Development and application of multidisciplinary workflows for geologically and/or petrophysically constrained geophysical inversion

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Signature:

Date: 14 September 2018
Abstract

Geophysical inversion has seen much progress in the past decades and has become a technique of choice to image the Earth’s subsurface. Recent developments in geological modelling include the calculation of probabilistic geological models (PGM) from field geological measurements through probabilistic geological modeling, which can be used in conjunction with other geoscientific disciplines such as petrophysics and geology. This thesis introduces an integrated inversion methodology exploiting the complementarities between probabilistic geological modelling, petrophysical measurements and geophysical inversion. The different sources of information are integrated into a 2D and 3D least-square inversion framework that captures data related to geophysics, petrophysics and geology. The proposed workflow offers a degree of modularity that allows several integration avenues. These are first investigated in depth using a synthetic case study before the application of a selected approach to real-world data.

When petrophysical constraints can be derived, PGMs can be used as a source of information to condition them spatially and to derive starting models. In such case, local petrophysical constraints are applied during inversion. To test this approach, we have generated a synthetic geophysical survey using field geological data from the Mansfield area (Victoria) to run probabilistic geological modelling, and values from the literature to populate the structural model and to generate the statistics of petrophysical measurements. In this case, results show that the integration of geological and petrophysical information in geophysical inversion can reduce uncertainty and improve imaging significantly. More precisely, the posterior sensitivity analysis to prior information shows that the application of petrophysical constraints sharpens the boundaries between geological units. It also enforces a degree of similarity between the statistics of inverted properties and petrophysical measurements. The integration of probabilistic geological modelling permits more accurate recovery of model structural features overall and to better constrain the solution. Our analysis also demonstrates that the best results are obtained in the joint inversion case, using locally conditioned petrophysical constraints.

These constraints, which are derived from geological and petrophysical measurements, are sensitive to measurement uncertainty. Models obtained from geologically and/or petrophysically constrained inversions are the result of complex interactions between
correspondingly diverse datasets. It is therefore important to understand how non-geophysical investigate input uncertainty impacts inverted models. To this end, we studied the influence of uncertainty in geological and petrophysical measurements onto geophysical inversion. Building up on the Mansfield synthetic survey, we simulate low, medium, and high geological and petrophysical uncertainty levels, combined into a series of nine case scenarios. We investigated the propagation of non-geophysical measurement uncertainty into geophysical inversion using misfit indicators and lithological models recovered a posteriori. This is complemented by the topological analysis of recovered lithological models. It is useful to quantify their conformity to the causative bodies, and allows the identification of geologically uncertain areas. Our work shows that the effect of geological measurement uncertainty dominates over that of petrophysical data uncertainty. It also indicates that while reducing uncertainty in geological measurements ameliorates inversion results, the effect of local entrapment is more pronounced for low petrophysical measurement uncertainty.

Our investigation of the proposed workflow extends to cases where petrophysical constraints cannot be derived from the available measurements. In such case, the PGM is used to calculate field measurement-based structural information characterizing uncertainty about the presence of observed lithologies. It is utilized to locally adjust the weights of a minimum-structure gradient-based regularization function. We first test this technique using the Mansfield synthetic study, for which results clearly demonstrate that it can reduce structural and model property differences between causative and inverted models. We then investigate a real-world case study using data from the Yerrida Basin (Western Australia), where we focus on prospective greenstone belts beneath sedimentary cover. Our results show that the proposed approach allows geophysical inversion to adapt the model preferentially in geologically less certain areas, where the PGM derived from field geological measurements is the least informative. Results also indicates that inverted models are consistent with both the PGM and geophysical data of the area, hence reducing interpretation uncertainty. Quantitative interpretation of inverted models finally reveals that the recovered greenstone belts may be shallower and thinner than previously thought.
Acknowledgements

According to the *Oxford Learner’s Dictionaries*, the word ‘acknowledgement’ refers to an ‘act of accepting that something exists or is true, or that something is there’. In this foreword, I digress from this definition and focus on expressing my thankfulness to those (besides my supervision team and university) who made it possible for me to complete my thesis and accompanied me along this journey. Please contact me if you want to hear an extensive list of grievances. I am a better person and scientist through those who support me and those that didn’t.

First and foremost, I am grateful to my partner in crime Danielle Sarah Su 徐莉蕤 for her invaluable support, especially towards the end of my candidature when patience has been a quality she has proven to have an unsuspected amount of.

My deep thanks also go to my parents, Philippe Giraud and Joëlle Giraud-Paul, my siblings Céline and Nathan Giraud, and my grandmother, Christiane Paul, for their continuous support to my studies, for pushing me and for their understanding.

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My appreciation is given to the Australian Federal Government who granted me an Australian Government Research Training Program (RTP) Scholarship, to the Australian Society of Exploration Geophysics and the Society of Exploration Geophysics who supported part of my research.

I am also grateful to geoscientists from previous stages of my career as a geophysicist who gave me the taste for geoscientific integration.
In accordance with the University of Western Australia’s regulations regarding Research Higher Degrees, this thesis is organized a series of journal papers.

The descriptions below summarize essential information the publications constituting chapters 2, 3, 4, of which the candidate is the leading author.

**Paper 1**

*General information*

*Publication type:* Journal article.

*Reference* (as provided by journal):

Jérémie Giraud, Evren Pakyuz-Charrier, Mark Jessell, Mark Lindsay, Roland Martin, and Vitaliy Ogarko (2017). "Uncertainty reduction through geologically conditioned petrophysical constraints in joint inversion." GEOPHYSICS, 82(6), ID19-ID34.

https://doi.org/10.1190/geo2016-0615.1

*Details of the work*

This publication introduces the concept behind the algorithm that was developed during the first year of the PhD. The student developed a prototype in 2D to test and illustrate the methodology to be used later during the project. The main object of this article is the introduction of a new modelling workflow and its testing on a simple model.

The publication starts with a literature review in the form of a relatively long introduction in order to introduce the methodology to be tested in this article. The result section shows the improvement brought by the introduced methods and illustrates the strengths of the presented workflow. The conclusion and discussion pave the road for the second paper and the work detailed in the other two papers.

*Location in thesis*

Chapter 2.
Student’s contribution to work

The student is the leading author of the publication. His contribution can be summarized as:
Development of the methodology for the integration of petrophysical data, geological modelling and geophysical joint inversion; Development of the prototype; Testing of the prototype; Creation of synthetic models; Participating in the creation of the geological model; Creation the petrophysical model; Redaction of the article (with revisions from co-authors).

Co-authors signatures and dates:

Evren Pakyuz-Charrier: Date: 10/09/2018

Mark Lindsay: Date: 10 September 2018

Mark Jessell: Date: 10/9/2018

Vitaliy Ogarko: Date: 12/09/2018

Roland Martin: Date: 13/09/2018

Student’s signature:

Jérémie Giraud Date: 14/09/2018
Paper 2

**General information**

*Publication type:* journal article (under review).

*Reference:*


**Details of the work**

This publication extends work presented in paper 1 to 3D and shows the algorithm’s capabilities through the simulation of a range of scenarios simulating different uncertainty levels. The work presenting relates to the extension of an existing inverse modelling platform (TOMOFAST3D) using the concepts tested in 2D in the first journal article. It also introduces and illustrates a new approach to the posterior analysis of inversion results.

**Location in thesis**

Chapter 3.

**Student’s contribution to work**

The student is the leading author of the publication. His contribution can be summarized as:

- Participation in the development of the inversion platform used: 2D prototype of the first author generalized to 3D in a different code developed in collaboration with a team member;
- Developing theoretical concept implemented in inversion platform relating to local constraints;
- Design of the workflow; Participation in the generation of the probabilistic geological models;
- Creation of petrophysical models and choice of uncertainty levels; Creation of reference density contrast and magnetic susceptibility model using reference structural model; Inversion code testing; Performing inversion runs; Development of posterior analysis methodology; Performing analysis and interpretation of results; Redaction of manuscript (with revisions from co-authors); Input/Output preparation and results analysis.

Co-authors signatures and dates (next page):
Paper 3

General information

Publication type: journal article (under review).

Reference

The corresponding article is under review for publication in Solid Earth and appears as a preprint discussion as (online public review for publication in Solid Earth):


Details of the work

This paper introduces a novel approach to the inversion of gravity data that uses information extracted from the results of probabilistic geological modelling when conditions necessary to
apply techniques introduced in paper 1 and 2 are not met. The proof-of-concept is investigated using the same geological structural model as paper 1 and 2, after which the methodology is applied to a real-world case.

**Location in thesis**

Chapter 4.

**Student’s contribution to work**

Development of the methodology for the integration uncertainty into geophysical inversion in collaboration with team member; Testing and benchmarking of the methodology on synthetic data; application to real-world data; Interpretation of results; Redaction of the article (with revisions from co-authors).

Co-authors signatures and dates:

Evren Pakyuz-Charrier: Date: 10/09/2018

Mark Lindsay: Date: 10 September 2018

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Roland Martin: Date: 13/09/2018

Student’s signature:

Jérémie Giraud Date: 14/09/2018
I, Mark Jessell, certify that the student statements regarding their contribution to each of the works listed above are correct.

Coordinating supervisor signature:

Date: 10/9/2018
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Dedication

To my family and loved ones.
To good and reproducible science.
And to C.C. F. Catus.
Chapter 1

Introduction

“Ce que nous connaissons est peu de chose, ce que nous ignorons est immense.”

“What we comprehend is slight, what we are incognizant of is immense.”

- Alleged last words of Pierre-Simon Laplace

Geophysical modelling and inversion have come to play an essential role in every large exploration project and Earth imaging initiative by imaging inaccessible volumes of rocks in a non-destructive and non-invasive manner. Geophysical inversion has been increasingly used since its conception in the 1960’s after (Verreault 1965) introduced the practical resolution of an inverse problem in the geosciences to calculate the Earth’s torque modes. He solved a problem that had long been recognised to be non-unique decades earlier (Hadamard 1902), long after Cramer’s rule was introduced (Cramer 1750) to solve systems of well-posed linear equations through what he called dérangement. The inversion process was then formalised and generalised to other problems in the seminal works of (Backus and Gilbert 1967) and (Jupp and Vozoff 1975). Both respectively refer to inversion as “trying to understand what is the totality of Earth models”, which “consists of operating directly on those [geophysical] data to to generate a view of the structure which causes them”. A few years later, (Tarantola and Valette 1982) proposed a general framework providing the theoretical basis for the robust incorporation of prior information into geophysical inversion.

In the light of the contributions that stemmed from these publications and other major works reviewed in this introduction chapter, the following PhD thesis proposes a new workflow for the integration of multiple geophysical data types with geological and petrophysical modelling.
1.1. Definitions

To standardize ideas before discussing concepts, some important terms require precise definition as their meaning can vary within sub-disciplines, or organisations (for instance, the Society of Exploration Geophysicists\(^1\), the Society of Petroleum Engineers\(^2\), the Dictionary of Earth Sciences\(^3\), Exploration Seismology\(^4\), the Encyclopedic Dictionary of Applied Geophysics\(^5\), and the Dictionary of Geological Terms\(^6\) provide definitions of *Petrophysics* that have different meanings). They are used consistently throughout the thesis, which includes published, accepted for publication and submitted journal articles (Chapter 2, 3, and 4, respectively).

- Petrophysical measurements

  *Petrophysical measurements*: the terminology refers to measurements of the physical properties of rocks, which can be obtained from surface samples or downhole surveys. For instance, density and magnetic susceptibility constitute petrophysical measurements, which characterise petrophysical properties of rocks useful to geological and geophysical modelling. By extension, petrophysical measurements also refer to the measures of the physical properties of rocks and are interchangeable. For example, measurements of density and magnetic susceptibility on rock samples constitute *petrophysical measurements*.

- Geological model

As an extension to the previously defined term *geological model* is sometimes broadly used to designate a representation of the subsurface in terms of physical properties, structural features or rock types. For this thesis, I limit the use of such term to structural models derived from geological field measurements *stricto sensu* (e.g., lithotype, foliation, age relationship, etc.), the interpretation of which can be assisted by other geoscience disciplines (petrophysics, geophysics, geochemistry, etc.). These models are populated with properties of interest derived

\(^{2}\) http://petrowiki.org/Petrophysics
\(^{3}\) Add ref of dictionary for earth sciences here.
from petrophysical measurements or reference values corresponding to the rock types in the area.

- Geological modelling

By extension to geological model, geological modelling refers to the process of deriving a geological model through construction of said geological model from, but not limited to, geological measurements as defined above. Figure 1.1 below illustrates the usage of geological measurements in geological modelling.

![Figure 1.1. Summary of geological modelling workflow. Modified from oral presentation associated with (Giraud et al. 2018a).](image)

- Uncertainty

The definition of uncertainty is field-dependent. It is generally admitted that it arises from imperfect knowledge of the studied object. In a scientific context, uncertainty is the reflection of potential errors in a measurement or in the modelling of a physical process or quantity. It refers to the degree to which the measurement (e.g., orientation data) or estimation of a given quantity (e.g., mass-density) or phenomenon (e.g., geological process) is expected to represent reality. Uncertainty is modelled using tools developed in statistics and information theory.

1.2. Research context in exploration geophysics and geoscience integration

1.3. Motivations for integrated geophysical inversion

Over the past two decades, numerous works have focused on the integration of different datasets in geophysical exploration and monitoring scenarios through exploitation of the complementarities between different geophysical techniques (Gallardo and Meju 2003; Brown et al. 2012; Lelièvre et al. 2012a) and geoscience disciplines (Li and Oldenburg 2000; Paasche and Tronicke 2007; Fullagar et al. 2008; De Stefano et al. 2011; Sun and Li 2015) (see introduction sections to Chapter 2 and 3 for more extensive discussion and exhaustive list of references). The main driver for such data integration in geophysical inversion is the need to
combine the strengths of different subsurface characterisation techniques to obtain a common earth model. Doing so may reduce the effect of non-uniqueness and decrease interpretation ambiguity with respect to separate, independent modelling procedures, as put forth by (Jupp and Vozoff 1975), who conceptualised joint inversion. More generally, the development of holistic approaches in geoscientific integration is based on the premise that modelling a physical system requires the use of all available information that characterises it (Hempel and Oppenheim 1948; Cartwright and McMullin 1984), which therefore justifies multidisciplinary integration in earth modelling (Nearing et al. 2016).

Practically, one of the main reasons for the recent development of integration techniques is that the exploration of natural resources is becoming increasingly challenging in basin and hard rock scenarios alike. It has become common knowledge that hydrocarbon discoveries are becoming rarer and smaller, as evidenced in 2014 having the fewest discoveries over a 60-year period (Ward and Crooks 2017). Likewise, the estimated amounts of newly discovered economic minerals show a decreasing trend since the mid 90’s (Schodde 2017) while deposits are found at increasing depths (Schodde 2015). In the meantime, the global demand for metals steadily increases (Backman 2008; Arrobas et al. 2017), and experts predict that the demand for hydrocarbon will increase until 2040 (BP Energy Outlook 2017).

Consequently, it has become necessary to push for exploration in areas that were previously considered either too risky or too challenging to maintain reserves and production levels. In this context, multi-disciplinary integration, geophysical joint or constrained inversions have been recognised as one of the tools of choice to reduce exploration risk in hydrocarbon and mineral exploration (Alfaro et al., 2007; Errey and Brabers, 2013). Meanwhile, the democratisation of supercomputing enabled by dramatic cost reduction in the production of CPUs now allows geoscientists to tackle increasingly large and/or complex problems. The development of massively parallel inversion codes enables application and usage of methodologies that were previously considered computationally expensive such as three-dimensional (3D) constrained inversions and stochastic geological simulations. The former and the latter present obvious complementarities, the exploitation of which present much potential in terms of characterisation of the subsurface, but which have, not been fully exploited yet. The possible gains have been highlighted by (Calcagno et al. 2008; Jessell et al. 2010) and integration is generally recommended in works advocating holistic modelling approaches. One
of the reasons for this is the challenge presented by the quantitative integration of data inherently different in nature, resolution, and spatial coverage. This can be attributed to a degree of disconnect and lack of interaction between the communities of numerical geological modelling, geophysical inversion, petrophysics and geochemistry (Pears et al. 2017).

In this thesis, I propose methodologies that take advantage of these recent developments to push integration strategies further towards a deeper level of integration between geophysical, petrophysical and geological measurements. In the next subsections, I briefly review various integration strategies relying on geophysical inversion and point out possible areas of improvements. This will then bring us to possible developments exploring integration avenues not investigated to date that the work presented in this thesis introduces.

1.3.1. Joint geophysical inversion: broad overview

The general approach to joint inversion of geophysical data is to jointly invert data from two or more geophysical methods by assuming a known relationship between the properties characterised by each method. Joint inversion is performed using constraints linking the different inverted models. It is commonly assumed that the spatial variations of the inverted properties are collocated, or that their respective variations can be linked using empirical, statistical petrophysical relationships or rock physics laws. These are based on prior knowledge and/or hypotheses about the petrophysical properties or the geology of the area, thereby effectively translating prior information into what can be interpreted as covariance functions between the models to be applied during inversion.

