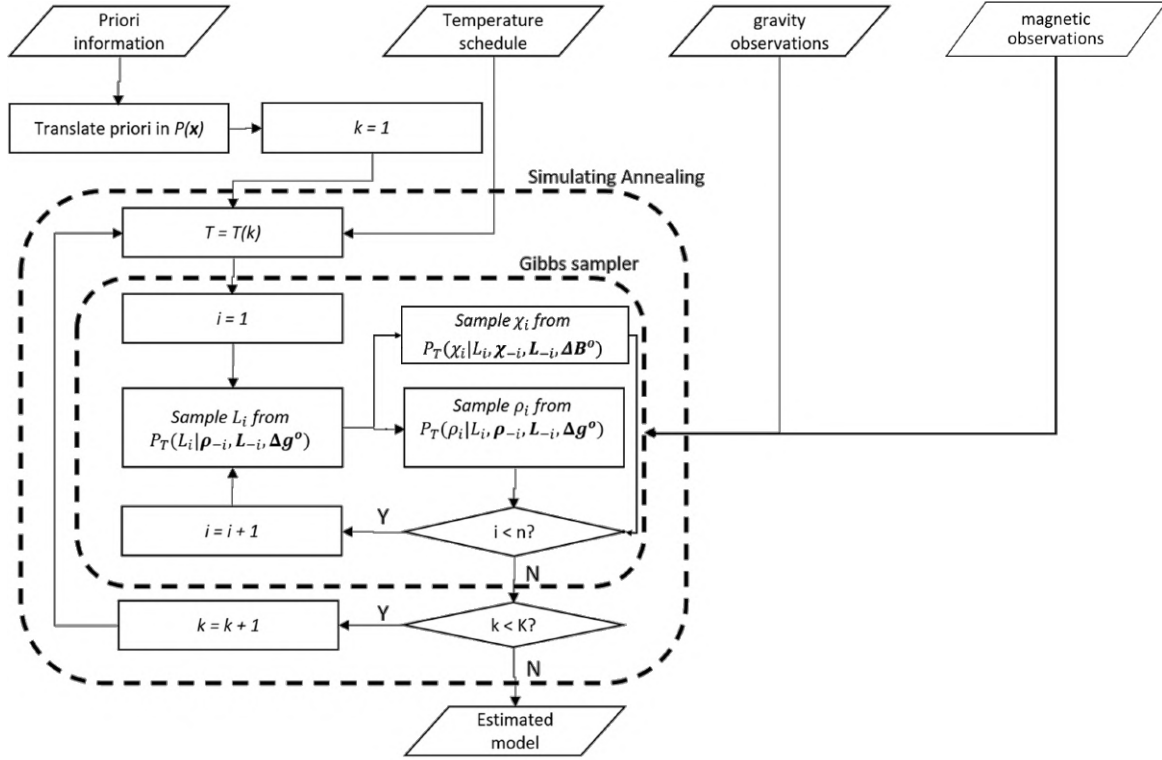


Figure 4.3.1: Flow chart of the proposed solution

from its conditional probability distributions. In the proposed solution, at each step of the iterative procedure a sample of the set label-density-susceptibility for the voxel i is drawn from their conditional distributions $P_T(\rho_i, \chi_i, L_i | \rho_{-i}, \chi_{-i}, L_{-i}, \Delta g^0, \Delta B^0)$. Here ρ_{-i} , χ_{-i} and L_{-i} represents all the density and labels apart those related to the voxel i . This is a three-dimensional conditional probability that can be decomposed into the product between the conditional probability of the density ρ_i given the label L_i , of the susceptibility χ_i given the label L_i and the marginal probability of the label L_i , namely:

$$\begin{aligned}
 P_T(\rho_i, \chi_i, L_i | \rho_{-i}, \chi_{-i}, L_{-i}, \Delta g^0, \Delta B^0) &= \\
 &= P_T(L_i | \rho_{-i}, \chi_{-i}, L_{-i}, \Delta g^0, \Delta B^0) P_T(\rho_i | L_i, \rho_{-i}, L_{-i}, \Delta g^0) P_T(\chi_i | L_i, \chi_{-i}, L_{-i}, \Delta B^0)
 \end{aligned}
 \quad (4.18)$$

where the statistical independence between density and susceptibility has been exploited. Therefore, the three-dimensional joint probability of label density and susceptibility shown in Eq. 4.18 can be sampled by first drawing a sample from the label marginal distribution $P_T(L_i | \rho_{-i}, \chi_{-i}, L_{-i}, \Delta g^0, \Delta B^0)$ and then, according to the extracted label value, from the density and susceptibility conditional ones $P_T(\rho_i | L_i, \rho_{-i}, L_{-i}, \Delta g^0)$ and $P_T(\chi_i | L_i, \chi_{-i}, L_{-i}, \Delta B^0)$. This procedure can be repeated iteratively for all the voxels, updating each time the previous parameters realisation. Once all the voxels are updated, the temperature is slowly decreased and a new stage of the Gibbs sampler is started again, as shown in the flow chart of Fig. 4.3.1. In details we select a geometrical cooling law for T with a variable cooling factor, namely $T(k) = T_e e^{(ak+b)^c}$, where k is the simulated annealing iteration and the constants T_e , a , b and c are estimated as described in Rossi (2017). For a more detailed description of the above optimisation algorithm, the interested reader can refer to sections 9.6 and 9.7 of Sansó and Sampietro (2021). Since the sampling of L_i , ρ_i and χ_i is a random process, it is possible to repeat the simulated annealing procedure several times starting from different random seeds. This is equivalent to perform a set of independent inversions, each arriving to a slightly different 3D model (in principle) close to the actual absolute MAP. We call L_i^n the solution of the inversion n

for the voxel i . Analogously we will have a set of ρ_i^n and χ_i^n with $n = 1, \dots, N$ and N the number of independent inversions performed. The final result is computed by taking the mode of the label of each voxel $\hat{L}_i = \text{mode}\{L_i^{n=1}, \dots, L_i^{n=N}\}$, and the average of the density and magnetic susceptibility considering only the solutions where $L_i^n = \hat{L}_i$.