In the absence of field geological information, several authors enforce constraints based on structural similarities, i.e., approaches introduced by (Haber and Oldenburg 1997; Gallardo and Meju 2003; Zhdanov et al. 2012; Molodtsov et al. 2013) between the models jointly inverted based on the assumption that some or all spatial variations in the inverted property are collocated. This approach, which relies on a simple hypothesis and requires little prior information. It has gained in popularity due to its conceptual simplicity and has been well explored, in particular through usage of the cross-gradient constraints introduced by (Gallardo and Meju 2003). Although this technique has been used mostly for basin studies involving the inversion of seismic jointly with non-seismic data (Gallardo and Meju 2004, 2007; Gallardo et al. 2005; Colombo and De Stefano 2007; Fregoso and Gallardo 2009; Hu et al. 2009; Abubakar et al. 2012; Molodtsov et al. 2013; Moorkamp et al. 2013; Ogunbo et al. 2018) and possibly
others, it has also been used in hydrogeophysical studies (Linde et al. 2006, 2008; Doetsch et al. 2010; Linde and Doetsch 2016), which rely more on the inversion of electromagnetic and seismic data, and hard rock terranes (Gallardo and Thebaud 2012; Leon-Sanchez et al. 2018), where gravity and magnetic inversion are commonly used. Applications of this technique can also extend to active faults (Bennington et al. 2015), crustal studies (Le Pape et al. 2017) and lithospheric structure characterisation (Deng et al. 2018).

Alternatively, when more prior information can be used, (De Stefano et al. 2011) offer the possibility to link multiple domains in joint inversion using either enforcing structural similarities or empirical relationships. When a geological interpretation or petrophysical data is available, several authors have developed approaches probabilistic approaches that account for such prior information (Bosch 2004; Lane and Guillen 2005; Mahardika et al. 2012; Shamsipour et al. 2012; Jardani et al. 2013; Reid et al. 2013; McCalman et al. 2014; Roberts et al. 2016). In a similar fashion, (Chen and Hoversten 2012) perform stochastic joint inversion to retrieve petrophysical properties (porosity, saturation). In exploration scenarios, another strategy has been introduced and used by (Hoversten et al. 2006; Gao et al. 2012; Giraud et al. 2013; Liang et al. 2016; Gase et al. 2018) who use constitutive rock physics equations (Carcione et al. 2007) to retrieve petrophysical properties from physical property models. Others extract information from petrophysical measurements for the different lithologies observed in the area to derive constraints linking the inverted models using clustering algorithms to encourage inverted model properties to cluster around predefined values. In addition, some studies (Paasche and Tronicke 2007; Sun and Li 2011, 2015, 2016; Lelièvre et al. 2012b; Carter-McAuslan et al. 2015; Giraud et al. 2016, 2017) use clustering approaches to constrain the values of inverted properties. This approach holds the potential for further developments and can be adapted to accommodate additional sources of information. For instance, the statistics of petrophysical measurements can be used in conjunction with results from probabilistic geological modelling to derive spatially varying petrophysical constraints.

As described in Chapter 2, this extension of existing techniques constitutes one of the novel approaches introduced in this thesis.

1.3.2. Guided inversions

An alternative to joint inversion can be found in what (Brown et al. 2012) proposed to label \textit{guided} inversion. It consists of constraining single-physics inversion by incorporating structural
information from the inversion results of another geophysical dataset in the smoothness regularization term of the cost function of the inversion to be performed. Unlike cases where authors simply remove regularisation constraints at interpreted surfaces (Favetto et al. 2007; Muñoz et al. 2010; Medina et al. 2012; Doetsch et al. 2012; García Juanatey et al. 2013), guided inversions relax the constraints (i.e., gradient regularisation) around assumed interfaces without allowing them to vanish completely, thereby giving more flexibility to the inversion algorithms to update the model and allowing it to account for uncertainty in the interfaces’ location. This approach can be applied under the same assumptions as the structurally-constrained joint inversions mentioned above to cases where one of the available methods (e.g., seismic or GPR) has a structural resolution that is far superior to another one (e.g., diffusive electromagnetic methods), somewhat diminishing the benefits of joint inversion using structural constraints over single-physics inversions. In such case, structural information (in the sense of the interpretable structures present or spatial property variations) from the better resolving method’s inverted model can be used to derive regularisation constraints for the inversion of the least resolving method.

The application of techniques relaxing regularisation constraints at specific locations determined from another inverted model is growing in importance in geophysics. In addition, there is a focus on the integration of information from geophysical methods relying on wave propagation such as seismics and GPR into the inversion of data resulting of predominantly diffusive electromagnetic data (Brown et al., 2012; Wiik et al., 2015; Guo et al., 2017; Yan et al., 2017). This illustrates that this integration strategy remains relatively unexplored to date. For instance, to the best of my knowledge, none of the related relevant work address the application of such technique to geological models or their uncertainty, nor do they consider potential field data inversion. This avenue is explored and extended to the application of guided inversion application through the usage of geological model uncertainty to constrain potential field data inversion (section 4.3 in Chapter 4).

1.3.3. Geological constraints for inversion

An alternative strategy to mitigate inversion’s inherent non-uniqueness is to strictly enforce specific geometrical relationships (i.e., contact locations or topologies) in the inverted models using hypotheses or prior information. Works published by (Bosch 1999, 2004; Gallardo et al. 2005; Bosch et al. 2006; Fullagar and Pears 2007; Guillen et al. 2008; Juhojuntti and Kamm
2015) develop inversion schemes allowing their inversion algorithm to deform structures in the inverted physical property model while keeping a constant topology. Likewise, (Lelièvre et al. 2012a, 2015) invert for contact surface geometries while keeping topology constant. Such continuity of concept is shown in (Li et al. 2009; Balidemaj and Remis 2010; Davis et al. 2012; McMillan et al. 2015; Zheglova and Farquharson 2016; Bijani et al. 2017; Zheglova et al. 2018), who parameterise the geometry of geological structures to recover the location of boundaries between regions through inversion in 2D by assuming topology and petrophysical properties known and fixed. These approaches, however powerful in certain scenarios, are still in development and have limitations. For instance, the necessity to explore different geological scenarios and topologies in 3D has been recognised by (Jessell et al. 2010, 2014, Lindsay et al. 2013b, a; de la Varga and Wellmann 2016; Wellmann et al. 2017; Pakyuz-Charrier et al. 2018), who sample the geological model space to produce a series of models sought to represent geological model space. Surprisingly, although it has been recommended by several works in recent years (i.e., Jessell et al., 2010, 2014, Lindsay et al., Wellmann et al., 2014, 2017; Linde et al., 2015, Pakyuz-Charrier et al., 2018), the integration of probabilistic geological modelling and geophysical inversion is still in its infancy and little geophysical inverse modelling work exploiting its results has been reported to date. As we will see in the next section and in Chapter 2, 3, and 4, one of the main foci of this thesis is to alleviate this by integrating the results of probabilistic geological modelling with geophysical inversion and petrophysical data in various ways.

1.4. Research focus and progression

1.4.1. Project objectives and proposed solution

The work presented in this thesis exploits developments in geological modelling and constrained inversion to develop a new holistic workflow integrating geological modelling and petrophysical measurements into geophysical inversion while accounting for geological and petrophysical uncertainty. More specifically, the project’s aim is to develop a general multi-stage, multi-disciplinary workflow exploiting standalone analyses of non-geophysical data to accommodate different scenarios in terms of data availability and to integrate geoscientific data in a robust and comprehensive way. The philosophy of this workflow is conceptualised in Figure 1.2.
The primary contribution of this thesis is to fill the gaps in integration highlighted in the previous subsections through the development of said workflow. The focus of the thesis is the development and application of a modular workflow capable of dealing with different levels of uncertainty and amount of data in terms of geological information, petrophysical measurements and geophysical data.

The input preparation stage involves petrophysical analysis through calculation of the statistics of the petrophysical measurements and/or probabilistic geological modelling to calculate probabilistic geological models and the related uncertainty indicators. Besides being informative about the studied area and often calculated for standalone applications, these inputs allow to derive robust constraints from inversion. Such constraints encapsulate the state of knowledge from non-geophysical sources, are petrophysically and/or geologically consistent while remaining statistically valid.

An illustration describing the geological modelling process is provided in Figure 1.3. For more background information, the reader can refer to Chapter 2, 3, and 4 for a general overview, and to (Pakyuz-Charrier et al. 2018) and the other references provided in Section 1.6.1 for detailed introduction and motivations for the development and usage of such modelling technique.
In the work presented here, the possible range of constraints for single physics and joint inversion consist of:

- homogenous and isotropic petrophysical constraints;
- locally varying petrophysical constraints;
- locally conditioned gradient regularisation;

where local (or locally) signifies that the properties are heterogeneously distributed in space (see Chapter 2, 3, 1.5.1 and 1.5.2). Conditioned (or conditioning) does not refer to matricial calculus but means that values are assigned using prior information (see Chapter 5 and 1.5.3).

At the inversion stage, constraints derived from prior information are applied to run the desired constrained inversion.

Lastly, posterior analysis of inversion results is performed accordingly with the constraints used for inversion and the non-geophysical datasets available. The posterior analysis tools available consist of the following:

- root-mean-square data misfit metrics and misfit maps;
- spatial analysis of physical property model update;
- analysis of recovered lithological model: simple topology analysis (e.g., adjacency).
The proposed workflow as described above is summarised in Figure 1.4. It can be read as a matrix showing the progression from input preparation (rows 1-3) to posterior analysis (lines 5-6) and how it integrates geophysical data (column A), petrophysical modelling (column B) and geological simulations (column C). Please note that data input preparation stages in lines 1 and 2 are not part of the focus of the work presented in this thesis. It will be succinctly discussed as established techniques already exist for elements B1-B2 (for instance through usage of expectation maximisation algorithm of McLachlan and Peel, 2000) and work allowing to perform C1-C2 was developed concurrently to the PhD project this thesis pertains to (see section 1.6.1). Essential information about probabilistic geological modelling is given in due course in Chapter 2, 3, and 4.

A point of note is that this workflow is sufficiently generalistic that it can be applied to datatypes not considered in this thesis (see concluding remarks in Chapter 5 for longer discussion). Here, it is applied to gravity and magnetic data inversion using petrophysical statistics based on density and magnetic susceptibility measurements from outcrop or downhole. Geological modelling is performed using orientation data, contacts and foliations. The data types considered are summarised in Table 1.1.

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**Figure 1.4.** General overview of the proposed workflow with reference to the thesis chapter for which the different branches are introduced. Note that the probabilistic geological model is obtained from MCUE as detailed in (Pakyuz-Charrier et al. 2018) while the statistics of petrophysics can be calculated from a mixture model derived using an expectation maximisation algorithm.
Table 1.1. Input datatypes of general workflow and chosen algorithms for main tasks.

<table>
<thead>
<tr>
<th>Input data to the proposed workflow</th>
<th>geophysics</th>
<th>petrophysics</th>
<th>geology</th>
</tr>
</thead>
<tbody>
<tr>
<td>ground and/or airborne gravity data</td>
<td>density measurements</td>
<td>contact and orientation data</td>
<td></td>
</tr>
<tr>
<td>ground and/or airborne magnetic data</td>
<td>magnetic susceptibility measurements</td>
<td>stratigraphy, fault relationships</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Input data to the proposed workflow</th>
<th>geophysics</th>
<th>petrophysics</th>
<th>geology</th>
</tr>
</thead>
<tbody>
<tr>
<td>complete Bouguer anomaly</td>
<td>density contrast mixture model</td>
<td>probabilistic geological model</td>
<td></td>
</tr>
<tr>
<td>total magnetic field anomaly</td>
<td>magnetic susceptibility mixture model</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Algorithm used</th>
<th>geophysics</th>
<th>petrophysics</th>
<th>geology</th>
</tr>
</thead>
<tbody>
<tr>
<td>ground and/or airborne magnetic data</td>
<td>magnetic susceptibility measurements</td>
<td>stratigraphy, fault relationships</td>
<td></td>
</tr>
</tbody>
</table>

1.4.2. Research progression

The first stage of the research presented here involves the development of a portable prototype to evaluate different strategies for the implementation of the proposed methodology in 2D synthetic cases. This prototype was developed using Matlab® during the first part of the PhD project to test hypotheses and to experiment with algorithms. This led to the submission of a manuscript now published in Geophysics. It is reported in Chapter 2 of this thesis.

The selected approach to integrating geological and petrophysical information was then deployed in a Fortran code called Tomofast-x⁷ to deal with 3D large-scale problems, which constitutes the second major stage of the research. Besides extension of the workflow to 3D, this part of the work also involves the extension of the methodology presented in Chapter 1 to the analysis of recovered of lithological models. The 3D inverse modelling stage is performed using Tomofast-x while the posterior analysis is, and remains after completion of the PhD project, performed used using my toolbox of Matlab® codes. This work was performed during year 2 and finalised in the first half of year 3. It was concluded with the submission of a manuscript for publication in Geophysical Journal International (further referred to as GJI), focusing on a sensitivity analysis to varying levels of uncertainty in petrophysical and geological input in gravity and magnetic joint inversion. It is reported in Chapter 3 of this thesis.

⁷ Performed in collaboration with Vitaliy Ogarko.
The third and final stage of the research summarised in this thesis explores a different integration procedure that can be applied to derive local constraints for inversion in the absence of petrophysical information suitable to derive constraints (see C1-C3 in Figure 1.4). It consists of the application of guided inversion to potential field data constrained by uncertainty information extracted from a probabilistic geological model. Note that this was implemented directly in Tomofast-x. This part of the work, which deals with the testing on synthetic data and application to a field case study, was performed in year 3. It was concluded with the submission of a manuscript for publication in *Solid Earth*. It is reported in Chapter 4 of this thesis.

1.5. Chapters description and publications

This thesis is articulated around three chapters relating to the main contributions of the work performed during the PhD project. Chapters 2, 3, and 4 are either published or under review in internationally peer-reviewed journals. The first page of all published work is given in Appendix 1. Note that the manuscripts have been reformatted to fit the format of this thesis.

1.5.1. Chapter 2: Uncertainty reduction through geologically conditioned petrophysical constraints in joint inversion

This chapter introduces the general inversion methodology for the integration of probabilistic geological modelling and petrophysical information and shows the advantages of the proposed integration technique. The methodology is tested through a realistic, complex synthetic example used as the proof-of-concept. A sensitivity analysis is performed in which the degree of integration is increased from single physics, non-constrained inversion to joint inversion constrained by petrophysical constraints conditioned by probabilistic geological information. The Chapter focuses on the use of probabilistic geological modelling to spatially condition petrophysical constraints. Results and findings allow us to conclude that the proposed integrated inversion approach is a powerful way of incorporating geological structural and petrophysical data into inversion, and was shown to be able to positively influence the inversion results.

The corresponding article has been accepted for publication in *Geophysics* and appears as:

Giraud, J., Pakyuz-Charrier, E., Jessell, M., Lindsay, M., Martin, R., Ogarko, V., 2017: Uncertainty reduction through geologically conditioned petrophysical constraints in joint
inversion. Geophysics, 82, ID19-ID34. doi:10.1190/geo2016-0615.1

1.5.2. Chapter 3: Sensitivity of constrained joint inversions to geological and petrophysical input data uncertainties with posterior geological analysis

This Chapter presents a 3D extension of the methodology introduced in Chapter 2 and extends the posterior analysis of inverted models. Chapter 3 investigates the impact of uncertainty in geological and petrophysical prior information on the integrated inversion of potential field. A sensitivity analysis to realistic levels of uncertainty in input geological and petrophysical data is performed. The geometry of the chosen 3D synthetic physical property is determined by geological field measurements and is populated using published values.

Detailed posterior analysis of the recovered petrophysical and lithological models reveals that the influence of uncertainty in geological measurement dominates over that of petrophysical data. It also shows that the inversion algorithm is more affected by local entrapment when petrophysical input data uncertainty is low.

The corresponding manuscript is under revision for publication in GJI. The provisional reference is given as:


1.5.3. Chapter 4: Integration of geological uncertainty into geophysical inversion by means of local gradient regularisation

This Chapter introduces a novel approach to the inversion of gravity data that uses information extracted from the results of probabilistic geological modelling. The proposed strategy consists of applying guided inversion (see 1.3.2 for brief definition) to gravity data using geological uncertainty information. The consequence of the chosen formulation is that inversion encourages preferential update of the model in geologically uncertain areas. See 1.4.1 for clarification about the usage of the words ‘local’ and ‘conditioning’.

The proof-of-concept is investigated using the same geological structural model (in the Mansfield area, Victoria) as Chapter 3, after which the methodology is applied to a case study
in the Yerida Basin (Western Australia). Results reveal that the proposed approach effectively integrates probabilistic geological modelling and geophysical inversion and that it allows refinement of the structural and geophysical models. The comparative analysis of results obtained in the application case study shows that the constraints introduced in this chapter allow to determine the geometry of prospective mafic greenstone belts in the studied area with increased confidence.

The corresponding article is under review for publication in *Solid Earth* and appears as a preprint discussion as (online public review for publication in *Solid Earth*):


1.6. **Additional contributions**

1.6.1. **Probabilistic geological modelling**

During the course of my PhD I have worked with Evren Pakyuz-Charrier, whose PhD project was focusing on the development and application of a probabilistic geological modelling scheme (as summarised in Figure 1.3). In the work presented in this thesis, I exploit the output of this process as a source of prior information and constraints (see Chapter 2, 3 and 4).

The impact in each other’s work led us to become co-author of our respective peer-reviewed publications. I am co-author of the following:


Pakyuz-Charrier, E., Giraud, J., Lindsay, M., Ogarko, V., and Jessell, M., 2018: Drillhole Uncertainty Propagation for three-dimensional Geological Modeling using Monte Carlo, Accepted for publication in Tectonophysics, 2018.
1.6.2. Large scale geological modelling

During the first part of my PhD I collaborated with researchers from the Centre for Energy Geosciences (University of Western Australia). I built a series of large-scale, fine-resolution geological models utilising interpreted seismic data alongside well-logs and geological knowledge. These models were subsequently populated with petrophysical properties to be used as a starting point for forward modelling and inversion of full-waveform seismic data. The activities related this project focusing on a workflow involving geological model building and the subsequent geophysical modelling helped frame my thesis research direction.