Moreover the frequency of L_i^n with $n = 1, \dots, N$ and the standard deviation of the extracted densities and susceptibilities, always considering only the solutions where $L_i^n = \hat{L}_i$, give a voxel-wise estimate of the accuracy of the retrieved model.

4.3.4 The Oka Case Study

As reported in the Introduction the proposed optimisation algorithm has already been intensively tested for the gravity-only inversion. We propose here a real case study on the Oka carbonatite Complex in the Monteregian Igneous Province, Canada (Gold, 1967; Thomas et al., 2016; Treiman & Essene, 1985) to show the quality of achievable results.

The Oka carbonatite Complex

The Monteregian Igneous Province (MIP) is a large area in the south of Québec, Canada, which consists in nine alkaline intrusions and dikes arranged in an approximately east-west direction, starting 60 km West of Montreal, across St. Lawrence Lowland. Its characteristic quasi-linear trend suggests that the pluton positioning was controlled by a deep-seated fault (Gold, 1986). Starting from the Easternmost intrusion, there's a progressive change from area with abundance in felsic rocks and quartz-saturated rocks towards more westerly carbonatites complex with silica-undersaturated rocks, while content in Fe increase from west to east (Gold, 1986). These differences in silica content between complex arose because of the different period of rocks emplacements, occurred in two different magmatic events, from 117 to 141 Ma, and in response to an upward transport of a metasomatic fluids in mantle (Eby, 1984). The Oka pluton is the westernmost and younger complex in the entire MIP. The intersection of two different tectonic lineaments, the northwest trending Beauharnois arch and eastward trending faults associated with the Ottawa-Bonnechere graben, is thought to have constrained the emplacement of the complex (Eby, 1975). Pluton is a bean-shaped body, composed in the central part by both carbonatite and Si-undersaturated rocks like okaite, ijoite, alnoite, and jacupirangite (Chen & Simonetti, 2014), boarded by strongly metasomatized rocks (feniti), as usual with carbonatites bodies, and intruded in a Precambrian gneiss an anorthosites ground. Oka carbonatite are mainly a coarse-grained calcite-carbonatite, which under these conditions are called sovite. It's composed by a high percentage of calcite, and other accessories minerals like apatite, biotite, wollastonite, magnetite, and pyrochlore. Presence of pyrochlore is very relevant as it is the main mineral from which Niobium is extracted. Mining activity in fact was carried out in the past in this area. Okaite is composed by a large volume of melilite, and a minor amount of apatite, biotite, perovskite, and magnetite. Ijolite includes wide variety of mafic rocks and is composed essentially by nepheline and pyroxenes, while jacupirangite made up of a great percentage of fassaite (a variety of augite, pyroxene) and other small percentages of nepheline and magnetite (Chen & Simonetti, 2014). Carbonatite rocks and Okaite have the largest percentages of magnetite in their composition, so we imagine they are the most magnetized rocks in the complex. Jacupirangite is the rock with the major density, while for the carbonatite system, densities go from 2840 kg/m³ for sovite, which forms the biggest part of the complex, to 3410 kg/m³ for the magnetite-carbonatite (Thomas et al., 2016).

The A-priori Model

As stated in the previous section the complex is made by two close intrusive centres resembling a distorted figure eight-shape in plan view. Each centre has a central plug of carbonatite surrounded by alkalic silicate rocks and an aureole of fenitization of the gneissic country rocks.

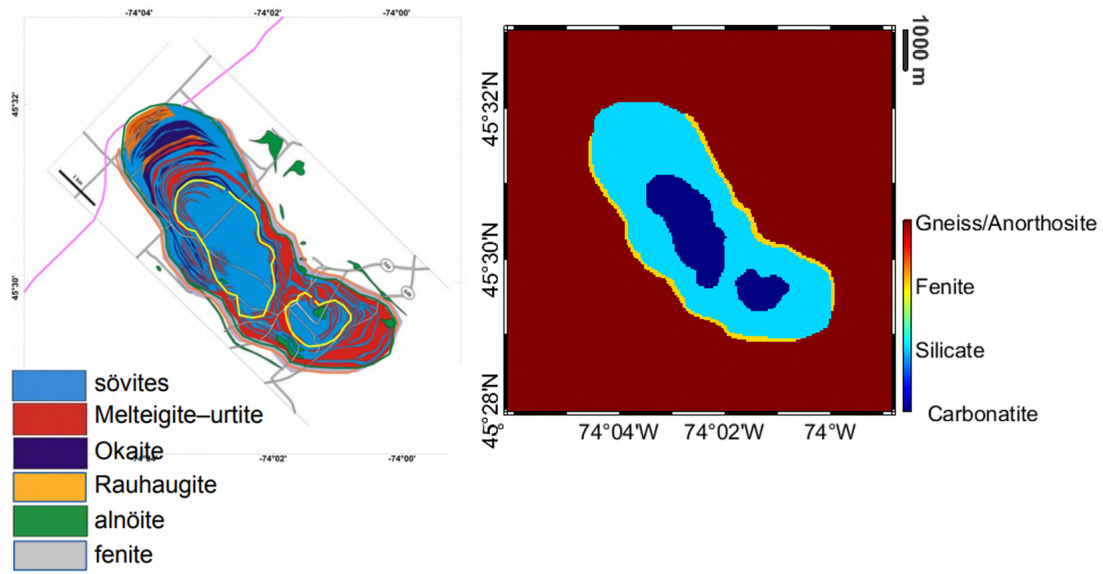


Figure 4.3.2: Detailed geological model of Oka Carbonatite complex from (Gold, 1986) (left) and simplified geological model used to build the *a-priori* model (right).

Table 4.3.1: A-priori model in terms of density, expressed as average values and variability.

Layer	Mean [kg/m^3]	Density variability σ [kg/m^3]
Carbonatite	2880	25
Silicate	2930	100
Fenite	2700	52
Gneiss/Anorthosite*	2740	52

* A lateral density variation is considered for the background with average density of $2740 \text{ kg}/\text{m}^3$ in correspondence of gneiss and of $2700 \text{ kg}/\text{m}^3$ in correspondence of anorthosite in the northwest corner of the study area.

In order to build the *a-priori* model, in absence of better knowledge, we started by adopting a simplified scheme (see Fig 4.3.2), accordingly to Sanders Geophysics (2019), continued up to a depth of 10 km in a constant cylindrical way. We suppose that each boundary between the different units can expand up to about 1 km or reduce to the boundary of the inner geological units. This will represent our *a-priori* information about the geometries. As for the *a-priori* densities and magnetic susceptibilities, they are supposed to be constant in the vertical direction with the value reported in Tab. 4.3.1 and Tab 4.3.2. We want to underline here that this simplified model represents the actual available information on the study volume. The inversion algorithm will modify the boundaries between the different geological units and will introduce voxel by voxel variations in the density and magnetic susceptibility coherently with the specified range of variability of each parameter.

Gravity and Magnetic Observations

Gravity and magnetic data have been downloaded from the Natural Resources of Canada webpage (Canada, 2016). In details, considering gravity observations we started from a set of point-wise ground Bouguer anomalies (corrected with a density value of $2670 \text{ kg}/\text{m}^3$), derived from several surveys and with accuracy ranging between 0.5 and 5 mGal. We build a complete grid

Table 4.3.2: A-priori model in terms of magnetic susceptibility, expressed as average values and variability.

Layer	Mean [S.I.]	Susceptibility variability σ [S.I.]
Carbonatite	0	$3 \cdot 10^{-6}$
Silicate	0.3	0.016
Fenite	0	$3 \cdot 10^{-6}$
Gneiss/Anorthosite	0.03	0.01

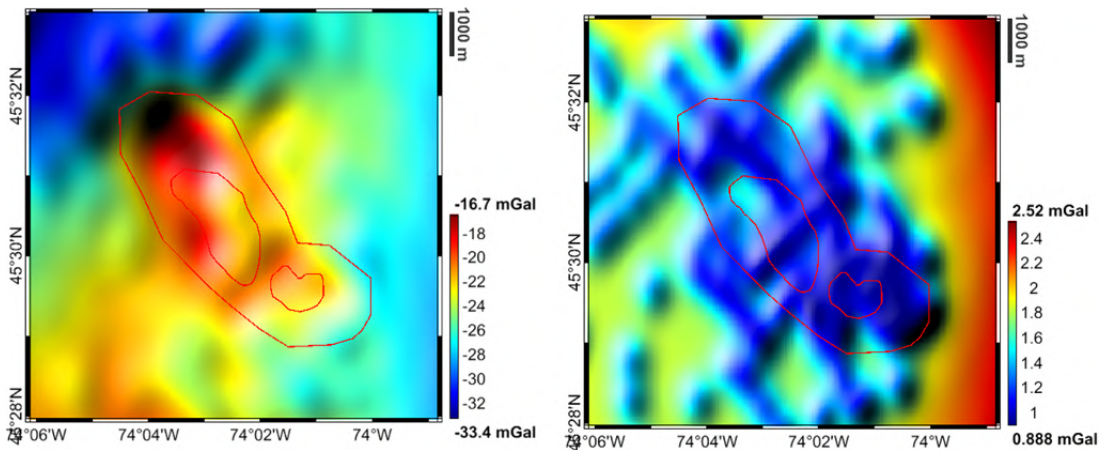


Figure 4.3.3: Computed grid of Bouguer gravity anomalies (left) and predicted accuracy (right). Red lines represents the boundaries of main units of the Oka complex.

on the study area with a spatial resolution of 100 m×100 m, together with its predicted accuracy (see Fig. 4.3.3) by exploiting a Least Square Collocation procedure (details can be found in Sampietro et al. (2017)). Looking to the gravity grid it can be seen how it well represents the main geological units in the area: we can notice the gravity low in the northwest corner corresponding to the presence of light anorthosite and the gravity high due to the silicated rocks. Looking to the predicted accuracy, we can recognise regions where gravity observations are actually available (blue regions in the map) from regions where the grid has been interpolated. Note also that in the easternmost area data are missing thus resulting in an inaccurate gravity estimate.