The reference of the related journal articles I am co-author of are given below:


1.6.3. Application and extension of developed workflow to other cases

During the course of my PhD, I have been working with Roland Martin on the development of the workflow summarised in Figure 1.4, which we extended to the utilisation of the cross-gradient technique (Gallardo and Meju 2003) to constrain gravity data inversion using full-waveform seismic inversion results across a transect in the Pyrenees mountain range in France and Spain. A manuscript intended for Geophysics of which I am a co-author of is being written.

1.7. Chapter 1 references


Cramer G (1750) Introduction à l’analyse des lignes courbes algébriques. Freres Cramer and
C. Philibert

Davis K, Oldenburg D, Hillier M (2012) Incorporating geologic structure into the inversion of magnetic data. ASEG Ext Abstr 26–29


Errey J, Brabers P Using Geophysics as a Tool for Mitigating Project Risk


Giraud J, Jessell M, Lindsay M (2018a) Impact of uncertain geology in constrained geophysical inversion. 1–6


Leon-Sanchez AM, Gallardo LA, Ley-Cooper AY (2018) Two dimensional cross-gradient joint inversion of gravity and magnetic data sets constrained by airborne electromagnetic resistivity in the Capricorn Orogen, Western Australia. Explor Geophys. doi: 10.1071/EG16069


Schodde R (2017) Long term trends in global exploration – are we finding enough metal?

Schodde R (2015) Exploration trends, finds and issues in Australia


Ward A, Crooks E (2017) Oil and gas discoveries dry up to lowest total for 60 years


22


Chapter 2

Uncertainty reduction through geologically conditioned petrophysical constraints in joint inversion

“There is analysis when from a complicated truth one deduces more simple truths.”

- André-Marie Ampère

"Il y a une analyse selon laquelle, d'une vérité compacte, on déduit des vérités plus simples."

Part of the work in this chapter was presented at the SEG 2016 Annual Meeting in Dallas (USA), and at the ASEG-PESA-AIG 2016: 25th Geophysical Conference and Exhibition in Adelaide (Australia). The first page of the related conference publications is shown in Appendix 1.

The full text¹ of this chapter has been published in GEOPHYSICS. It has been reformatted to fit this thesis. Relevant references have been added accordingly with advances that occurred since publication. Minor amendments were made accordingly.

2.1. Abstract

We introduce a joint geophysical inversion workflow that aims to improve subsurface imaging and decrease uncertainty by integrating petrophysical constraints and geological data. In this framework, probabilistic geological modelling is used as a source of information to condition the petrophysical constraints spatially and to derive starting models. The workflow then utilises

¹ Link to publication: https://library.seg.org/doi/abs/10.1190/geo2016-0615.1
petrophysical measurements to constrain the values retrieved by geophysical joint inversion. The different sources of constraints are integrated into a least-square framework to capture and integrate information related to geophysical, petrophysical and geological data. This allows us to quantify the posterior state of knowledge and to calculate posterior statistical indicators. To test this workflow, using geological field data we have generated a set of geological models, which we used to derive a probabilistic geological model. In this synthetic case study, we show that the integration of geological information and petrophysical constraints in geophysical joint inversion can reduce uncertainty and improve imaging. In particular, the use of petrophysical constraints retrieves sharper boundaries and better reproduces the statistics of the observed petrophysical measurements. The integration of probabilistic geological modelling permits more accurate retrieval of model geometry, and better constrains the solution while still satisfying the statistics derived from geological data. The analysis of statistical indicators at each step of the workflow shows that 1) the inversion methodology is effective when applied to complex geology, and 2) the integration of prior information and constraints from geology and petrophysics significantly improves the inversion results while decreasing uncertainty. Lastly, the analysis of uncertainty to the integration of the conditioned petrophysical constraints also shows that, for this example, the best results are obtained for joint inversion using petrophysical constraints spatially conditioned by geological modelling.

2.2. Introduction

Over the last 15 years, significant research efforts have been directed towards the integration and use of the complementarity between different geophysical datasets in geophysical exploration to better constrain the properties of the subsurface [see (Gallardo and Meju 2011; Gyulai et al. 2013; Lelièvre and Farquharson 2016; Moorkamp 2017) for more information about the different joint inversion approaches in exploration geophysics]. The main interest of joint inversion is to use and combine the strengths of different geophysical techniques to reduce the effect of non-uniqueness and uncertainty with respect to single domain inversions (Jupp and Vozoff 1975). One of the motivations for developing these techniques is that the exploration of natural resources is becoming increasingly challenging. Hydrocarbon discoveries are becoming rarer and smaller (Ward and Crooks 2017), and economic mineral deposit discoveries also show a decreasing trend since the
mid 90’s (Schodde 2010) while deposits are found at increasing depths (Schodde 2015). Geophysical joint inversion is one of the tools used to mitigate the risk of inaccurate interpretation of geophysical data in exploration scenarios (Rubin and Hoversten 2006).

The usual approach to performing geophysical joint inversion is to jointly invert datasets of two or more geophysical methods using selected constraints and links between the datasets that depend on the amount and type of prior knowledge. When minimum geological information is available, several authors enforce structural constraints between the models jointly inverted (Gallardo and Meju 2003, 2004, 2007; Gallardo et al. 2005; Linde et al. 2006; Colombo and De Stefano 2007; Fregoso and Gallardo 2009; Hu et al. 2009; Moorkamp et al. 2011, 2013; Abubakar et al. 2012; Lelièvre et al. 2012; Boucheddha et al. 2012; Molodtsov et al. 2013; Bennington et al. 2015). Alternatively, when more external information is available, (De Stefano et al. 2011) offer the possibility of linking multiple domains during joint inversion using either structural constraints or empirical petrophysical laws. When probabilistic geological or petrophysical data are available, several authors developed approaches involving statistical tools that account for prior information (Bosch 2004; Gloaguen et al. 2004; Lane and Guillen 2005; Mahardika et al. 2012; Shamsipour et al. 2012; Jardani et al. 2013; Reid et al. 2013; McCalman et al. 2014; Roberts et al. 2016). In a similar fashion, (Chen and Hoversten 2012) performs stochastic joint inversion to retrieve petrophysical properties.

In the deterministic realm, (Paasche and Tronicke 2007; Lelièvre et al. 2012; Sun et al. 2012; Sun and Li 2015) use clustering approaches to constrain the values of inverted properties. (Garofalo et al. 2015) use a physical relationship and impose similar layer geometry during joint inversion. Another strategy has been introduced and used by (Hoversten et al. 2006; Gao et al. 2012a; Giraud et al. 2013; Liang et al. 2016) who use constitutive equations linking petrophysical properties to physical properties to retrieve petrophysical properties. Alternatively, (Dell’Aversana et al. 2011, 2016; Medina et al. 2015; Miotti and Giraud 2015; Miotti et al. 2015) estimate petrophysical relationships using well-log data before running joint inversion to retrieve petrophysical properties (e.g., porosity, water saturation, and volume of shale).
Successful case studies have shown the relevance of integrating different geophysical datasets in complex scenarios using some of the methodologies listed above (see for example Colombo and De Stefano 2007; De Stefano et al. 2011; Gallardo et al. 2012; Reid et al. 2013; Medina et al. 2015).

However, while geological measurements and orientation data can be used as constraints during inversion (Fullagar et al. 2008; Lelièvre and Oldenburg 2009; Scholl et al. 2016), less effort has been put on the quantitative integration of geostatistical modelling into geophysical joint inversion. Several studies show examples where different disciplines of geology and geophysics are integrated in a cooperative manner using expert knowledge (Jessell and Valenta 1996; Betts et al. 2003; Mantovani et al. 2016; Tschirhart and Pehrsson 2016). Quantitative integration of these two disciplines is an active, yet underexplored research area. Recent research works (Revil et al. 2015; Zhang and Revil 2015; Zhou et al. 2016) illustrate the increase of interest from the community, and show that integration of multiple datasets is a way forward in tackling the limitations of current inversion methodologies.

Recent advances in geostatistical modelling enable geologists to quantitatively generate more realistic geological models from surface and borehole data (Calcagno et al. 2008; Jessell et al. 2014; de la Varga and Wellmann 2016). However, quantitative validation using geophysical and petrophysical data is necessary (Jessell et al. 2010, 2014, Lindsay et al. 2013b, a, 2014).

To mitigate the lack of quantitative integration between geology and geophysics, several authors developed geophysical inversion algorithms addressing the geometry of the inverted models. For instance, (Gallardo et al. 2005; Fullagar and Pears 2007; Guillen et al. 2008; Wellmann and Finsterle 2013; Zhang and Revil 2015) developed geology-geophysics inversion algorithms that allow the geometry of the geological structures to vary in order to honour geophysical data. Alternatively (Balidemaj and Remis 2010; Li et al. 2010; Davis et al. 2012; McMillan et al. 2015) parameterise geology to include model geometry in inversion. To cope with the additional variables introduced by geological modelling, (Doetsch et al. 2010) allow their algorithm to discretise the medium in layers. Similarly, (Juhojuntti and Kamm 2015) introduce a layered joint inversion scheme. These layered schemes attempt to solve hydrogeological problems, and the investigated models do not have the same geological complexity encountered in hard rock scenarios. With this

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regard, (Lelièvre et al. 2015) developed a more general method inverting for contact surface geometry.

In joint inversion, the hypotheses underlying structure-based approaches (e.g. the curvature of the models as introduced by (Haber and Oldenburg 1997), or the cross-product of the gradients of the model as introduced by (Gallardo and Meju 2003), may exert little influence on the inversion depending on the geological setting of the area, in cases where gradients of the considered properties are not parallel. A possible strategy to complement joint inversion approaches relying on structural similarities is to link the different geophysical methods through constraints derived from non-geophysical field measurements. In this work, we propose such a methodology which we apply to a general case where some of the assumptions commonly made to link models in joint inversion are not valid across the entire model.

As discussed above, the use of petrophysical laws can be used to link different domains in joint inversion and to avoid making hypotheses on the structural setting of the medium. However, accurate determination and upscaling of these laws to the entire model is challenging and sufficient prior information is necessary to determine and tune them. On the other hand, statistical petrophysical analysis is a powerful tool to derive correlations between physical properties. In addition to the templates using mechanical properties, petrophysical templates have been produced to classify rocks according to their mineral content or lithology using, among others, density and magnetic susceptibility. Some authors (Hatfield et al.; Barlow 2004; Rao and Delhi 2008) also use plots of density and magnetic susceptibility to discriminate lithologies, although in hard rock scenarios lithological classes may overlap (Williams 2009). In this article, we use the statistics of the petrophysical properties in cross-plot domain and link it to lithology from probabilistic geological modelling to constrain inversion. We address the petrophysical constraints in the same spirit as the clustering approaches introduced by (Lelièvre et al. 2012; Sun et al. 2012, 2013). The clustering approach has been further investigated (Carter-McAuslan et al. 2015), applied to field data by (Sun and Li 2015, 2017a), and extended, for single domain inversion, to the use of geological interpretation by and (Rapstine et al. 2016). We adapt and extend these concepts to a joint least-square inversion framework, in which we integrate probabilistic geological information.
Inverse problems in geosciences typically have a high dimensionality and are under-constrained (Li and Oldenburg 1998; McCalman et al. 2014). The workflow we present integrates complementary sources of information to constrain geophysical inversion in order to reduce both uncertainty and non-uniqueness due to the effect of the ill-posedness of the inverse problem. Geological prior information is commonly used to mitigate non-uniqueness and as a means to derive starting and reference models. However, the reliability of geological prior information is tied to the geologist’s expertise, and is therefore affected by biases (Bond et al. 2007, 2015). To alleviate this, we introduce a methodology that integrates probabilistic geological modelling, petrophysical measurements and geophysical joint inversion in a fully integrated workflow. In this way, our methodology accounts quantitatively for prior uncertainty relating to geology, petrophysics and geophysics. We obtain spatially conditioned petrophysical constraints by combining surface petrophysical measurement and the geological model resulting from what we refer to as Monte Carlo Uncertainty Estimation (MCUE) as introduced by (Pakyuz-Charrier et al. 2018a, c, b). The novelty of the work presented in this article is that not only do we take advantage of complementary geophysical methods in joint inversion, we also combine probabilistic geological modelling and petrophysical measurements to derive constraints for inversion. We use this to integrate the statistics of the petrophysical measurements, geological modelling and geophysical data. This allows us to calculate posterior uncertainty indicators and to evaluate the quality of the results.

In this manuscript we first introduce the theoretical background describing the methodology we have used, detailing the inversion algorithm and how geological modelling and petrophysical constraints are derived and integrated. Then, prior to introducing the synthetic case study we generated to test our workflow we explain our choice of statistical tools for uncertainty analysis. The final section of the paper analyses the results using the selected statistical tools. This section shows the improvements and limitations of the integration of geological modelling and petrophysical constraints in geophysical inversion.
2.3. Methodology

To integrate geological measurement in the inversion we use a probabilistic geological modelling approach accounting for geological uncertainty. We use what we refer to *Monte Carlo Uncertainty Estimator* (MCUE) (Pakyuz-Charrier et al. 2018a, c, b). It utilises probabilistic modelling to obtain a probabilistic geological model (i.e. a lithology probability set for each voxel in the model). MCUE is based on a Monte Carlo perturbation of geological input data used to produce a relatively large number of possible geological models (typically between several hundred to a few thousand), which we couple with the statistics of the petrophysical measurements to constrain the inversions (joint and single domain). As a statistical description of a wide range of possible geological models, MCUE removes the need for a best guess model.

The workflow we present here can be divided into several steps. The first two steps of the workflow are to perform MCUE analysis and in parallel derive statistical laws that reproduce the statistics of petrophysical measurements (see subsection on petrophysical constraints, equation 2.6). The next step consists of combining the geological statistical model with the former statistical laws to obtain starting models and constraints for inversion. Then, geophysical inversions are performed. After joint inversion, the last step of the workflow is the calculation of uncertainty indicators. This allows us to quantify the reduction of uncertainty, to evaluate the effect of integrating geology and petrophysics in single domain and joint inversion. Zones of higher uncertainty, which remain poorly constrained, can be identified as the foci for further study (Wellmann et al. 2010b; Lindsay et al. 2012).

The test data set uses a geological model computed from actual surface structural measurements (rock type, foliations, dip and strike and surface contact geometry) but for which we increased the complexity by adding additional structures in order to test the robustness of the methodology. We use GeoModeller® to generate models. This relatively complex synthetic case study allows us to evaluate the behaviour of the inversion algorithm in real cases studies, where there is no control on the actual model. To test and illustrate the workflow we simulate gravity and magnetic surface data.
2.4. Workflow summary

The workflow is summarised in Figure 2.1. Before inversion, the first step is to translate prior geological and petrophysical data into information that can be used during the inversion. In the MCUE approach, geological modelling uses geological data to produce a probabilistic geological model. A mixture model that reproduces the statistics of the petrophysical measurements is derived. The probabilistic geological model and the mixture model are used to derive starting models, global (spatially invariant) and geologically conditioned petrophysical constraints. Once these are available, constrained single domain inversions are performed first. These are used as controls to assess the improvement brought by constraints and to compare with joint inversion. The next step of the workflow is to run joint inversion. After joint inversions have been performed, the last step of the workflow is the estimation of posterior uncertainty using uncertainty indicators for the inverted models.

![Figure 2.1. Integrated joint inversion workflow summary illustrating the interaction between geology, petrophysics and geophysics.](image)
2.4.1. Inversion framework

2.4.1.1. Objective function

We formulate the inverse problem in a least-square sense as detailed in (Tarantola 2005). We derive the following objective function (equation 2.1):

\[
\theta(m) = (d - g(m))^T C_d^{-1} (d - g(m)) + (m - m_p)^T C_m^{-1} (m - m_p)
\]

\[
+ \delta^G(p_{\text{max}} - p(m))^T C_p^{-1} (p_{\text{max}} - p(m))
\]

\[
+ \delta^M(p_{\text{max}} - p(m))^T C_p^{-1},
\]

where

\[
g(m) = \begin{bmatrix} g_G(m) \\ g_M(m) \end{bmatrix}, m = \begin{bmatrix} m_G \\ m_M \end{bmatrix}, d = \begin{bmatrix} d_G \\ d_M \end{bmatrix}, \]

\[
C_d = \begin{bmatrix} C_{d_G} & 0 \\ 0 & C_{d_M} \end{bmatrix}, C_m = \begin{bmatrix} C_{m_G} & 0 \\ 0 & C_{m_M} \end{bmatrix}.
\]

(2.1)

In equations (2.1) and (2.2), \(m\) represents the model of inverted properties while \(d\) represents the geophysical measurements to be inverted. The forward operator \(g\) calculates the data model \(m\) produces; \(m_p\) is the prior model, which we also use as starting model; \(C_m\) and \(C_d\) are spherical covariance matrices corresponding to model and data noise, respectively; and G and M superscripts and subscripts refer to gravity and magnetics, respectively.

Here, \(C_p\) is what we call the petrophysical probability covariance matrix (see subsection 2.4.3); \(p\) is the probability density function derived from petrophysical measurements, calculating the likelihood of model \(m\), \(p(m)\); and \(p_{\text{max}}\) is the mode of \(p(m)\). Superscript \(T\) denotes the transpose operator. The scalars \(\delta^G\) and \(\delta^M\) are set either to 0 or 1 depending on the type of inversion.