As for the magnetic field an helicopter borne grid of Total Magnetic Intensity anomalies at 137 m above sea level have been used (Fig. 4.3.4). The original grid downloaded from the

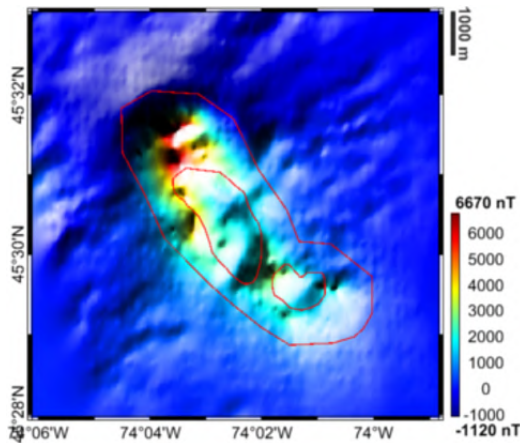


Figure 4.3.4: grid of Total Magnetic Intensity anomalies downloaded from the Natural Resources of Canada (2016). Red lines represents the boundaries of main units of the Oka complex.

Natural Resources of Canada (2016) has a spatial resolution of $50 \text{ m} \times 50 \text{ m}$ and comes from data acquired with line spacing of 200 m at a bearing of $\text{N}16^\circ\text{W}$. In our work the original grid has been downsampled to a spatial resolution of 100 m.

Also in this case the observations well correlate with the *a-priori* model, showing high magnetisation values for silicate. No information on the accuracy of the magnetic grid is provided by the Natural Resources of Canada webpage. The inducing magnetic field is computed from the CHAOS-7.8 model (Finlay et al., 2020).

Inversion Results

Starting from the *a-priori* information described in Section 4.3.4, namely geometries of the main geological units, average density and susceptibility and the corresponding expected accuracy, we are able to build the *a-priori* density and susceptibility cubes of our volume. In doing this we considered a spatial resolution in the planar direction of about 100 m both in x and y . As for the vertical we considered voxels with a thickness ranging between 50 m at the surface to 500 m at the base of the model here fixed at a depth of 10 km for a total number of volumetric elements of $100 \times 100 \times 61 = 6.1 \cdot 10^5$ corresponding to about $1.8 \cdot 10^6$ unknowns. The discretization has been assumed following the principles explained in Sampietro and Capponi (2019) also extended to the magnetic field, here supposed to be known with an accuracy of 2 nT. The λ and γ parameters in Eq. 4.14 has been fixed at 0.005 and 0.011 by empirically equalising the order of magnitude of the different terms of Eq. 4.14. As for the computational time, the inversion arrives at convergence after 200 iterations of the SA, taking about 10 hours on an Intel i3 8 Gb Ram computer. In order to estimate the accuracy the SA optimisation has been repeated 10 times starting from different random seeds, however this is a parallel procedure which does not requires extra computational time if enough CPUs are available. Some tests have shown that down-sampling the problem to a resolution of 150 m or even to 200 m gives same major features in terms of results, reducing the computational time to about 2 hours (for the 200 m resolution) with just a slightly worse fitting of the data in the high frequencies.

We report in Fig. 4.3.5 the residuals for the gravity and magnetic fields of the *a-priori* (before applying the inversion) and of the *a-posteriori* (after applying the inversion) models. What we can observe is that the inversion has been able to noticeably reduce the misfit with respect to the observed fields from 2.2 mGal and 1130 nT of the *a-priori* model to 0.28 mGal and 210 nT of the final solution. Focusing on the gravity residuals, we see that the residuals of the *a-priori* model is dominated by high negative values, close to the southernmost limit of the Oka formation and by a general southwest-northwest trend. These main characteristics have been properly corrected in the final results which just shows two small anomalies, opposite in sign, in correspondence of the core and in the northern part of the carbonatite complex. In any case we can see, comparing Fig. 4.3.5 and Fig. 4.3.3, that the obtained residuals are compatible with the predicted accuracy, namely they are always smaller than the three times the standard deviation reported in the accuracy map.

As for the magnetic field we can see that higher residuals of the *a-priori* model are found for the core and in the southernmost part of the complex and are remarkably reduced in the final results with very small features probably associated to detailed geology of the area. These residuals are indicative of a too poor *a-priori* modelling of that specific region. In this sense our solution tends to force the cooperation between geophysicists and geologists for a good formalisation of the *a-priori* model and of the relative constraints. To improve the fitting of the magnetic fields two possibilities can be foreseen: either to suppose, in contrast with the available geological information, a low magnetisation also in the sovite core, or to have a slightly less dense carbonatite core with intrusion of more magnetised bodies. Small intrusions of few hundreds metres thickness magnetised silicate could in principle explain these residuals. However this is something that can be hardly discriminated by potential fields alone without any constraints based on further geological or geophysical evidences.

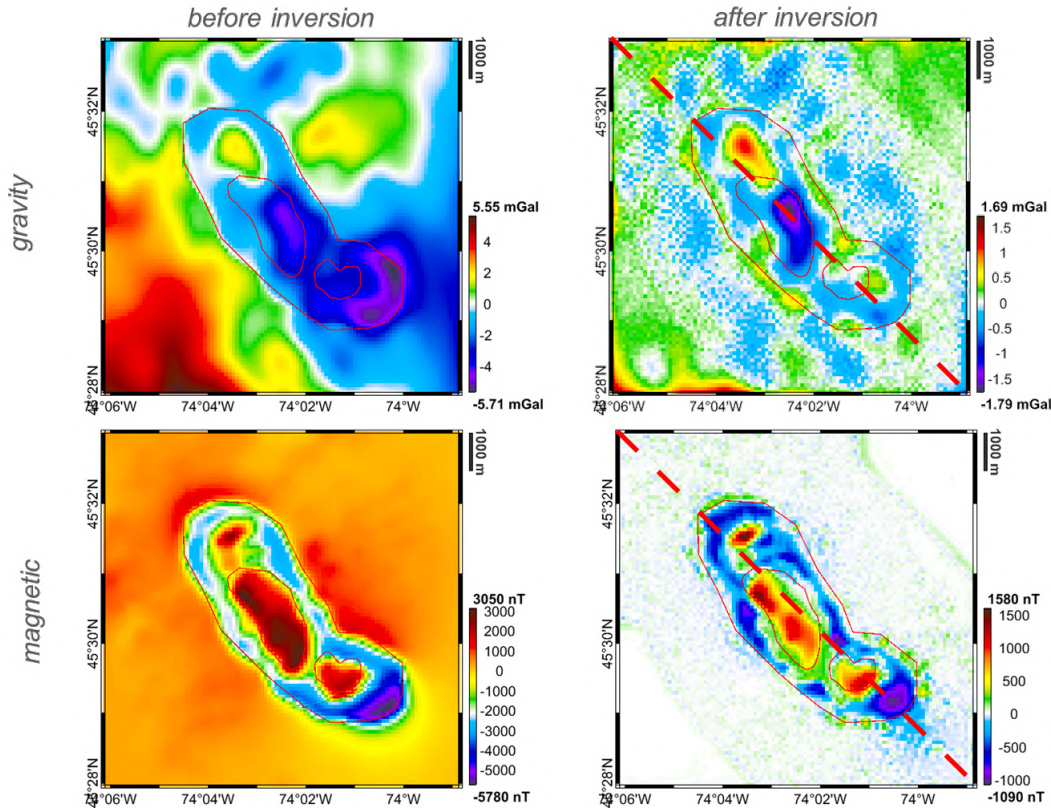


Figure 4.3.5: Residuals before (left) and after (right) applying the joint inversion for the gravity (up) and magnetic (down) fields. Red lines represents the boundaries of main units of the Oka complex. Red dashed line is the profile shown in Fig. 4.3.9

Looking to the results in terms of geometries of geological units, we found a fanning of silicate and fenitized rocks in the shallowest part (up to a depth of about 4.5 km) of the model. Here the fenitized gneiss extension has been increased from about 100 m of the a-priori model to about 600 m. This is coherent with what described in Lentz et al. (2006). The inversion also slightly reduced here and there the silicate annular rings in favour of carbonatite and fenitized gneiss. Fig. 4.3.6 shows the density and susceptibility distribution obtained by the joint inversion at 1 km depth. We can notice in both the maps the presence of well defined sharp variations of the specific property at the boundary of different geological units. Looking to the density maps we can also see high density values (of about 3000 kg/m^3) in the northern part of the complex that can be associated to the presence of the okaite series while, when moving south, lower density values around 2900 kg/m^3 are found in correspondence of the melteigite-urtite series. This corresponds well to the detailed geological maps and to our knowledge of the detailed

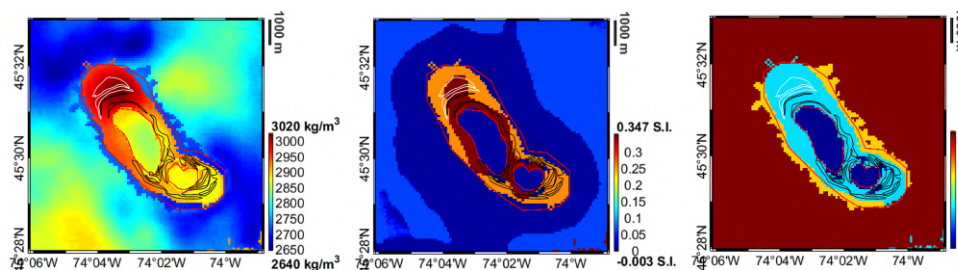


Figure 4.3.6: density, susceptibility distributions and label model from the final solution at 1 km depth. White lines are boundaries of known main okaite formations and black lines are boundaries of main melteigite-urtite formations digitized from Fig. 4.3.2.