In the objective function, the first two terms in equation (2.1) relate to data and model misfit, respectively. The third and fourth terms are specific to petrophysical constraints on gravity and magnetic data inversion, respectively. They relate to the probabilistic description of the model based on independent, non-geophysical sources of information. Term \(p\) encapsulates the coupling in joint inversion. It is a function of both \(m_G\) and \(m_M\) and is defined such that \(p : N \times N \rightarrow N\) with \(m\) as input, returning the corresponding \(p(m)\) values.
2.4.1.2. Optimisation scheme

We minimise the joint objective function $\theta(m)$ (equation 2.1) using a least-squares algorithm, adapting the solution proposed by (Tarantola 1984) to our joint inversion problem. The model is iteratively updated using a fixed-point method as follows (equation 2.3) for gravity and magnetic data:

$$m^G_{k+1} = m^G_k + \left[ A^G_k C^G_d^{-1} A^G_k + C^G_m^{-1} + f^G_k C^G_p^{-1} f^G_k \right]^{-1} \left[ A^G_k C^G_d^{-1} \left( d_G - g_G(m^G_k) \right) - C^G_m^{-1} \left( m^G_k - m^G_p \right) + f^G_k C^G_p^{-1} \left( p_{\text{max}} - p(m_k) \right) \right],$$

and

$$m^M_{k+1} = m^M_k + \left[ A^M_k C^M_d^{-1} A^M_k + C^M_m^{-1} + f^M_k C^M_p^{-1} f^M_k \right]^{-1} \left[ A^M_k C^M_d^{-1} \left( d_M - g_M(m^M_k) \right) - C^M_m^{-1} \left( m^M_k - m^M_p \right) + f^M_k C^M_p^{-1} \left( p_{\text{max}} - p(m_k) \right) \right],$$

with

$$A_k = \begin{bmatrix} A^G_k \\ A^M_k \end{bmatrix} = \begin{bmatrix} A^G_{k=0} \\ A^M_{k=0} \end{bmatrix} = \begin{bmatrix} \frac{\partial g_G(m_k)}{\partial m_G}, \frac{\partial g_M(m_k)}{\partial m_M} \end{bmatrix}^T,$$

$$J_k = \begin{bmatrix} f^G_k(m_k) \\ f^M_k(m_k) \end{bmatrix} = \begin{bmatrix} \frac{\partial p(m_k)}{\partial m_G}, \frac{\partial p(m_k)}{\partial m_M} \end{bmatrix}^T,$$

(2.4)

where $A_k$ and $J_k$ are, respectively, the matrices of the partial derivatives of $g$ and $p$ with respect to $m$. Subscript $k$ denotes the $k$-th iteration. The inverse of the Hessian matrix (the left part of the second term in equation 2.3) is calculated using a Cholesky direct solver based on Gauss pivot rules. Partial derivative matrices $A_k$ are calculated analytically while the elements of $J_k$ are calculated using first order finite difference derivatives.

2.4.1.3. Stopping criteria

The number of iterations is controlled by two criteria: iterations stop when the model updates stabilise below a chosen threshold; or when the Bravais-Pearson correlation (BP, also called linear correlation) between the inverted models and the BP correlation between the magnitudes of the spatial gradients of inverted models have both reached a plateau.
We calculate the BP correlation as follows (equation 2.5):

\[
r(T^{(1)}, T^{(2)}) = \frac{T^{(1)} T^{(2)} - \overline{T^{(1)}} \overline{T^{(2)}}}{\left(\left(\overline{T^{(1)}}^2 - \overline{T^{(1)}}^2\right) \left(\overline{T^{(2)}}^2 - \overline{T^{(2)}}^2\right)\right)^{1/2}}
\]

where \(T^{(1)}\) and \(T^{(2)}\) are the properties for which the correlation is calculated, and the horizontal bar operator is the arithmetic average operator.

We calculate \(r\) for \(T^{(1)}\) and \(T^{(2)}\) being the inverted models or the magnitude of their gradients. In the second case, \(T^{(1)}\) and \(T^{(2)}\) are calculated as \(T^{(1)} = |\nabla m^{(1)}|\), \(T^{(2)} = |\nabla m^{(2)}|\) for a given set of models. \(r\) can be interpreted as the cosine similarity between the vectors \(T^{(1)} - \overline{T^{(1)}}\) and \(T^{(2)} - \overline{T^{(2)}}\). It reaches its maximum value when the two vectors have the same orientation in the entirety of the model. Therefore, we can use \(r(|\nabla m^{(1)}|, |\nabla m^{(2)}|)\) to characterise the geometrical convergence of the inverted models during inversion. Similarly, \(r(m^{(1)}, m^{(2)})\) provides a metric characterising the degree of linear relationship between the two models during inversion. When \(r\) reaches a plateau, the changes in the models are not sufficient to have an impact on \(r\), meaning that, with regards to geometrical considerations, inversion has converged.

### 2.4.2. Geological modelling

Building geological models from geological observations depends on the interpreter (Bond et al. 2007), on the type of data (Bond et al. 2015) and of the quality of the data and how well it represent nature (Alcalde et al. 2017). Under these conditions, rigorous prior uncertainty estimation on geological prior models is difficult to obtain even with error estimates on input data. Thus, following the recommendations of (Lindsay et al. 2012, 2013b; Wellmann and Regenauer-Lieb 2012; Jessell et al. 2014), we use a geological modelling scheme capable of generating a ‘suite’ of geological models, which allows the quantification of uncertainty inherent in a 3D model.

In the MCUE approach of (Pakyuz-Charrier et al. 2018a, c), geological models are drawn from probability distributions defined by basic assumptions about the statistics of the errors on
Chapter 2

geological data using a Monte-Carlo simulation. Topological rules prevent unstructured behavior, ensuring that the models are geologically plausible. The data replacement and perturbation procedure used in the Monte Carlo simulation is described in detail in (Pakyuz-Charrier et al. 2018c), to which the reader can refer for more information.

The probability of presence of a lithology is calculated for each cell of the model. For the \( i \)-th cell of the medium, the probability of presence of rock unit \( k \) is \( \psi_{k,i} \). That is, the end product of MCUE is analogous to a ‘geological model with an uncertainty estimate’. In the workflow we present in the paper, the results from of MCUE are used to calculate several terms in equation (2.1): \( p(m), p_{\text{max}} \).

2.4.3. Petrophysical constraints

The petrophysical constraints are applied to inversion through the minimisation of the third term of equation (2.1) simultaneously to the minimisation of the data and model misfit terms. To maximise the similarity between the statistical properties of the measured petrophysical data and the inverted model we follow concepts introduced by (Lelièvre et al. 2012; Sun et al. 2012, 2013). We assume that the petrophysical properties are normally distributed for each rock type. Therefore, there exists a statistical model that can represent the probability distribution of the overall measurements. \( p(m) \) is formulated using a mixture model as (equation 2.6):

\[
p(m) = \sum_{k=1}^{n_f} \omega_k N(m|\mu_k, \sigma_k)
\]

In equation (2.6), \( n_f \) is the number of lithologies observed in the petrophysical measurements. The parameters of \( N(m|\mu_k, \sigma_k) \), \( \sigma_k \) and \( \mu_k \), are estimated using an expectation maximisation algorithm. Although there are no constraints on the type of distribution to be used, we assume, to fix ideas, a normal distribution \( N \). As described in (Grana et al. 2015, 2017), Gaussian mixture models can be used in statistical of rock physics modelling. In equation (2.6), each distribution is characterised by a mean value vector, \( \mu_k \), which corresponds to the clusters’ centers, and the associated covariance matrix, \( \sigma_k \). \( \omega_k \) is the relative weight of the \( k \)-th lithology in the measurements. \( \mu_k \), \( \sigma_k \) and \( \omega_k \) are obtained by fitting equation (2.6) to the petrophysical measurements. The correlation between petrophysical properties of different nature (for example
density and magnetic susceptibility) is captured in the off-diagonal elements of $\mathbf{\sigma}_k$, which is a full matrix. After the mixture is characterised we calculate the diagonal matrix $\mathbf{C}_p$ as follows:

$$\mathbf{C}_p = \left( \text{max}_{k=1:n_f} \text{diag}(\mathbf{\sigma}_k) \right)^{-1} \mathbf{I}. \quad (2.7)$$

This method of weighting is chosen to enhance the contribution of well-defined components of the mixture model in the model update.

Model covariance matrix $\mathbf{C}_m$ is preconditioned through the application of a depth-weighting inverse power law function following (Li and Chouteau 1998; Li and Oldenburg 1998) for gravity, and following (Li and Oldenburg 1996) for magnetic data, to balance decreasing sensitivity with depth. For the conditioning of petrophysical constraints by geological modelling, $\mathbf{p}(\mathbf{m})$ is calculated using both the results from MCUE and the mixture estimated in equation (2.6).

The probability of presence of the different rock units $\psi_{k,i}$, in each cell of the medium, is accounted for. In such case, $\mathbf{p}(\mathbf{m})$ is calculated as follows (equation 2.8):

$$\mathbf{p}(\mathbf{m}) = \left[ \begin{array}{c} p_1(m_1) \\ p_2(m_2) \\ \vdots \\ p_{n_m}(m_{n_m}) \end{array} \right], \text{with: } p_i(m_i) = \sum_{k=1}^{n_f} \psi_{k,i} \mathbf{N}(m_i|\mu_k, \mathbf{\sigma}_k), \quad (2.8)$$

where $n_m$ is the total number of cells of the model. The conditioning of the petrophysical constraints is illustrated as follows (Figure 2.2):

![Figure 2.2. Principle of conditioning of petrophysical constraints by MCUE.](image-url)
After conditioning of $p(m)$ (equation 2.6 and 2.8) the term $p_{\text{max}}$ (in equation 2.1 and 2.3) can be calculated. It is calculated as follows (equation 2.9), for the $i$-th cell of the medium:

\[
\begin{align*}
    k^* &= \left\{ k | \psi_{k,i} = \max_{n=1:n_f} \psi_{n,i} \right\}, \\
    p_{\text{max},i} &= \psi_{k^*,i} \sum_{j=1}^{n_f} N(\mu_{k^*}, \mu_j, \sigma_j).
\end{align*}
\]

(2.9)

MCUE is also used to calculate starting models for inversions using conditioned petrophysics. In such case, the starting model is determined by calculating the mathematical expectation of $p(m)$ after it is conditioned by geological modelling. The use of the mathematical expectation is convenient here because it represents the average model obtained after a sufficiently large number of draws using Monte Carlo sampling in model space, which is performed during MCUE.

The starting model is calculated as follows for the $i$-th cell (equation 2.10):

\[
m_{0,i} = \sum_{k=1}^{n_f} \psi_{k,i} \mu_k
\]

(2.10)

In the case of global petrophysical constraints, $p(m)$ is calculated assuming equiprobability for all lithologies (all $\psi_{k,i}$ being equal to $\frac{1}{n_f}$), and $m_0 = 0$.

2.4.4. Uncertainty analysis and inversion uncertainty indicators

In our workflow, we monitor inversion and perform posterior statistical analysis that incorporates geological and petrophysical information. We study the convergence of the algorithm, the increase of model likelihood and assess the reduction of non-uniqueness. To this end, we calculate the petrophysical likelihood of the inverted model and indicators it allows us to derive. In addition, the posterior analysis of the correlations introduced in the previous subsection provides information on the degree of coupling between the inverted models. For tests on synthetic models, we calculate the root-mean-square (RMS) model misfits. For geophysical (field or synthetic) data we calculate the first term in equation (2.1), corresponding to the data misfit term.
The petrophysical likelihood function of the inverted models is calculated a posteriori for each cell of the medium, using geologically conditioned petrophysical constraints (equation 2.8):

\[ L = p(m_f), \quad (2.11) \]

where \( p \) is conditioned by MCUE (as in equation (2.8)) and \( m_f \) is the model obtained after convergence of the algorithm.

In the definition of the petrophysical likelihood \( L \) (equation 2.11) we do not include the term related to geophysical data fit in order to isolate the reduction of geological and petrophysical uncertainty brought by geophysical inversion. As stated above, \( L \) is used to derive other indicators. It is straightforward to show that, assuming that the observables are constituted of the parameters defining \( p \) in equation (2.8).

Final values for the different inversions and analysis of the value of \( L \) allow us to estimate the amount of information from the petrophysical constraints that contributed to the inversion.

2.5. Synthetic geophysics with real geology

2.5.1. Geological context and modelling

We generated a 3D geological model derived from surface data from the Mansfield area (Victoria, Australia). The original model is the Mansfield sedimentary basin located North-West to Mansfield, Victoria, Australia. It presents itself as a Carboniferous mudstone and sandstone syncline oriented N170. It abuts a faulted contact with a Silurian-Devonian folded sandstone basement to the South West. After we obtained a geological model that reproduces field geological data we increased the complexity of the model to better test the inversion algorithm by the addition of a fictitious North-South fault across the Carboniferous basin and of an imaginary mafic intrusion to the South West corner of the model, in the Devonian basement; details on the original model can be found in GeoModeller User Manual, Tutorial case study H (Mansfield).

The reference geological model was constructed without addressing errors in geological data (e.g. using unperturbed input data), and is shown on Figure 2.3.
In Figure 2.3, the map view shows that the model contains faults that intersect. Cross-section A-B was chosen for the testing the geophysical part of the workflow as it shows complex, realistic structures that can be challenging to retrieve through inversion. Since we are only solving a 2D problem, the obliquity of the section to the regional structures does not pose a problem.

We applied the MCUE method to the geological reference model by assuming that errors on orientation data can be modelled using the von Mises-Fisher distribution, using a solid angle of approximately 0.1 steradians. This corresponds to the case scenario where 99% of the orientation data lies within a 22 degree aperture cone. 300 samples generated by the Monte-Carlo simulation in MCUE allowed us to obtain a stable 3D statistical model, shown in Figure 2.4 for cross-section A-B.
Figure 2.4. Probability of presence for the different lithologies for cross-section A-B. These probabilities have been obtained from MCUE on the whole geological model and extracted along the cross-section to be used in a 2D setting.

Figure 2.4 shows the resulting probability of the presence at a given location of each of the modelled lithologies after applying MCUE. Comparing the results for different lithologies it is interesting to note that some parts of the model are better constrained at depth than closer to ground level. This can be explained by the fact that geological complexity can be more important closer to ground level depending on orientation data, thus increasing uncertainty in such cases. For instance, lithology 3 shows high probability of presence around 2.5 km depth in the bottom left corner of the corresponding plot. Lithology 1 represents the basement, and is defined as the lack of observation of the other units. As such lithology 1 is a proper unit, it embodies the limits of our knowledge where other units are not observed.
2.5.2. Simulating geophysical and petrophysical data

Using the reference geological model, we assigned values of density contrast and magnetic susceptibility to each lithology of section A-B consistently with the structural setting. We assigned a low density contrast and limited magnetic susceptibility to basin fill (lithologies 4, 5 and 6). We assigned higher density contrast and magnetic susceptibilities to lithologies 1, 2 and 3. The petrophysical model, as shown in Figure 2.5, is directly derived from the reference geological model by assigning values to each lithology (Figure 2.3). The values we assigned to lithologies have been chosen to obtain contrasts that are close to what could be observed in real scenarios. For density contrast, the background density is set at 2.6 g/cc (or 2600 kg/m³). This model is used to generate geophysical data for inversion, and is referred to as the reference model.

Magnetic and gravity data were computed at the same horizontal location along the section but at two different altitudes as the aim here is to simulate magnetic airborne (data acquired at 50 m elevation) and gravity ground surveys (data acquired at ground level). Magnetic data are simulated following the same approach as (Guo et al. 2015). Gravity data are simulated following (Boulanger and Chouteau 2001). We inverted for the horizontal component of the total magnetic field and the vertical component of the Bouguer anomaly assuming a flat topography.

![Figure 2.5. True petrophysical model (top) and simulated geophysical data (bottom). Gravity density contrast (left) is expressed in kg/m³ while magnetic susceptibility has no units. The numbers on the Figure indicate the index assigned to the lithologies as per Figure 2.3.](image-url)
In this synthetic dataset we simulated petrophysical measurements using a Gaussian mixture model (GMM). The individual Gaussian distributions making up the simulated petrophysical data have a variance of $(40 \text{ kg/m}^3)^2$ for density contrast, $(0.01 \text{ SI})^2$ for magnetic susceptibility, and a cross-covariance of 0.04 (SI·kg/m³). In this example we describe magnetic susceptibility using Gaussian distributions (although it could also be done using another type of distribution such as lognormal distributions, depending on the petrophysical measurements). Table 2.1 summarises the statistical properties of the distributions describing the simulated petrophysical data.

Table 2.1. Parameters of the mixture model describing petrophysical measurements

<table>
<thead>
<tr>
<th>Lithology index</th>
<th>Mean density contrast (kg/m³)</th>
<th>Variance on density contrast ((kg/m³)²)</th>
<th>Mean magnetic susceptibility (SI):</th>
<th>Variance on magnetic susceptibility ((SI)²)</th>
<th>Cross-covariance (SI·kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>300</td>
<td>1600</td>
<td>0.075</td>
<td>1e-4</td>
<td>0.04</td>
</tr>
<tr>
<td>2</td>
<td>300</td>
<td>1600</td>
<td>0.05</td>
<td>1e-4</td>
<td>0.04</td>
</tr>
<tr>
<td>3</td>
<td>200</td>
<td>1600</td>
<td>0.025</td>
<td>1e-4</td>
<td>0.04</td>
</tr>
<tr>
<td>4</td>
<td>100</td>
<td>1600</td>
<td>0.05</td>
<td>1e-4</td>
<td>0.04</td>
</tr>
<tr>
<td>5</td>
<td>0</td>
<td>1600</td>
<td>0.025</td>
<td>1e-4</td>
<td>0.04</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>1600</td>
<td>0</td>
<td>1e-4</td>
<td>0.04</td>
</tr>
</tbody>
</table>

The corresponding cross-plot is shown in Figure 2.6, where the center of the Gaussians correspond to physical property values assigned to the different lithologies of the true model as shown in Figure 2.3 and Figure 2.5. In Figure 2.6, one would notice that the projection of cluster centers on the magnetic susceptibility and density contrast axes overlap. For example, clusters pairs 1, 2 and 5, 6 (2, 4 and 3, 5) have the same center along the density contrast (magnetic susceptibility) axis. In such case, because of this ambiguity, the six geological units cannot be resolved properly without joint interpretation.
Figure 2.6. Plot of the mixture model describing petrophysical measurements, as per properties summarised in Table 2.1. The crosses indicate the centre (mean) of the individual distributions making up the mixture model; the associated numbers refer to lithology number as shown on Figure 2.3.

2.6. Results: from unconstrained single domain inversion to constrained joint inversion

2.6.1. Inverted models

We performed a sensitivity analysis to evaluate the influence of prior information and constraints on the inverted model. For single domain inversion we evaluate: unconstrained inversion; inversion with global (e.g., spatially invariant and geologically un-constrained) petrophysical constraints; and inversion with geologically conditioned petrophysical constraints. For joint inversion, we evaluate the use of petrophysical constraints and geologically conditioned petrophysical constraints. The classification of inversion types is summarised in Table 2.2 (next page).

The comparison and analysis of results obtained from inversion (a) through (e) (Table 2.2) constitutes the sensitivity analysis of inversion subject to increasing degrees of integration. It allows us to estimate the contribution of various constraints to inversions and improvements they might bring to the inverted models. The inverted models for inversion (a) through (e) as per Table 2.2 are shown in Figure 2.7 below for qualitative analysis.
Gravity data (Figure 2.5) contains long wavelength information, which explains why in this case only the largest structure is resolved by unconstrained gravity inversion (a) (Figure 2.7a). In contrast, the magnetic data (Figure 2.5) is able to resolve smaller structures, even though in the case of unconstrained magnetic inversion (a) (Figure 2.7a) it still only retrieves the largest structures of the model.

From Figure 2.7 (next page), qualitative comparison of inversions (a) through (e) shows that the use of global petrophysical constraints in single domain inversion (Figure 2.7b) does not resolve the geometry of lithologies accurately. More structural complexity is resolved when petrophysical constraints are applied to joint inversion (Figure 2.7c), and when petrophysical constraints are conditioned by geological modelling in single domain inversion (Figure 2.7d). Besides showing models that are consistent with each other, Figure 2.7e shows improvements in terms of structural geology. Even if noticeable differences occur only at a few locations, unit 1 (basement) is better constrained and unit 4 is better defined and does not link to unit 2 anymore. This improvement is critical because this link could lead to misinterpretation of the basin size.

Results from Figure 2.7 show that joint inversion allows us to better retrieve complex geometries than single domain inversions, while the use of geologically conditioned petrophysical constraints increases the agreement of retrieved geometries with the reference model. Petrophysical constraints allow us to retrieve values that respect the statistics of surface measurements. As the petrophysical
units are well defined in the mixture model matching the statistics of the petrophysical data we simulate, the effect of the constraint is to sharpen the contacts between units.

Thus, as can be observed in Figure 2.7c, petrophysical constraints sharpen the inverted models. As can be seen in Figure 2.7d geological conditioning makes the inverted model’s geometries closer to that of the reference model. Joint inversions in Figure 2.7c and Figure 2.7e increase geological complexity in the inverted model while increasing resemblance to the reference model (when comparing to single domain inversion in Figure 2.7b and Figure 2.7d, respectively). Visually, Figure 2.7e shows results that are closest to the reference model.
Figure 2.7. Inversion results for gravity data (left) and magnetics (right). Left column: density contrast, in kg/m³. Right column: magnetic susceptibility. Inversion types are referred to as (a) through (e) as per Table 2.2. Black dotted lines represent the interfaces between lithologies in the reference model.
2.6.2. Uncertainty analysis

We analysed the uncertainty of the results obtained from the different types of inversion in Table 2.2 and shown in Figure 2.7 through the calculation of the indicators introduced above. These indicators are the likelihood $L$ (equation 2.11). This assessment allows us to quantify qualitative observations from the inverted models shown in Figure 2.7. First, we compare the inversion results by displaying the inverted models using cross-plots where inverted physical property values are color-coded by corresponding likelihood values (a-e next page). As an additional indicator, we used the absolute value of the cross-product of the gradients (f) to compare the different inversions.

Comparing cross-plots in a and in b it is observed that petrophysical constraints sharpen the model as inverted data are clustered around specific values. Single domain inversions (b) are run separately and the inverted models do not interact: the geometry of inverted models does not match. Therefore, in this case, the ambiguity of cluster centers in single domain inversion is affecting the resulting cross-plot. Results shown in b are affected by the ambiguity existing on values of the center of clusters (lower likelihood points shown in blue). On the other hand, to honour the petrophysical constraint in joint inversion (c and e), inverted values must be clustered around values that belong concurrently to cluster centers along the gravity contrast and magnetic susceptibility axes (higher likelihood points shown in red). Consequently, joint inversion results are less affected by ambiguity.
Figure 2.8. Cross-plots of inverted models for the different levels of integration. Inversion types are referred to as (a) through (e) as per Table 2.2. The color coding represents likelihood values for each point in the cross-plot. Colored lines are contour levels of the GMM shown in Figure 2.6. The bottom right plot (f) shows the comparison of cross-product values for different inversions with the true value.
Ambiguities observed in b disappear in c as in the latter global petrophysical constraints are applied jointly to the inverted properties. However, ambiguity appears again on d when geologically conditioned petrophysical constraints are applied to single domain inversion. Finally, e shows that inverting geophysical datasets jointly reduces the remaining ambiguity and the number of low likelihood points). f shows the average cross-gradient is, for all 5 inversion types we ran, higher than for the true model. For this indicator, the final product of our workflow (e.g. joint inversion using geologically conditioned petrophysical constraints, inversion (e) as per Table 2.2) shows values closest to those calculated for the reference model.


2.7. Constrained joint inversion with inaccurate starting model

In this subsection, we investigate the influence of a starting model that does not accurately incorporate information from geological modelling. Instead of deriving starting models using the result of MCUE combined with petrophysical measurements (equation 2.10), we use a one-dimensional starting model constituting a vertical positive gradient of density and magnetic susceptibility distributions. The values of the starting model range from 0 g/cc to 3 g/cc and 0 SI to 0.075 SI. shows the inversion results obtained used for inversion type (e) (Table 2.2). Inversion results shown in show that, except in the deepest, least constrained parts of the model where structural features of the model are guided by the starting model, the inversion methodology is robust to the starting model containing minimum prior information we used. Although the retrieved model lacks the complexity of results shown on Figure 2.7e, it still retains important features of the geological model. The analysis of quality indicators reveals that the model RMS misfit is in the same order as for inversion (c) (Table 2.1) and that the values of $I_F$ and $S_{rms}$ are intermediate to inversion (c) and (d).
Figure 2.9. Inverted model obtained through inversion type (e) (bottom) using a 1D starting model following a positive vertical gradient (middle). For comparison, the starting model derived from MCUE and petrophysical measurements is also shown (top).
2.8. Discussion

In the examples we showed we assumed that the petrophysics of the models can be described by petrophysical measurements. However, in real case scenarios it is possible that some lithologies have not been sampled by either petrophysics or geology; one approach to mitigating this is to consider this source of uncertainty in the estimation of the mixture model describing petrophysical measurements. We also assumed that the petrophysical measurements show distinct clusters, which is not always the case in nature. When clusters are not easily distinguishable, it is more difficult to differentiate the corresponding geological units through inversion. In such cases, the concerned units might be undistinguishable after conditioning of the petrophysical constraints, thus decreasing the complexity of the geological information contained in the constraints and the influence they may exert on inversion.

We made the arbitrary choice of Gaussian mixtures to describe the petrophysical measurements. Nevertheless, there is no restriction to the type of function used to describe the statistics of these measurements. In the workflow we introduced, the only requirement is for the mixture model to be differentiable, which is the case for almost all the functions that can characterise the statistics of petrophysical measurements.

One of the motivations behind the use of geologically conditioned petrophysical constraints is the incorporation of probabilistic geological information. A less computationally expensive strategy is to estimate the value of an attribute characterising the medium using geological modelling (for instance MCUE) or expert knowledge to derive less strong constraints for inversion. For example, when using the cross-gradient approach (Gallardo and Meju 2003), a non-zero objective value reflecting the geology of the area could be used. In the same fashion, when maximising the correlation between models (Lelièvre et al. 2012) and/or the gradient of the models during joint inversion, an optimum value different from unity can be used to honor prior geological information. In such case, another possibility is to calculate the BP correlation \( r \) for the orientation of the gradients in the model. This could be useful in cases similar to the model we used because the cross-product and the correlations we calculate for the true model are different from 0 and 1, respectively (see f). In such case, a possible strategy to combine the cross-gradient technique with
geological information is to derive local cross-gradient constraints in a fashion similar to the conditioning of petrophysical constraints.

2.9. Conclusion

We have developed a new inversion workflow that integrates probabilistic geological modelling, petrophysical measurements and geophysical data in a statistical sense. We evaluated the efficacy of the workflow and found that it successfully reduces uncertainty. The sensitivity analysis conducted on prior information and inversion constraints shows that inclusion of petrophysical data significantly improves results. Also, the use of geological information from MCUE to condition petrophysical constraints shows better uncertainty and model misfit reduction than when only global petrophysical constraints are applied to inversion, and was particularly effective when used on single-domain constrained inversion. Small differences in the petrophysics of retrieved models and in geophysical data fit between petrophysically conditioned single-domain and joint inversion do not indicate that joint inversion improved results significantly. Nonetheless, from a geological point of view, joint inversion produces results that are more consistent than single-domain inversions. This result is important because decisions made using one or the other of these two models could result in different outcomes (e.g., error in basin size estimation, wrong interpretation of blocking or open fault, etc). In covered terranes, complex regions may be subject to inconsistencies in model construction or be undetectable without surface evidence. In such cases, the use of MCUE in inversion would lead, in portions of the model that depart most from reality, to non-constructed zones where geological structures are difficult to identify. This can reveal the necessity to acquire additional data, to adapt the modelling of these areas, or show the need for targeted exploration.

Some studies focus on one particular aspect of integrated inversion, such as the improvement of a specific joint inversion approach or an original way of using either geological or petrophysical information. More holistic, our approach combines quantitatively, and gives equal importance to petrophysical, geological and geophysical data. Besides providing improved imaging consistent across the different disciplines involved, this workflow allows quantitative evaluation of uncertainty reduction. The adaptability of the described methods permits possible further
uncertainty reduction through the integration of additional datasets, adaptation to 3D inversion and implementation on supercomputing platforms for large datasets. One of the main issues we will have to face is the indirect computation of Hessian matrices by using more sophisticated gradient-based iterative procedures, because direct solvers like Cholesky decomposition are very difficult to scale.

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2.11. Chapter 2 References


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2. See Chapter 3 and 4 of this thesis.

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Chapter 3

Sensitivity of constrained joint inversions to geological and petrophysical input data uncertainties with posterior geological analysis

"真正的認知是知道自己的無知"

"True knowledge is the knowledge of one's ignorance”

- 孔子(Confucius)

The full text of this chapter is under peer-review for publication in Geophysical Journal International and has been reformatted to fit this thesis. In this Chapter, (Giraud et al. 2017) refers to Chapter 2 and (Giraud et al. 2018a) refers to Chapter 4.

3.1. Abstract

The integration of petrophysical data and probabilistic geological modeling in geophysical joint inversion is a powerful tool to solve exploration challenges. Models obtained from geologically and/or petrophysically constrained inversions are the result of complex interactions between correspondingly diverse datasets. It is therefore important to understand how non-geophysical input uncertainty impacts inverted models. In this article, we propose to study the influence of uncertainty in geological and petrophysical measurements used to derive prior information and constraints onto geophysical inversion. Starting from geological field data from the Mansfield area (Victoria, Australia), we simulate low, medium, and high uncertainty levels in geological measurements and petrophysical data, combined into a series of nine realistic case
scenarios. This allows us to investigate the impact and propagation of uncertainty in non-geophysical measurements into geophysical inversion. To analyse inversion results, we calculate misfit indicators and reconstruct lithological models a posteriori. We complement the examination of inverted models with the topological analysis of lithological models, which we use to quantify the resemblance between the recovered and reference models in a geological fashion. Our work reveals that the influence of uncertainty in geological measurement dominates over that of petrophysical data. Our results show that the effect of geological measurement uncertainty dominates over that of petrophysical data uncertainty. It also suggests that while reducing uncertainty in geological measurements ameliorates inversion results, the effect of local entrapment is more pronounced for low petrophysical measurement uncertainty.

### 3.2. Introduction

The premise that modeling a physical system requires the use of all available information about it (Hempel and Oppenheim 1948; Cartwright and McMullin 1984; Nearing et al. 2016) justifies the integration of various disciplines in geophysical inverse modeling. It is motivated by the need to improve the models’ geological reliability and to mitigate geophysical inversions’ inherent limitations. With minimum non-geophysical information, geophysical integration efforts focus on inverting several geophysical datasets jointly by enforcing structural similarities between inverted models, i.e., (Haber and Oldenburg 1997; Gallardo and Meju 2003). In the past years, the ever growing need to improve subsurface imaging, to reduce and analyse uncertainty increased the interest of the geoscientific community for multi-disciplinary integration (Moorkamp 2017). Numerous works have explored integration strategies to improve geophysical imaging for mineral, hydrocarbon, near surface and multiscale geophysics, as reviewed by (Parsekian et al. 2015; Lelièvre and Farquharson 2016; Moorkamp et al. 2016; Linde and Doetsch 2016), respectively.

More specifically, recent works highlight the advantages of integrating either petrophysical constraints (Lelièvre et al. 2012b; Carter-McAuslan et al. 2015; Zhang and Revil 2015; Kamm et al. 2015; Heincke et al. 2017; Sun and Li 2017) or geological information or data (Fullagar and Pears 2007; Lelièvre et al. 2012a, 2015; Lelièvre and Farquharson 2013; Revil et al. 2015; Scholl et al. 2016; Bijani et al. 2017; Lipari et al. 2017; Giraud et al. 2018b) in inversion. Alternatively, (Brown et al. 2012; Zhou et al. 2014, 2016; Wiik et al. 2015; Guo et al. 2017;
Giraud et al. (2018b) propose the integration of structural information from geophysical or non-geophysical images in geophysical inversion to guide the inverse modeling process.

Concurrently, several authors developed methodologies to characterize geodiversity (Lindsay et al., 2013a, 2013b, 2014), which is the geological counterpart of biodiversity in biological sciences applied to geological modeling. Meanwhile, others focus on the study of geological uncertainty (Wellmann and Regenauer-Lieb 2012; Lark et al. 2013; Park et al. 2013; Kinkeldey et al. 2015; de la Varga and Wellmann 2016; Schneeberger et al. 2017; Schweizer et al. 2017).

In particular, (Pakyuz-Charrier et al. 2018a, c) produce probabilistic geological models from statistically uncertain inputs. These authors calculate probabilistic geological models (PGMs) through a technique called Monte-Carlo Uncertainty Estimator (MCUE). Their methodology relies on the sampling of a probability distribution representing geological measurements and their uncertainty. It is coupled to a geological modeling engine to produce a series of geologically plausible models. From this suite of geological models, the observation probability (i.e., the observed relative frequency) of each lithology is calculated in each model cell across the studied area, thus constituting a probabilistic geological model (PGM).

When available, such PGM can be utilized to condition petrophysical constraints spatially, which has the potential to greatly improve inversion results (Giraud et al. 2016a, b, 2017). Consequently, models calculated through constrained geophysical inversion encapsulate geophysical and petrophysical information. In such cases, as it is often the case in inverse modeling, integrated inversion suffers from non-linearity. Although it is a key factor for model evaluation in exploration scenarios (Bosch et al. 2010, 2015), there has been little study of the propagation in and sensitivity of inversion results to varying uncertainty in both geological and petrophysical input measurements in exploration scenarios. Utilisation of inaccurate information to derive petrophysical constraints has been investigated by (Sun and Li 2015, 2017) and (Carter-McAuslan et al. 2015). Nevertheless, the role of uncertainty in prior information (i.e., how data is scattered around the true value) is only partially addressed as published works mostly consider biased prior information (i.e., with systematic errors).

Previous works have investigated the effect of noise in geophysical data inversion, i.e., (LaBrecque et al. 1996; Fernández-Martínez et al. 2014a, b) and its removal, i.e., (Yuan et al. 2012; Pilkington and Shamsipour 2014). To date, much less work has been done, however, to investigate the propagation of uncertainty in geological and petrophysical field measurements.
in constrained inversion. Understanding the respective influence of petrophysical and geological data uncertainty onto the inversion process is elementary to reduce the risk of misinterpretation of results and to sound decision making. Integration approaches considering petrophysical and geological constraints simultaneously are relatively recent and have not been thoroughly studied yet.

In this work, we develop a study that intends to alleviate the scarcity of studies focusing on the propagation of petrophysical and geological uncertainty in integrated inversion. We use a re-designed version of the 3D inversion platform Tomofast-x (Martin et al. 2013, 2018) to integrate statistical petrophysical constraints and probabilistic geological models, extending the 2D inverse modeling workflow of (Giraud et al. 2017). The primary objective of this article is to investigate and understand how uncertainty propagates from the geological and petrophysical input measurements to the recovered lithological model. We perform a sensitivity analysis to study how variations in the statistics of petrophysical and geological measurements affect the inverted models and the lithologies recovered a posteriori. We interpret inversion results qualitatively through visual inspection and quantitatively by calculating indicators quantifying the discrepancies between the true and inverted models in terms of physical properties as well as recovered lithologies.