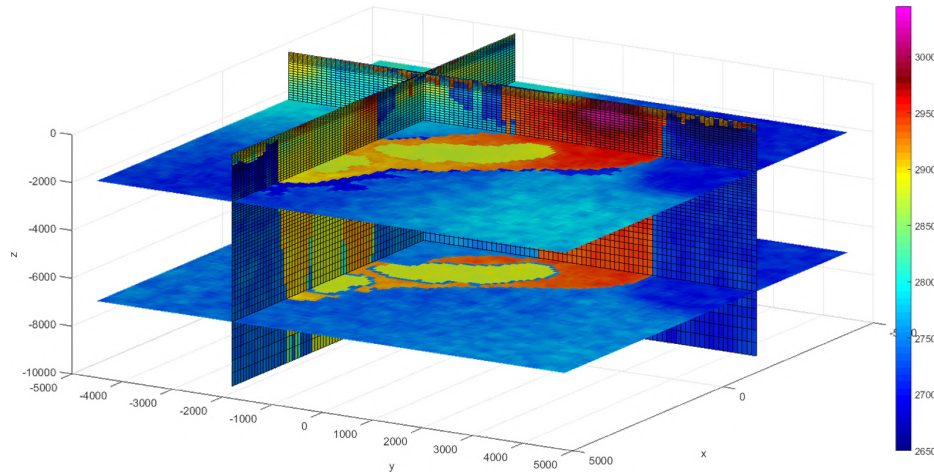


Figure 4.3.7: Estimated 3D density model. Units are kg/m^3

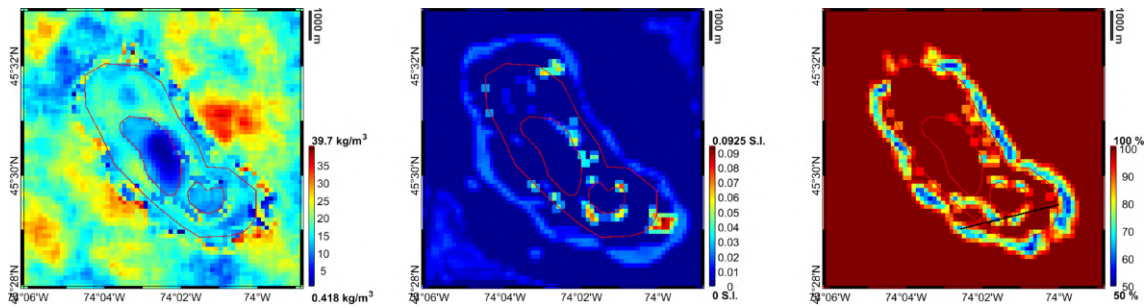


Figure 4.3.8: Predicted accuracy at 1 km depth in terms of density (left), susceptibility (centre) and label (right)

geological formations retrieved from literature (which foresees densities of 2970 kg/m^3 and 2880 kg/m^3 , see Gold (1967)). The estimated sovite density is of about 2860 kg/m^3 which is again well aligned with literature (see e.g. Ramberg (1973)). Looking to the susceptibility map we can observe how the inversion predicts significant susceptibility only in the silicate rocks with values radially decreasing from the core of the anomaly. Fig. 4.3.7 shows some slices of the full 3D density model. We can observe from the figure that the Oka complex extends downwards in a cylindrical way for at least 10 km and possibly more. Okaite seems to be presents only in the first few kilometres (up to a depth of 2 km), while fenitized rocks slightly decrease their thicknesses with depth and disappears at a depth of about 4 km. The Bayesian inversion also allows obtaining the accuracy of the model. We report in Fig. 4.3.8, as an example, the accuracy map of density, susceptibility and label at 1 km depth. We can observe that the largest uncertainty in terms of density are in the background where in any case the uncertainty has been reduced from 100 kg/m^3 (see Tab. 4.3.1) to less than 40 kg/m^3 . As for the susceptibility very localised uncertainties are found mainly close to the boundary of the silicate rings. Finally looking to the labels we can see that the most uncertain region is the fenitized rocks which bounded the complex.

The developed software allows to perform also gravity only or magnetic only inversions, by considering only the corresponding terms in the objective function (Eq. 4.14). We report in Fig. 4.3.9 the gravity and magnetic signals along the profile shown in Fig. 4.3.5 for the gravity only, magnetic only and joint inversion. We can see that all the inversions are able to predict the observations, with slightly worse performance for the joint results. This is expected since the joint inversion fitting at the same time the gravity and magnetic fields puts more constraints on the final solution. However, comparing the results of the different solutions in terms of labels, we can note that there are important differences between the joint and the gravity only, magnetic only inversions. We report in Fig. 4.3.10 the results of the three inversions in terms