This paper develops in five sections as follows. In the methodology section (Section 3.3), we provide a summary of the different steps of the proposed workflow (subsection 3.3.1). This is followed by the formulation of the inverse problem (subsection 3.3.2), where we give a short introduction to our inversion platform. We then provide essential information about the probabilistic geological modeling procedure, the calculation of local petrophysical constraints and starting models (subsection 3.3.3). In ensuing section (Section 3.4), we detail the metrics that we calculate to analyse inversion quality and retrieved lithological models. In Section 3.5, we introduce the geological context, the simulated case scenarios we test and practical information about the synthetic geophysical survey. In the results section (Section 3.6), we first perform qualitative interpretation and examination of inversion results. We subsequently validate our observations using a series of posterior indicators. We then finish with the discussion and conclusion. Section 3.9 provide information allowing complete reproducibility of the work presented in this article.
3.3. Inverse problem formulation and integration of constraints

3.3.1. Integration procedure summary

The main steps of the modeling procedure are summarised in Figure 3.1. As said above, the inversion algorithm is similar in spirit to (Giraud et al. 2017), which we extend to large-scale 3D problems and complement with the posterior recovery of lithological models and topological analysis. A prerequisite to inversion is to translate petrophysical and geological data into information that can be used in the inverse modeling process. The first step is to calculate the PGM using MCUE and to derive a mixture model (i.e., a weighted sum of density functions) representative of the petrophysical measurements. The PGM and the mixture model are then combined to derive local petrophysical constraints and to calculate starting models for inversion (step 2 in Figure 3.1). The next of the workflow is to perform constrained geophysical inversion (step 3). The posterior analysis in step 4 comprises a lithological reconstruction procedure that allows the recovery of a lithological model and the subsequent topological analysis. The calculation of a series of indicators provides metrics for the assessment of inversion results in terms of geological plausibility and misfit.

Figure 3.1. Modeling workflow summary.
3.3.2. Cost function and optimization process

3.3.2.1. Problem formulation

The objective function $\Theta$ that we optimize is derived from the formulation of a probability density function accounting for data and prior information (Tarantola 2005). It can be expressed as a product distribution as follows:

$$
\Theta(d,m) = \Theta_d(d,m) \Theta_m(m) \Theta_c(m),
$$

(3.1)

where subscript $d$ relates to the geophysical measurements $d$ to be inverted, subscript $m$ relates to the inverted model $m$, and subscript $c$ to the petrophysical constraints. In this equation, $\Theta_d(d,m)$ is the density function corresponding to geophysical data misfit, $\Theta_m(m)$ is the prior density function on model $m$, and $\Theta_c(m)$ is the probability density relating to constraints derived from petrophysical information.

Our working assumption is that density functions $\Theta_d(d,m)$ and $\Theta_m(m)$ can be expressed as:

$$
\begin{align*}
\Theta_d(d,m) &= A \exp \left( -\left( d - g(m) \right)^T C_d^{-1} (d - g(m)) \right), A \in \mathbb{R}^+ \\
\Theta_m(m) &= B \exp \left( -\left( m - m_p \right)^T C_m^{-1} (m - m_p) \right), B \in \mathbb{R}^+,
\end{align*}
$$

(3.2)

with

$$
\begin{align*}
g(m) &= 
\begin{bmatrix}
g_G(m_G) \\
g_M(m_M)
\end{bmatrix}, 
\begin{bmatrix}
m_G \\
m_M
\end{bmatrix}^T, 
d = 
\begin{bmatrix}
d_G \\
d_M
\end{bmatrix}, 
\begin{bmatrix}
C_d & 0 \\
0 & \delta C_d
\end{bmatrix}, 
\begin{bmatrix}
C_m & 0 \\
0 & \delta C_m
\end{bmatrix},
\end{align*}
$$

(3.3)

where superscript $T$ denotes the transpose operator. Superscripts and subscripts $G$ and $M$ refer to gravity and magnetic data and model, respectively. In our particular case, $\Theta_c(m)$ is expressed using a mixture model where each subpopulation corresponds to a specific rock type. $A$ and $B$ are the normal distributions’ normalization constants, while $C_d$ and $C_m$ are covariance matrices corresponding to data and model weighting, respectively. $m_p$ is the prior model, which we also use as starting model for our inversions in the examples shown in this paper. The scalar $\delta$ is a positive real number representing the relative weight of the two problems being inverted jointly.

Substituting equation (3.2) in equation (3.1), we obtain:

$$
\Theta(d,m) = AB \exp \left( -\left( d - g(m) \right)^T C_d^{-1} (d - g(m)) - \left( m - m_p \right)^T C_m^{-1} (m - m_p) \right) \Theta_c(m).
$$

(3.4)
From equation (3.4), it is straightforward to show that maximizing $\Theta(d,m)$ is equivalent to minimizing the following cost function $\theta$:

$$
\theta(d,m) = (d - g(m))^T C_d^{-1} (d - g(m)) + (m - m_p)^T C_m^{-1} (m - m_p) + \log(\Theta_c(m)^{-1}).
$$

Generally speaking, the constraint term $\phi_c(m)$ can be utilized to incorporate prior information in the inverse problem and to enforce constraints. In this article, it encapsulates local information derived from probabilistic geological modelling combined with the statistics of the physical measurements of the lithologies sampled in the studied area. Calculation of this term is detailed in section 3.3.3.2. In the remainder of this paper, we assume that $C_d$ and $C_m$ are spherical covariance matrices. We set each diagonal element of $C_d$ as the sum-of-squares of geophysical data. It remains necessary to estimate $C_m$, the parameters controlling the weight of the petrophysical constraints in inversion, and to determine the relative weight between the gravity and magnetic problems. This procedure is discussed in subsection 3.5.3 as applied to our dataset.

3.3.2.2. Inversion algorithm

The form of $\theta(m)$ as per equation (3.5) allows us to solve the inverse problem in a least-square sense using the least-square-root (LSQR) algorithm (Paige and Saunders 1982; Chapman and Pratt 1992; Pratt and Chapman 1992; Gerhard Pratt et al. 1998; Hicks and Pratt 1998; Martin et al. 2013).

For the purpose of this work, we extended the parallel code TOMOFAST3D (Martin et al. 2013, 2018). This extended new implementation, which we call Tomofast-x, follows the object-oriented FORTRAN 2008 standard. The design of Tomofast-x utilizes classes designed to account for the mathematics of the problem, which permits to reduce software complexity, thereby facilitating the addition of new functionalities (see Hammond et al., 2014, and references therein).

3.3.3. Geological conditioning of petrophysical constraints

3.3.3.1. Probabilistic geological modeling

Several studies showed that multiple sources of uncertainty can impact geological modeling, and that quantitative uncertainty estimation of individual geological models is difficult to
obtain (Bond et al. 2007, 2015; Alcalde et al. 2017). To mitigate this, (Pakyuz-Charrier et al. 2018a, c, b) extend previous works, i.e., (Jessell et al. 2010; Lindsay et al. 2012, 2013b; Wellmann and Regenauer-Lieb 2012) to generate a collection of geological models reflecting the range of geologically possible models. We calculate PGMs using outputs from MCUE as detailed in (Pakyuz-Charrier et al. 2018c) as part of the pre-requisite to inversion (step 1 as per Figure 3.1).

The PGM is obtained by sampling probability distributions thought to best represent input measurements and their uncertainty using a Monte-Carlo approach. MCUE perturbs a reference model under the assumption that uncertainty on measurement position can be modelled using a normal distribution and that measured orientation data (i.e., foliations through dip and strike converted into a vector in three-dimension) used to build the model can be modelled using spherical statistics. This can be achieved using the von Mises-Fisher distribution (vMF) (Davis 2002). In three dimensions, it is given by (Mardia and Jupp 2008):

$$vMF(x | y, \kappa) = \frac{\kappa}{4\pi \sinh(\kappa)} e^{\kappa y^T x}, \kappa \in \mathbb{R}^+ ,$$

where \( x \) is the orientation data vector; \( y \) is a unit vector representing the mean measurement direction. The term \( \kappa \) is called the concentration parameter. It characterizes the spread in orientation measurements. It can be interpreted as an analogous of the inverse of the standard deviation for normal distributions. In principle, it is possible to assign an individual uncertainty estimate to each measurement depth- or location dependent uncertainty (e.g., for borehole data or for seismic horizons). In the work presented here, we assume independent surface measurements that present similar levels of uncertainty.

Geological plausibility of model realizations is enforced through the application of topological rules and plausibility filters that force the model to honour age relationships and the stratigraphic column. The resulting set of models – typically several hundreds of models – is then combined into a PGM constituted of the observation probability of all modelled lithologies in each cell. This applies to all lithologies to the exception of the basement, which is assigned in the absence of other units under the hypothesis that it fills space when no other lithology is present.
In the work presented here, the results from MCUE are to condition petrophysical constraints \( \Theta_c(m) \) term in equations 3.1-3.5) and to compute starting models. This is detailed in Subsection 3.3.3.2 below.

### 3.3.3.2. Local petrophysical constraints

Petrophysical constraints are applied to inversion through the minimization of the constraint term \( \phi_c \) in equation (3.5) simultaneously to the other terms. To maximize statistical closeness between inverted properties and measured petrophysical data we follow concepts introduced and used by (Paasche and Tronicke 2007; Doetsch et al. 2010; Lelièvre et al. 2012b; Sun and Li 2013). We condition the petrophysical constraints geologically to derive local constraints following the procedure introduced in (Giraud et al. 2017).

Assuming that the physical properties are normally distributed for each lithology, petrophysical measurements can be represented using a mixture model. Therefore, we can use such statistical description to define a probability distribution to be used to constrain inversion. Let the statistics of petrophysical measurements be represented by a mixture distribution of the form (equation 3.7):

\[
p(m) = \sum_{k=1}^{n_l} p_k(m) = \sum_{i=1}^{n_m} \sum_{k=1}^{n_l} p_k(m_i) = \sum_{i=1}^{n_m} \sum_{k=1}^{n_l} \omega_k N(m_i | \mu_k, \sigma_k).
\]

In equation (3.7), \( n_l \) is the number of lithologies observed in the petrophysical measurements; \( p(m) \) is obtained for the whole model by summing the contribution of all the lithologies observed in each of the \( n_m \) model-cells; \( k \) denotes the index of the corresponding lithology. The kernels \( N(m_i | \mu_k, \sigma_k) \) of the mixture are normal distributions. Each normal distribution is characterized by a mean value vector for the considered property, \( \mu_k \), and the associated covariance matrix, \( \sigma_k \). The relative weights of the corresponding lithologies, \( \omega_{k=1...n_l} \), are non-negative weights called mixing coefficient summing to 1. Note that in our implementation, \( \sigma_k \) is a full matrix, thereby accounting for correlation between density contrast and magnetic susceptibility of rocks.

Introducing \( \rho \in \mathbb{R}^+ \) and defining \( \Theta_c(m) = p(m)^{-\rho} \) for the gravity or magnetic problem, we obtain \( \phi_c(m) = \rho \log(p(m)) \). This corresponds to the log-likelihood of the distribution representative of the petrophysical measurements multiplied by a positive scalar weighting the petrophysical constraints term in equation (3.5). From equation (3.7) it becomes clear that
such petrophysical constraints constitute soft constraints favouring model changes towards the most likely configuration as indicated by the expression of $p(m)$. For joint inversion, we use $\rho = [\rho^G \rho^M]$. In real world scenarios, the parameters of $N(m|\mu_k, \sigma_k)$, $\sigma_k$, and $\mu_k$, can be estimated from petrophysical data using an expectation maximization algorithm (i.e., McLachlan and Peel, 2000). A normal distribution is commonly expected to describe the physical measurements of rocks. It is clear that the assumption that the statistics of measured petrophysical properties can be represented or approximated using such distribution is not always valid (e.g., bimodal susceptibility distribution of certain rocks), and that the choice of distribution remains case-dependent.

The conditioning of petrophysical constraints by geological modeling consists in calculating $\Theta_C(m)$ using observations probabilities from the PGM to weight the elements of the mixture model defined in equation (3.8) below. We define the observation probability matrix $\psi$ of dimensions $n_l \times n_m$ containing the observation probabilities of the different rock units. Substituting $\omega_k$ as per equation (3.7) with the probability of the respective lithology in each cell of the model provides a local mixture model depending on both geological modeling results and petrophysical measurements. We can rewrites $p(m)$ as (equation 3.8):

$$p(m) = \sum_{i=1}^{n_m} \sum_{k=1}^{n_l} \psi_{k,i} \ N(m_i|\mu_k, \sigma_k). \quad (3.8)$$

This process, which corresponds to the second stage of the workflow (Figure 3.1), is illustrated in Figure 3.2 (next page).

In addition to the calculation of $\Theta_C(m)$, the PGM is useful to calculate starting models. For the $i$-th model cell, the starting model $m_0$ is set as the average model from the PGM populated accordingly with petrophysical measurements. It is calculated as:

$$m_0 = \psi \cdot \mu \quad (3.9)$$
The consequences of the formulation of the petrophysical constraints in equation (3.8) and of the starting model in equation (3.9) for inversion are the following. Inversion will be strongly influenced by the petrophysical constraints in model cells where geology is well determined (e.g., one observation probability dominates the others) and the locally weighted mixture shows well-separated lithologies. In contrast, local petrophysical constraints are similar to global petrophysical constraints in model cells were geology remains undetermined after MCUE. Also note that model updates during inversion are largely driven by geophysical data where the locally weighted mixture model does not exhibit a sufficiently clear distinction between the different lithologies.

3.4. Quality indicators

In this Section, we detail the posterior analysis of inversion results, which constitutes the fourth and final step of the workflow (Figure 3.1). We base our interpretation of inverted models on two types of quality indicators on global and local indicators. All the inversions we present achieve a similar geophysical data misfit, indicating that little can be learned from comparing models with this particular metric (see subsection 3.6.2.1). We observed that the incorporation of prior information with varying degrees of uncertainty has limited impact on final geophysical data misfit values. This is in agreement with (Gallardo and Meju 2004, 2007, 2011; Abubakar et al. 2012; Gallardo et al. 2012; Gao et al. 2012; Molodtsov et al. 2013; Moorkamp et al. 2013; Jardani et al. 2013; Juhojuntti and Kamm 2015; Sun and Li 2016a, 2017; Rittgers et al. 2016;
Demirel and Candansayar 2017; Giraud et al. 2017) who do not expect nor observe dramatic data misfit improvements through data integration, and point out that improvements mostly occur in model space.

3.4.1. Global indicators: model misfit and lithological resemblance

Indicators derived from the difference between reference and inverted models are commonly used as a metric to assess inverted models in synthetic studies and to characterize the resemblance between causative bodies and retrieved models. Invoking Laplace’s first law of errors (Laplace 1774; Wilson 1923; Stigler 1986), the first indicator we calculate is equivalent to the mean absolute deviation around the reference model, or mean absolute model misfit (MAMM). It is less sensitive to isolated outliers than the more common root-mean-square indicators. Let us express this indicator as follows:

$$\varphi_m(m) = \frac{1}{n_m} \sum_{i=1}^{n_m} |m_i^{ref} - m_i^{inv}|, \quad (3.10)$$

where $m_i^{ref}$ and $m_i^{inv}$ correspond to the $i$-th cell of the inverted reference and inverted models, respectively.

In complement, we assess inverted models using reconstructed lithological models recovered from inverted physical property models. Lithologies are recovered, for each cell of the medium, from a membership analysis using equation (3.7) similarly to (Doetsch et al. 2010; Sun et al. 2012), which we restrict locally to cells characterized by $\psi_{k,i} > 0$. This allows us to evaluate the lithological resemblance between recovered lithological model $l^{inv}$ as the proportion of recovered cells that are in agreement with the reference lithological model $l^{ref}$. We define what we term the lithological resemblance $r$ as follows:

$$r(l^{inv}, l^{ref}) = \frac{1}{n_m} \sum_{i=1}^{n_m} 1_{l_i^{ref}}(l_i^{inv}), \quad (3.11)$$

where $1_{l_i^{ref}}$ symbolises the indicator function for $l_i^{ref}$.

3.4.2. Local indicator using the topology of inverted models

The set of cells assigned with recovered lithologies constitute a lithological model characterized by discrete values representing rock types. Topology records the geological relationships between adjacent objects within a model, which can be represented in terms of its topology
(Perrin and Rainaud 2013). It can be used as “tool for quantifying differences between geological models in uncertainty analyses” (Thiele et al. 2016a). Topological analysis allows us to interpret and compare results in a way that also accounts for changes in geological relationships regardless of the scale considered. It is therefore well-suited to detect local differences between models, and complements indicators reflective of bulk properties (i.e., values averaged over the whole model). This can be useful to identify areas of the recovered models that are geologically implausible and to highlight poorly constrained lithologies. Such analysis of inverted models complements works of (Doetsch et al. 2010; Sun et al. 2012; Carter-McAuslan et al. 2015; Sun and Li 2015, 2017; Martinez and Li 2015; Li and Sun 2016; Melo et al. 2017), who infer lithologies from inverted models but whose study do not extend to the quantitative geological assessment of recovered models. One of the key advantages of topological analysis over qualitative interpretation is that it presents a systematic way to analyse results and to detect features that cannot be measured using mean model indicators and which may be challenging to impossible to detect through visual inspection of three-dimensional models (Pellerin et al. 2017).

In the present case, we perform the topological analysis of recovered lithological models to compare basic geological features of models recovered from inversion results. Following the nomenclature proposed by (Thiele et al. 2016a), we use ‘lithological topology’. It is defined in the framework introduced by (Burns 1988), who addresses the relationship between adjacent rock volumes (in our case, cells assigned with a given lithology). The different kinds of topological relationships, for instance, “contains”, “is inside”, “meets”, etc., are characterized using the Egenhofer relations (Egenhofer and Herring 1990), generalized to 3D by (Zlatanova 2000).

In the workflow presented here, we limit our investigations to the adjacency of units (i.e., “unit A is in contact with unit B”), which is the most common Egenhofer relation used in geology (Thiele et al. 2016a). We represent adjacency following the matrix representation of (Godsil and Royle 2001), which can be summarized as follows. For a model consisting of \( n \) lithologies, the adjacency matrix can be reduced to a positive strictly lower triangular \( n_l \times n_l \) matrix \( M \), where element \( M_{i,j} \) are non-zero if and only if a contact between lithologies \( i \) and \( j \) is observed.
To make the adjacency matrix more suitable to the comparison of lithological models, we attach, to each element $M_{i\geq j,j}$ of the matrix, the number of occurrences of the respective contacts. Let the resulting adjacency matrix elements be:

$$M_{i>j,j} = n_{ij}, M_{i\leq j,j} = 0,$$

where $n_{ij}$ is the number of contacts between lithology $i$ and $j$, for node $M_{i>j,j}$. $n_{ij} = 0$ indicates that lithology $i$ and $j$ are disjoint.

In the synthetic case study we present, we use adjacency matrices to compare recovered lithological models with the reference model, while in real world studies, it can be used to compare scenarios or departures from selected geological models (Perrin and Rainaud 2013; Thiele et al. 2016b; Pellerin et al. 2017). Besides reflecting global features of the lithological model, the adjacency matrix $M$ is also a local indicator because its (mathematical) properties can change dramatically with small, local alterations in the lithological model.

To estimate deviations from the reference lithological model, we calculate the difference between the adjacency matrices of the recovered and reference model, normalized by the highest number of contacts observed in the reference model. Let us define the matrix $M^{rel}$ as follow:

$$M^{rel} = \frac{1}{\max M^{ref}} (M^{inv} - M^{ref}),$$

where $M^{inv}$ and $M^{ref}$ represent the adjacency matrices calculated from inversion results and the reference model, respectively.

From equation (3.13), $M^{rel}_{i,j} > 0$ indicate that the recovered lithologies overestimate the contact surface area between lithology $i$ and lithology $j$. On the contrary, $M^{rel}_{i,j} < 0$ indicate that the recovered lithologies underestimate the contact surface area between between lithology $i$ and lithology $j$.

3.5. Simulated Case study and uncertainty scenarios

3.5.1. Geological context

We built the unperturbed geological model from contact data and surface orientation (i.e., contact points and foliations, respectively) collected in the Mansfield area (Victoria, Australia) in Geomodeller® (Lajaunie et al. 1997; Calcagno et al. 2008; Guillen et al. 2008). It presents a Carboniferous sedimentary syncline oriented N170, abutting a faulted contact with a
Silurian-Devonian folded basement. Structural complexity was artificially increased to better challenge the inversion algorithm through the addition of a north-south oriented fault and an ultramafic intrusion to the south. Information used to derive the original model is detailed in the GeoModeller User Manual, Tutorial case study H (Mansfield). Figure 3.3A shows the unperturbed (or reference) geological model. The base structural model was made available online by (Pakyuz-Charrier 2018)(see section 3.9 for details about availability of data and models shown here). The utility of this model for testing purposes has been shown by (Giraud et al. 2017, 2018b; Pakyuz-Charrier et al. 2018c).

3.5.2. Simulated physical properties

We populate the reference geological model by assigning low density contrast and limited magnetic susceptibility to basin fill (lithologies 3, 5 and 6). Using values from the literature (Hatfield et al.; Hunt et al. 1995; Airo 2005; Clark and Emerson 2006) we assigned higher density contrast and magnetic susceptibilities to ultramafic rocks (lithology 1), diorite (lithology 2) and dolerite (lithology 4). Modelled lithologies and physical properties are provided in Table 3.1. The reference density and magnetic susceptibility models are shown in Figure 3.3B and Figure 3.3C, respectively. A reference density value of 2670 kg/m³ was used.

Table 3.1. Stratigraphic column showing geological topological relationships and average physical properties. Lithologies are indexed from 1 through 6 by age. Lithology 1 is the oldest and 6 is the most recent.

<table>
<thead>
<tr>
<th>Lithology index</th>
<th>Geological relation</th>
<th>Geological unit</th>
<th>Density contrast (kg/m³)</th>
<th>Magnetic susceptibility (SI)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>Sedimentary</td>
<td>Basin fill 3</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>5</td>
<td>Sedimentary</td>
<td>Basin fill 2</td>
<td>110</td>
<td>0.01</td>
</tr>
<tr>
<td>4</td>
<td>Intrusive</td>
<td>Dolerite</td>
<td>300</td>
<td>0.025</td>
</tr>
<tr>
<td>3</td>
<td>Sedimentary</td>
<td>Basin fill 1</td>
<td>110</td>
<td>0.01</td>
</tr>
<tr>
<td>2</td>
<td>Intrusive</td>
<td>Diorite</td>
<td>170</td>
<td>0.05</td>
</tr>
<tr>
<td>1</td>
<td>Basement</td>
<td>Ultramafic rocks</td>
<td>240</td>
<td>0.08</td>
</tr>
</tbody>
</table>

In real world scenarios, different lithologies encountered in basins may share similar characteristics in the petrophysical domain, such as low density contrast and magnetic susceptibilities, and in some cases cannot be differentiated in a density contrast – magnetic susceptibility cross-plot. To account for this, we assign the same properties to lithologies 3 and 5, which become undistinguishable.
3.5.3. Geophysical Survey

3.5.3.1. Synthetic geophysical data and forward modeling

Magnetic and gravity data were computed to simulate and gravity and magnetic ground surveys. We inverted for the total magnetic field anomaly and the vertical component of the complete Bouguer anomaly. Magnetic data are simulated following the same approach as (Bhattacharyya 1964). Gravity data are simulated following (Boulanger and Chouteau 2001). We model a magnetic field strength equal to 57700 nT, which approximates the International Geomagnetic Reference Field for the locality of Mansfield (Victoria, Australia).

We add zero-mean normally distributed random noise with standard deviation equal $\sigma^G_d = 0.3$ mGal (i.e., 2.25% of the average amplitude of the data) and to $\sigma^M_d = 10$ nT (i.e., 2.5% of the average amplitude of the data) to gravity and magnetic measurements, respectively, to simulate noise contamination of the data. The synthetic geophysical data we invert is shown in Figure 3.3D and Figure 3.3E for gravity and magnetic data, respectively. To balance the decreasing sensitivity of potential field data with depth, we use the inverse integrated sensitivities technique of (Li and Oldenburg 2000; Portniaguine and Zhdanov 2002).

The study area is discretised into $128 \times 128 \times 32$ cells (dimensions $130\text{m} \times 130\text{m} \times 90\text{m}$), making up a total of 524,288 elements. To avoid dispersion effects, we sampled geophysical data on a $128 \times 128$ grid, for a total of $n_d = 16,384$ measurement points per geophysical dataset.
### 3.5.3.2. Hyperparameter estimation

The values defining the weights of the different terms in the cost function as per equation (3.2) through equation (3.5) constitute hyperparameters of the inverse problem. We estimate them using the L-curve principle (Hansen and O’Leary 1993; Hansen and Johnston 2001; Santos and Bassrei 2007), seeking geophysical data misfit superior or equal to noise level. We determine $C_m$ and $\rho$ in a two-stage heuristic process that partially avoids the limitations of L-curve analyses in 3D constrained joint inversion scenarios due to high computation requirements (see Bijani et al. 2017) or the difficulty to visualise hypersurfaces. The first stage involves the estimation of optimum weights for single-physics inversion on a 3D subset of the full model. It is comprised of $48 \times 48 \times 32$ cells with the corresponding $48 \times 48$ surface data points. The subset we chose is located in the central part of the model. There, the reference model is made fairly complex by an ultramafic inclusion and faulted units. The corresponding data is representative.
of the full models’. The subset comprises approximately 14% of the total volume and data points, thereby reducing the computational cost of a single significantly. This allows us to run hundreds of constrained inversions. The outline of the model is shown in top view in Figure 3.3D and Figure 3.3E.

Manual tuning of $C_m$ and $\rho$ for single-physics inversions provides an initial estimate of the parameters sought for. We refine our search by sampling values spaced at regular intervals in logarithmic scale around these initial estimates. This led us to perform series of 400 and 1032 separate gravity and magnetic inversions, from which we generate the corresponding L-surfaces for identification of the optimum weights (corresponding L-surfaces are available in Appendix B1).

The second stage of hyperparameter estimation pertains to joint inversion. The values obtained for single domain inversion are transferred to joint inversion of the subset of the full model. The relative weight between the gravity and magnetic problems is obtained through L-curve analysis of 50 different weights. A series of 625 inversions sampling values of $C_m$ and $\rho$ from single domain inversion is then performed to determine optimum values. Finally, fine tuning of the resulting values using the full model allowed us to obtain the set of optimum hyperparameters which we used to run the inversions shown in this paper.

3.5.4. Case scenario evaluation

In real world scenarios, statistical geological and petrophysical models derived from geological and petrophysical measurements are dependent upon the quality of data and on the geology of the area. The evaluation of the sensitivity of our inverse modeling procedure to varying uncertainty levels in geological and petrophysical data is performed through the simulation of a range of possible case scenarios. To this end, we simulate three base uncertainty levels for both geological and petrophysical data to represent extreme and average cases representative of real scenarios. Note that we simulate measurements and uncertainty levels using values reported in the literature (see references provided in the caption of Table 3.2). In our idealized experiment, we assume that the statistics of physical properties are derived from a representative population. Likewise, we assume that measurement uncertainty on orientation data or contact position are based on outcrop and/or borehole condition and measuring tool specifications. Table 3.2 below gives the tested uncertainty levels on geological and
petrophysical measurements, assuming that density contrast and magnetic susceptibility are not correlated (i.e., cross-correlation equal to zero).

Table 3.2. Input uncertainty for geological input data (first block) and physical properties (second block). Cases (a), (b) and (c) correspond to cases scenarios where 95% of the orientation data is contained within 52, 37 and 30 degrees aperture cones, respectively. For petrophysics, cases α, β and γ characterize different levels of spread of the measurements around the mean values. Chosen standard deviations for case α (most uncertain case) in terms of magnetic susceptibility are of the same order of magnetic as (Sanger and Glen 2003), larger than (Törnberg and Starkell 2005) for density contrast, and conform to (Barlow 2004) for both density contrast and magnetic susceptibility. Chosen concentration parameters are in agreement with metrological studies (Allmendinger et al. 2017; Novakova and Pavlis 2017).

<table>
<thead>
<tr>
<th>Geological input data uncertainty</th>
<th>Orientation data uncertainty (concentration parameter)</th>
<th>Contact position uncertainty (standard deviation, in m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a – most uncertain case</td>
<td>80</td>
<td>50</td>
</tr>
<tr>
<td>b – Intermediate case</td>
<td>20</td>
<td>50</td>
</tr>
<tr>
<td>c – least uncertain case</td>
<td>25</td>
<td>25</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Physical property uncertainty</th>
<th>Standard deviation of density contrast (km/m³)</th>
<th>Standard deviation of magnetic susceptibility (SI)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a – most uncertain case</td>
<td>60</td>
<td>0.02</td>
</tr>
<tr>
<td>β – Intermediate case</td>
<td>45</td>
<td>0.015</td>
</tr>
<tr>
<td>γ – least uncertain case</td>
<td>33.75</td>
<td>0.0113</td>
</tr>
</tbody>
</table>

Combining the base uncertainty levels as per Table 3.2, we obtain a total of nine cases representative of the range of simulated case scenarios (Figure 3.4 below). The comparison and analysis of results obtained using these nine cases shown in Figure 3.4 constitutes our sensitivity analysis of integrated inversion subject to varying geological and petrophysical uncertainty.

Figure 3.4. Simulated case scenarios classification matrix representing the combinations of uncertainty levels on geological and petrophysical input for inversion as per Table 3.2. Each line corresponds to a given geological input measurement uncertainty scenario while each columns corresponds to a given petrophysical uncertainty case.
Figure 3.5 shows the observation probability of the most probable lithology in each model cell, calculated, in each case, from a suite of 300 plausible geological models. It is reflective of the amount of information brought by geological measurements across the different parts of the model. In Figure 3.5, one can notice that for case (a), interfaces between geological units are not distinguishable in large portions of the model (darker regions), while case (b) seems less affected, case (c) being the best determined. This clearly illustrates the propagation of input measurement uncertainty to the PGM.

*Figure 3.5. Maximum observation probability model corresponding for PGMs corresponding to cases (a), (b) and (c) (i.e., decreasing measurement uncertainty) as per Table 3.2. High values (in white) indicate well determined areas while low values materialized by darker shades (i.e., lower values) indicate poorly constrained areas where no lithology dominates.*
Figure 3.6 below shows the resulting mixture model as per equation (3.7) where all lithologies are equally weighted. As can be seen in Figure 3.6, although the geological model comprises six distinct units, lithologies 3 and 5 present exactly the same density contrast and magnetic susceptibility (Table 3.1). This simulates cases where geological units cannot be differentiated by attributes the available petrophysical measurements are sensitive to.

Figure 3.6. Simulated global mixture models, with increasing standard deviations (in equation 3.7) from case α to γ as per Table 3.2. The mean value for each lithology is marked by a cross, of which the color corresponds to the respective lithology as per Figure 3.3A. Lithologies 5 and 3 completely overlapped because they present the same density contrast and magnetic susceptibility.

3.6. Sensitivity analysis to uncertainty in petrophysical and geological input data

3.6.1. Inverted models

In this Section, we qualitatively analyse the inverted models. We examine the differences between reference and inverted models in terms of density contrast for (a, β), (b, β) and (c, β) (Figure 3.7) and magnetic susceptibility for (b, α), (b, β) and (b, γ) (Figure 3.8). In addition, we perform visual inspection of the recovered lithological models corresponding to the cases shown in Figure 3.7 and Figure 3.8 in Figure 3.9A and Figure 3.9B, respectively. The complete set of results for all cases (Figure 3.4) in terms of inverted models, differences with the true model and recovered lithological models is given in Appendix B2.
Figure 3.7. (A) Inverted density contrast models (left-hand side rectangle) for cases (b, α), (b, β), (b, γ), and (B) corresponding absolute difference with reference model (right-hand side rectangle). Outlined portions of the model show areas of the inverted model most sensitive to changes in the uncertainty in input petrophysical measurements.

From Figure 3.7A and Figure 3.7B, one would notice that differences between the cases shown are relatively small. However, visual comparison of inversions (b, α), (b, β) and (b, γ) in Figure 3.7A indicates that decreasing uncertainty in petrophysical data increases the contrasts in inverted physical properties. This is because the different lithologies are increasingly well differentiated in the cross-plot from case α to γ (Figure 3.4). To a lesser extent, it also modifies the geometry of the contacts between structures in the model (small scale changes in lithological models shown by arrows in Figure 3.9A). In particular, changes are more noticeable in the central part of the model where Figure 3.3 and Figure 3.5 respectively show higher geological complexity and uncertainty.
Although the same mixture model is used to define petrophysical constraints for cases (a, β), (b, β) and (c, β), results shown in Figure 3.8A exhibit only a slight increase in sharpness from (a, β) to (c, β). This is due to increasing differences between the observation probabilities weighting the different lithologies in the respective petrophysical constraints. Visually, it is noticeable in Figure 3.8A that decreasing geological input uncertainty results in increased inverted model complexity associated with lower discrepancies with the true model (Figure 3.8B). This is particularly noticeable in areas corresponding to the most uncertain parts of the model as per Figure 3.5. Inversion becomes increasingly guided by geology in these regions as large portions of the model undergo a significant decrease in geological uncertainty from case (a) to (c). This results in geologically conditioned petrophysical constraints increasingly encouraging inversion to update the model preferentially in the most geologically uncertain parts of the model. The consequence of this is an indirect focusing effect of geophysical inversion on uncertain areas.
Figure 3.9. (A) Recovered lithological model for cases (b, α), (b, β), (b, γ) (left hand side rectangle) and (B) recovered lithological model for cases (a, β), (b, β), (c, β) (right hand side rectangle). Note that lithology 5 does not appear as it is merged with lithology 3. The recovered models are overlaid with the boundary of the geological units from the reference model.

Comparison of inversion results obtained for scenarios (b, α), (b, β) and (b, γ) (Figure 3.7) and (a, β), (b, β), (c, β) shows (Figure 3.8) that larger structures corresponding to ultramafic rocks (lithology 1), diorite (lithology 2), and basin fill are coherent for all cases. It also shows that the differences occur at interfaces and in regions where geological uncertainty varies the most. This translates in pronounced differences between the recovered lithological models in Figure 3.9B, notably in areas marked by arrow. It also corroborate previous observations, showing that the most noticeable changes are related to variations in geological uncertainty while changes related to uncertainty in petrophysics are limited to small scale or low magnitude changes. This is also reflected in Figure 3.9A where the recovered lithological models show largely similar features. To complete and confirm our interpretations, the next subsection focuses on quantitative quality indicators and on the topological analysis of recovered lithological models.
3.6.2. Quality indicators

3.6.2.1. Model misfit and lithological resemblance

The mean absolute model misfit (MAMM) $\varphi_m$ is derived from the absolute model misfit (equation 3.10) and reflects the average differences between inverted and reference models. As can be seen Figure 3.10B, for both density contrast and magnetic susceptibility, the main control on this indicator is uncertainty in geological input, which dominates over changes in petrophysical uncertainty. The effect of petrophysics is therefore to tune and sharpen the model while geology strongly influences the structural features recovered by inversion. This confirms observations made in 3.6.1.

The effect of petrophysics is therefore to tune and sharpen the model towards which geology guides inversion to.