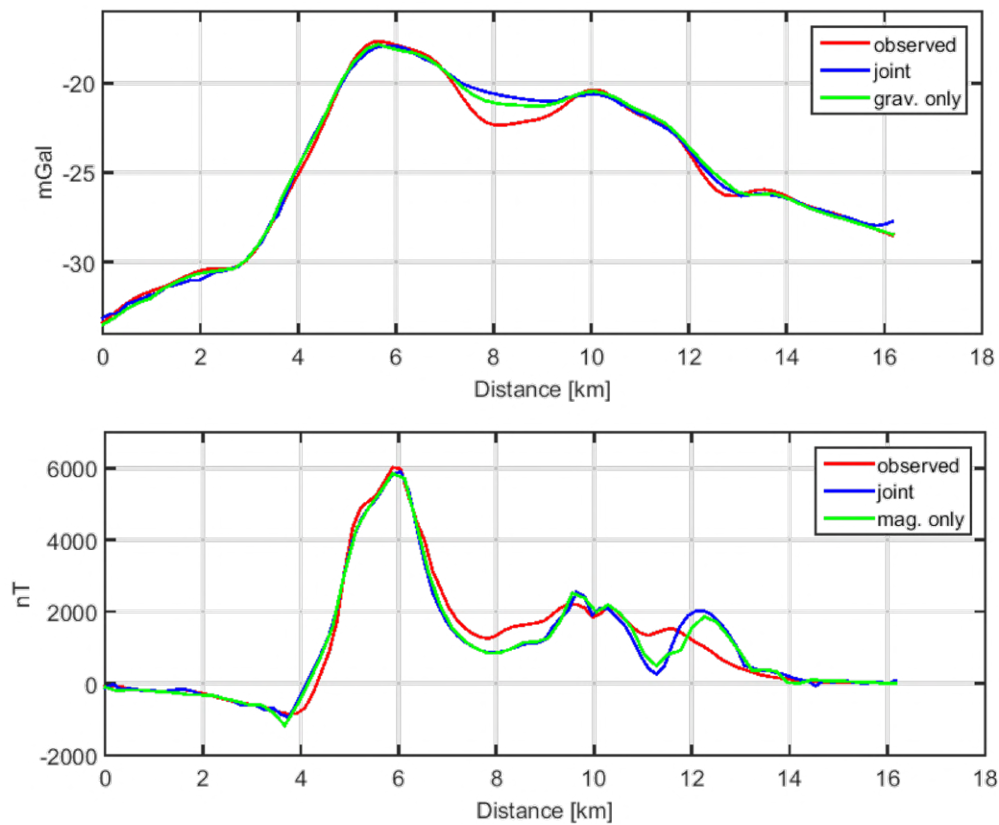


Figure 4.3.9: Predicted gravity and magnetic signal from gravity only, magnetic only and joint gravity magnetic inversions.

of labels at 1.5 km depth. We see that the gravity only inversion is not able to discriminate in a proper way between the different layers. This is somehow an expected result looking to the important overlays in terms of *a-priori* densities of the different layers. On the contrary the magnetic field is able to discriminate between the layers but shows only almost constant susceptibilities within each single layer (see also Fig. 4.3.6).

In order to understand the impact of the *a-priori* model on the inversion results, two further inversions, degrading the *a-priori* model, have been performed. In the former we assume a non-informative prior model considering just one label for the whole volume with constant *a-priori* density and susceptibility. In the latter test we remove the hypothesis of cylindrical geometry of the carbonatite complex. Both these inversions (reported in the supplementary material), give results well aligned with those presented in this section, thus giving robustness to our solution.

4.3.5 Conclusion

In the current work we presented a Bayesian approach to perform joint gravity and magnetic inversion. The algorithm can effectively change density and magnetic susceptibility distribution together with the geometries of the main geological units in a full 3D approach, fitting the gravity and magnetic data and respecting all qualitative and quantitative constraints. If compared with classical solutions the proposed method is superior for different points:

- once the *a-priori* model and constraints have been formalised, starting from the available information, the algorithm is able to properly manage the complexity of the problem providing meaningful new solutions in terms of geometries preserving sharp (in terms of density and susceptibility distribution) boundaries between different lithologies;

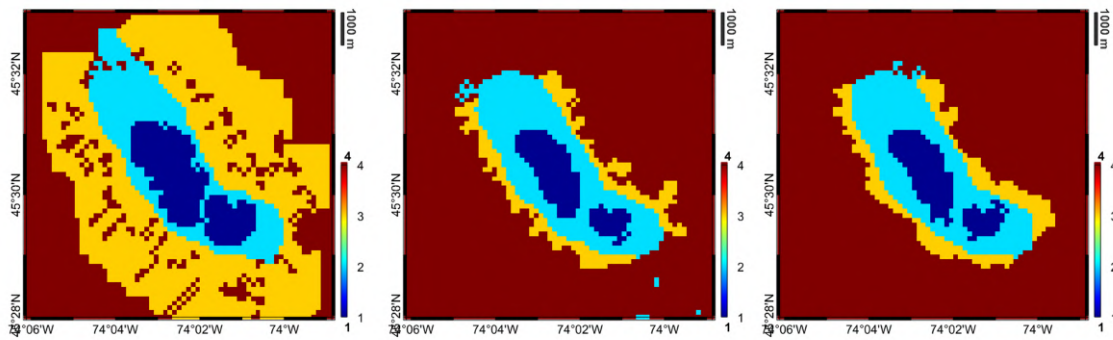


Figure 4.3.10: Estimated labels at 1.5 km from gravity only inversion (left), magnetic only inversion (centre) and joint inversion (right).

- results will not require an additional interpretation step (e.g. the selection of equi-density or equi-susceptibility surfaces to delineate the boundary of geological units);
- available information (e.g. interpreted seismic profiles, boreholes, etc.) and a-priori knowledge can enter in a easy and coherent way inside the inversion algorithm, allowing to obtain results statistically coherent with the a-priori model;
- the proposed solution is also able to estimate information about the accuracy of the final results, in terms of density, susceptibility and geometries.

Looking to the Oka complex example we can see how the ground Bouguer anomaly and the helicopter-borne total magnetic intensity maps well correlated with the available simplified geological knowledge: with expected density and susceptibility of the sovite core lower than that of the annular rings of silicate rocks and of the background gneiss. The inversion of gravity and magnetic data confirms the cylindrical shape of the complex, at least up to 10 km depth, with a small radial expansion at the surface of the fenitized layer.

The 3D magnetic susceptibility distribution suggests that only the silicate rocks have an important magnetisation while the carbonatite core and the background are almost no magnetic. The obtained 3D density distribution well correlated with detailed geological information available in the area (which was not included into the *a-priori* model), for instance retrieving high-density values of the okaite series, or the presence of the melteigite-urtite silicate rocks in the southern part of the Complex. Residuals in terms of magnetic field in the obtained solution suggest the possible presence of highly magnetised bodies (with few hundred metres thickness) in the carbonatite core.

Authors Contribution

D.S. supervised the study; M.C. and D.S. conceived and performed the study; D.S., M.C. and G.M. performed the bibliographic research; M.C., D.S. and G.M. wrote the paper.

Chapter 5

Conclusions

This thesis focused on locating critical raw materials essential for the green transition by exploiting advanced geophysical techniques. The research address the problems of the non-uniqueness in the interpretation of potential fields and of the uncertainties in the geophysical exploration, with the aim to realize crustal models as reliable as possible, and to link the results with the geology of the selected area, focusing on mineral prospecting.

We tested different inversion processes in different scales of detail, so as to understand which approach might be the most appropriate, and we analyze the inversion results depending on the scale investigated and on prior geological knowledge.

Considering the two inversion methods used, we can say that both have different advantages. Bayesian inversion allows for sharp boundaries between the different layers into which we can divide the crust. It emerges as a very effective method when we want to define the exact geometries of an area, when we already have some a-priori information. However, this necessity of information can also be seen as a disadvantage, together with the higher computational time. BFGS optimization method with limited memory, on the other hand, has the advantage of being faster in execution and requiring less a-priori information to invert the data, also if the lack of information does not allow the algorithm to identify the different crustal layers, but requires an additional interpretation step. It is definitely a good strategy to invert an area lacking a-priori information.

Further considerations can be made about the differences in the results according to the scale investigated. To do this, we first briefly look at the results of the three inversions performed:

- The large-scale investigation of the Iranian lithosphere demonstrated the effectiveness of integrating seismic tomography with gravity and magnetic data in reconstructing lithospheric structures. By applying a Bayesian joint inversion method, the study refined the density and magnetic susceptibility models, revealing significant tectonic features. Moreover, the calculated rigidity model revealed a strong correlation between lithospheric rigidity and seismic activity. Regions characterized by higher rigidity exhibited lower seismicity, suggesting a stabilizing effect of mechanical strength on tectonic deformation. These findings provide a valuable framework for assessing seismic hazards in tectonically active regions. They also highlight potential zones for mineral exploration associated with tectonic lineaments and magmatic intrusions.
- The medium-scale study focused on a resource-rich area in Great Britain, and led to the definition of the physical characteristics of the granitic batholith present in the area. The research delineated the density and susceptibility distribution in the area, connecting them to the principal geological features and to the mining potential in the zone, and allowing the isolation of the crustal granitic body. The ability to target specific geological formations reduces exploration uncertainty and provides actionable insights for the sustainable exploitation of resources.
- The detailed analysis of the Oka Carbonatite Complex highlighted the potential of joint inversion techniques in resolving fine-scale geological features critical for mineral exploration. The results provided a high-resolution model of the complex, identifying

minerals-rich zones and their spatial relationships. This case study demonstrates the versatility of Bayesian inversion framework, which seamlessly integrates different datasets and accounts for geological uncertainties. The methodology is adaptable to a wide range of geological contexts, making it a valuable tool for site-specific investigations.

The three different inversions yielded different types of results, which we can generalize as follows:

- regional scale inversion favors a better definition of the macro-structures in the area, and its geodynamic behavior. This is an important aspect to obtain a complete overview of the area, which is fundamental if we want to identify mineralization. In addition, an analysis at these scales is favored by the large availability of data, collected from the various satellite missions measuring the gravity field, and from the many global magnetic field models. This kind of inversion allows for reliable information on lesser-known areas, going to increase knowledge of those areas that are inaccessible to other geophysical investigations;
- medium scale analysis permits to get a deeper insight into the zone and to examine the various features on a more superficial level. As example, this allows to isolate a surface crustal body based on the densities distribution in the area. In this way we are able to obtain more detailed information of the depths with greatest interest for mineral exploration, which allows to make initial estimates of the actual mining potential of a terrain;
- local scale inversion allows the 3-D reconstruction of a single deposit, highlighting its distribution of densities and magnetic susceptibilities. This enables to improve the geological knowledge given by field analysis, allowing the identification of the different mineralizations in the deposit, based on their physical characteristics. Such a detailed analysis provides information not only from a qualitative point of view as in previous cases, but also from a quantitative ones.

Across all three case studies, the integration of gravity and magnetic data through joint inversion methods emerged as a powerful approach for understanding subsurface structures and provides geologically plausible models that align with observed data. By improving the resolution and accuracy of crustal models, the research supports the sustainable exploration of critical raw materials (CRMs). The identification of zones interesting for mining purposes with these kinds of geophysical methods reduces exploration costs and minimizes environmental impact, aligning with the principles of responsible resource management. Furthermore, the ability to link the results with geological structures and tectonic processes contributes to the understanding of lithospheric dynamics, offering insights that extend beyond resource exploration.

Further work to improve inversions might involve defining a more accurate a-priori model, to better constrain the geology of the area we want to investigate, acting for example on the mantle composition, or on the empirical velocity-density conversion relationships, which we have used on several occasions to define the characteristics of the a-priori model. Also the computational demands of joint inversion techniques remain a challenge, particularly for large-scale problems, which could be addressed by developing parallel computing or machine learning techniques. These advances could help overcome these limitations, enabling more efficient processing of complex datasets.

In conclusion, this thesis has demonstrated the potential of advanced geophysical inversion techniques in the study of the Earth's crust for exploration of critical raw materials. By integrating gravity and magnetic data with prior geological knowledge, the research provides a robust framework for the modeling of the crust, resolving subsurface structures and identifying areas of potential interest from a mining perspective. The case studies highlight the versatility of the methodology, and demonstrate its applicability in different scales and geological settings. As

global demand for CRMs continues to rise, the results of this research contribute to the broader goal of achieving sustainable resource management. By advancing the tools and techniques available for geophysical exploration, this work supports the transition to a greener and more resource-efficient future.

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