![Figure 3.10. Metrics for inversion results analysis: MAMM indicator for density contrast (A) and magnetic susceptibility (B), lithological resemblance $r$ (C), for the different uncertainty scenarios as per Figure 3.4. Each color corresponds to a separate geological uncertainty scenario (a, b, and c) (e.g., a lines in Figure 3.4). Petrophysical uncertainty scenarios ($\alpha$, $\beta$, and $\gamma$) (i.e., columns in Figure 3.4), are differentiated by marker type. Coloured lines connect values attached to the corresponding geological uncertainty scenario for visualisation purposes but do indicate a continuum between the points.](image)

In all three geological uncertainty scenarios, Figure 3.10 also indicates that the lowest MAMM values for both density contrast and magnetic susceptibility correspond to the intermediate petrophysics case ($\beta$). From these observations, we can argue that case ($c$, $\beta$) is the optimum inverted model of this study and that in general, intermediate petrophysical uncertainty similar to case ($\beta$) provides optimum results, while inverted model quality is directly related to geological input uncertainty. This interpretation is also valid for lithological resemblance $r$ (equation 3.11) in Figure 3.10C, for which the main control is geological input uncertainty. A possible explanation to this is that while potential field data inversion is highly affected by non-uniqueness, local entrapment is more likely to occur when the elements of the mixture...
model present the narrowest standard deviations. This reduces possible changes in the model during inversion, while on the contrary, normal distributions with broad standard deviations constrain inversion weakly. This interpretation is not contradicted by the inverted data root-mean-square error (RMSE) values (equation 3.14 below), which reaches similar values for all inverted models (see values in Table 3.3). We calculate the data RMSE as:

\[
RMSE(m^P, d^P) = \left[ \frac{1}{n_d} \frac{1}{\sigma_d^P} \phi_d(m^P, d_P) d_P^T d_P \right]^{\frac{1}{2}} ,
\]

where \( P \) denotes the problem considered, e.g., gravity (G) or magnetic (M) as per equation 3.3. Values of \( \sigma_d^P \) are given in subsection 3.5.3.1 and \( \phi_d \) is the corresponding data misfit obtained as explained in subsection 3.3.2.1.

### Table 3.3. Data RMSE for the tested scenarios.

<table>
<thead>
<tr>
<th>Uncertainty case scenario</th>
<th>(a,a)</th>
<th>(a,a)</th>
<th>(a,a)</th>
<th>(a,a)</th>
<th>(a,a)</th>
<th>(a,a)</th>
<th>(a,a)</th>
<th>(a,a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gravity data</td>
<td>1.026</td>
<td>1.028</td>
<td>1.003</td>
<td>1.043</td>
<td>1.045</td>
<td>1.034</td>
<td>1.033</td>
<td>1.039</td>
</tr>
<tr>
<td>Magnetic data</td>
<td>1.023</td>
<td>1.01</td>
<td>1.055</td>
<td>1.033</td>
<td>1.014</td>
<td>1.009</td>
<td>1.021</td>
<td>1.032</td>
</tr>
</tbody>
</table>

Finally, examination of model misfit and lithological resemblance (Figure 3.10) clearly illustrates the non-linearity of the process leading to the lithological model. For instance, MAMM for scenarios (c) is significantly lower for scenarios (a) (Figure 3.10A and Figure 3.10B). Meanwhile, \( r \) increases from 87% to 93% between scenarios (a) and (c) (Figure 3.10C). While geological uncertainty seems to be the main influencing factor, visible differences between the simulated scenarios occur primarily in the more geologically complex areas. This makes their geological interpretation challenging and highlights the necessity to study reconstructed lithological models in a geology-related manner. The next subsection develops the topological analysis.

#### 3.6.2.2. Topology of lithological models

The topology of lithological models is calculated following the technique detailed in Section 3.4.2. Figure 3.11 shows the relative difference between the adjacency matrix of the reference model and that of inverted models, encapsulated in \( M^{rel} \) (equation 3.13).
In Figure 3.11, adjacency matrices consistently exhibit higher relative difference for contacts between lithology 4 and (3+5) (we remind that 3 and 5 are indistinguishable in petrophysical domain, see Figure 3.6) than for other lithological relationships. A possible explanation is that lithology 4 (dolerite) has a lower thickness than other lithologies (see Figure 3.3) in the more complex and uncertain regions of the model (Figure 3.5). Therefore, it may not be recovered by inversion in areas where geophysical inversion cannot resolve it given the constraints applied. In such cases, because lithology (3+5) is intruded by dolerite (lithology 4), the geological meaning and topology of the model are strongly impacted as one may expect the intrusive lithology to be in contact with all the units it cuts. Negative $M_{rel}$ values for lithologies 4 and (3+5) indicate an underestimate of the number of contacts, suggesting that the intrusion is poorly recovered for cases (a) and (b) but that it is better constrained by cases (c).

Figure 3.11. Relative difference between the adjacency matrices of the recovered lithological model and of the reference model for the different uncertainty scenarios.
The interpretation of Figure 3.11 confirms results from other metrics. For geological uncertainty scenarios (a), (b) and (c), the best results are obtained with petrophysics case (β). Comparison of the different adjacency matrices indicates that results obtained with petrophysics case (β) shows better agreement with the reference model. It also demonstrates that geology is the main constraining factor for inversion, and that case (c, β) is optimum in terms of model recovery. Topological analysis as shown in Figure 3.11 also corroborates the observations made in subsection 3.6.2.1. in that geological input data uncertainty is the principal factor affecting the recovered models and that petrophysics is tuning the model. Furthermore, this confirms that knowledge of local changes in retrieved models induced by changes in petrophysical uncertainty are important for interpretation, and that the ‘sharpest’ petrophysical distributions does not necessarily lead to optimum results.

3.7. Discussion

Contrarily to intuitive assumptions, a reduction in the spread of physical properties around the mean value measured for each of the lithologies used to derive local constraints does not necessarily improve inverted models. As we have seen in Subsection 3.6.2.1 and 3.6.2.2, for each of the PGMs that we tested, petrophysics case β leads to better results in terms of model misfit $\varphi_m$ and lithological resemblance $r$ than case γ. In contrast, we observed that a decrease in geological uncertainty is directly related to improvements in the recovered model. This difference resides in that more certain geology leads to a starting model closer to the causative model. Importantly, reducing geological uncertainty decreases the effect of non-uniqueness further by reducing the range of models honouring the local constraints.

The laws governing geological modeling and geological processes are ‘highly’ non-linear. Consequently, the PGM is not simply a smooth version of the reference (or causative, in real-world studies) model as it encapsulates the complexity of all the geologically plausible models from MCUE. This is why topological analysis of the inverted models might reveal the presence of features different from the reference model(s) or from the interpreted geology of the area. Lower geological uncertainty level reduce the variability of possible models and the associated biases. Consequently, as we have seen, inverted models are strongly impacted by the level of certainty in geological field measurements.

Petrophysical constraints refine the model by controlling physical property contrasts between units and reduce interpretation uncertainty. However, the downside of such constraints is that
they might enhance the risk of local entrapment in local optimization schemes around scenarios resembling the starting model if the separation between lithologies is too pronounced. This might be because the topography of the cost function is made more complex by the addition of petrophysical constraints. In the example we show, this is illustrated by petrophysical case \( \gamma \), which does not provide better results than cases \( \alpha \) and \( \beta \) despite having a lower level of uncertainty.

Although the description of physical measurements using normal distributions cannot be applied to all scenarios, our findings regarding the influence of the related uncertainty may be extrapolated, to a certain extent, to the general case. Uncertainty in geological and petrophysical measurements affect inversion largely through their influence on the topography of the constraint term. Consequently, our results can be generalized to other types of distribution describing physical or petrophysical measurements provided that the related uncertainty impacts petrophysical constraints in a similar way. Our utilisation of Gaussian mixture models relies on a soft clustering technique that shares a number of characteristics with the fuzzy c-means algorithms (Bordogna and Pasi 2011). We can therefore assume that our findings would hold true for inversions utilizing petrophysical constraints relying on soft clustering techniques such as the fuzzy c-means algorithms of (Paasche and Tronicke 2007; Carter-McAuslan et al. 2015; Sun and Li 2015, 2016b; Maag and Li 2018).

The main differences between inversions results shown here are characterized during inverted model analysis since ameliorations brought by constrained joint inversion occur primarily in model space. This confirms observations of (Giraud et al. 2017), and to a lesser extent, (De Stefano et al. 2011; Medina et al. 2012; Heincke et al. 2014, 2017; Linde and Doetsch 2016; Sun and Li 2016a; Colombo et al. 2017) who highlight the interest of joint inversion for improved geological interpretation, and (Gallardo and Meju 2004, 2011; Abubakar et al. 2012; Gao et al. 2012; Jardani et al. 2013; Molodtsov et al. 2013; Juhojuntti and Kamm 2015) who stress the fact that improvements brought by joint inversion occur predominantly in model space. Complementing these works, we utilised a series of metrics to assess the reliability of inverted models for geological interpretation. Our analysis of lithological models complements the work (Sun and Li 2016a), who conclude that “no additional analysis [of geology differentiation] after inversion is needed” in a case where geological information is limited. This needs to be amended in cases where geological information or modelling is available. As we
have demonstrated, geological analysis of recovered lithological models is useful to identify implausible parts of the model or to suggest alternate geological hypotheses. In our case, posterior model examination allows us to highlight poorly constrained areas or lithologies, thus confirming observations of (Paasche 2016).

Future developments of the methodology introduced here include the matching of recovered lithological models with the closest geological realization from the suite of models which is used to derive the PGM. A possible extension of the presented methodology that furthers integration between the three disciplines we considered here is the incorporation of topological rules from area-specific geological knowledge directly in inversion. This would provide a theoretical framework unifying the inversion strategy we proposed with the works of (Lelièvre et al. 2015; Miernik et al. 2016; Bijani et al. 2017) and (Fullagar and Pears 2007), where the inverse model is formulated using surface geometry on one hand, and (Carter-McAuslan et al. 2015; Sun and Li 2015, 2016a, 2017) who use petrophysical information on the other hand. Nevertheless, the applicability of such a modeling scheme is currently limited by the high computational requirements of level sets and wireframe inversion (Lelièvre et al. 2015; Lelièvre and Farquharson 2016; Bijani et al. 2017), or hypothesis limiting possible application to specific scenarios (Juhojuntti and Kamm 2015). The same remark applies to the formulation of our joint inversion problem in a multi-objective global optimization scheme, which, while presenting the advantage of being less affected by non-uniqueness, is limited by high computational cost of such approach. Nonetheless, we believe that the implementation of such methodology in 3D is within reach.

Future works include the application of the method presented here to real world geophysical data. Ongoing development of Tomofast-x include the integration of spatial trends, geochemical information in the geological conditioning process and locally varying $C_m$ matrices. Further work also includes tests involving lithology-dependent petrophysical uncertainty to better account for spatial variability of rock properties.

Our topological analysis is a first step towards quantitative posterior geological evaluation of inversion results. It is, however, restricted to the most common and simple geological relationships. Ideally, it should account for as many topological relationships as possible to provide comprehensive topological analysis. In addition, the study presented here could be extended by increasing the complexity of our geological model further through the addition of
one or more intrusive bodies not sampled by surface geology or not sampled by petrophysics. In such case, we expect to observe less sharp contrasts in the physical properties and a topological signature incompatible with the measured geological data in the neighborhood of the intrusion.

3.8. Conclusion

We have studied how petrophysical and geological uncertainty feed into and influence geophysical inversion results using a realistic synthetic case study. We have presented the capabilities of our integrated inversion platform and shown how it integrates uncertain petrophysical and geological data in 3D geophysical inversion.

We explored a relatively new and sparsely documented area of inversion and integrated studies by simulating a series of uncertainty levels in prior information. Our results clearly indicate that in geoscientific integration studies similar to ours in philosophy, the main control on the inverse models’ geological features is geological information. Meanwhile petrophysics exerts a significantly lower influence that is, as a first order approximation, restricted to enhancing model resolution. We have also shown that the topological analysis of recovered lithological models is a useful step in geological interpretation. Topological analysis is also crucial for the utilization of inverted models for further modeling because it can reveal poorly constrained geological units, thereby allowing the identification of alternative scenarios and zones to be investigated in more details.

3.9. Data, models and code availability

Reference property models, synthetic geophysical data, inversion model and recovered lithological models shown or discussed in this paper are made available by (Giraud et al. 2018a) in an ASCII format usable by Tomofast-x using doi: 10.5281/zenodo.1003105. The source code and the parameter files will be available on Github, project Tomofast-x. We used the publicly available structural geological model of the Mansfield area (Victoria, Australia) of (Pakyuz-Charrier 2018) as the reference geological structural framework.

3.10. Acknowledgements

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perceptually uniform colorcet maps” P. Kovesi (Good Colour Maps: How to Design Them, arXiv:1509.03700 [cs.GR] 2015). The authors are thankful to the Australian federal government for granting an International Postgraduate Research Scholarship to J. Giraud. The authors acknowledge the state government of Western Australia for supporting M.W. Jessell and M. D. Lindsay through the Geological Survey of Western Australia, Royalties for Regions, and the Exploration Incentive Scheme. M. W. Jessell is supported by a Western Australian Fellowship. M. D. Lindsay is supported by the Mineral Research Institute of Western Australia.

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Chapter 4

Integration of geological uncertainty into geophysical inversion by means of local gradient regularization

“Sono stato impressionato dall’urgenza del fare.
Conoscere non è abbastanza; dobbiamo applicare.
Essere volenteroso non è abbastanza; dobbiamo fare.”

“I have been impressed with the urgency of doing.
Knowing is not enough; we must apply.
Being willing is not enough; we must do.”

- Leonardo da Vinci

Part of the work in this chapter was presented at the EAGE 2018 Annual Meeting in Copenhagen (Denmark). The first page of the related conference publications is shown in Appendix A.

The full text of this chapter is under peer-review for publication in Geophysical Journal International. It has been reformatted to fit this thesis. The first page of the article as it appears in the journal is shown Appendix A.

4.1. Abstract

We introduce a workflow integrating geological uncertainty information in order to constrain gravity inversions. We test and apply this approach to data from the Yerrida Basin (Western Australia), where we focus on prospective greenstone belts beneath sedimentary cover. Geological uncertainty information is extracted from the results of a probabilistic geological modelling process
using geological field data and their uncertainty as input. It is utilized to locally adjust the weights of a minimum-structure gradient-based regularization function constraining geophysical inversion. Our results demonstrate that this technique allows geophysical inversion to update the model preferentially in geologically less certain areas. It also indicates that inverted models are consistent with both the probabilistic geological model and geophysical data of the area, reducing interpretation uncertainty. The interpretation of inverted models finally reveals that the recovered greenstone belts may be shallower and thinner than previously thought.

4.2. Introduction

The integrated interpretation of multiple data types and disciplines in geophysical exploration is a powerful approach to mitigating the limitations inherent to each of the datasets. For instance, gravity data, which has poor horizontal resolution, can be integrated with seismic inversion to mitigate the poor lateral resolution of seismic inversion (Lelièvre et al. 2012). Likewise, geological modelling and geophysical inversions are routinely performed in the same area to obtain an subsurface model consistent with geological and geophysical measurements (Guillen et al. 2008; Williams 2008; Lelièvre and Farquaharson 2016; Pears et al. 2017). When sufficient prior information is available, petrophysical constraints can be derived for inversion (Paasche and Tronicke 2007; Lelièvre et al. 2012), and integrated with geological modelling to derive local constraints (Giraud et al. 2017). However, in exploration scenarios, this might be impractical as the available petrophysical information may be insufficient to allow us to derive such constraints (Dentith and Mudge 2014). In such cases, when more than one geophysical dataset is available, practitioners may rely on joint inversion using structural constraints (Haber and Oldenburg 1997; Gallardo and Meju 2003; Zhdanov et al. 2012).

Alternatively, when one of the datasets has a spatial resolution that is superior to the others, structural information can be transferred into the gradient regularization constraint for the inversion of the lesser resolving method(s), thus mitigating some of the challenges faced by joint inversion in such cases into what (Brown et al. 2012) termed guided inversion. This strategy has been applied in recent years using the interpretation of predominantly propagative data (e.g., seismics, ground-penetrating radar) to constrain the inversion of diffusive data (e.g., diffusive
electromagnetic methods), see (Yan et al. 2017) and references reported therein. However, this avenue remains relatively unexplored to date.

In this article, we broaden the applications of guided inversion and explore the integration of non-geophysical information in inversion, such as geological uncertainty, into what we call uncertainty-guided inversion where we focus on the complementarity of information content between the datasets. We introduce a new technique that integrates local uncertainty information derived from probabilistic geological modelling in the inversion of potential field data, following recommendations of (Jessell et al. 2010; Lindsay et al. 2013a; Jessell et al. 2014; Lindsay et al. 2014; Wellmann et al. 2014, 2017). In contrast to (Giraud et al. 2016, 2017) who derives local petrophysical constraints from petrophysical measurements and geological modelling results, constraints used in uncertainty-guided inversion are based solely on the local conditioning of a gradient regularization function, thereby offering the possibility to integrate probabilistic geological modelling into geophysical inversion in the absence of sufficient petrophysical information. This conditioning relies on the calculation of local weights derived from prior geological information. In this study, we utilize a probabilistic geological model (PGM) (Pakyuz-Charrier et al. 2018) consisting of the observation probability of the different lithologies of the area in every model cell. More specifically, we utilize the information entropy (Shannon 1948; Wellmann and Regenauer-Lieb 2012), which measures geological uncertainty in probabilistic models. We calculate it in each model cell of the PGM to derive spatially varying weights applied to the gradient regularization function used during inversion.

The integration methodology we develop is similar in philosophy to (Brown et al. 2012; Wiik et al. 2015; Guo et al. 2017), who extract continuous structural information from seismic data to adjust the strength of the regularization term locally in order to promote specific structural features during electromagnetic inversion. However, our work differs from these authors in four main respects. Firstly, the geophysical problem we tackle is different in nature as we constrain potential field data in hard rock scenario instead of electromagnetic data in soft rock studies. Secondly, we use a metric encapsulating geological uncertainty derived from geological measurements, whereas, in contrast, previous studies use other geophysical attributes. Thirdly, we allow inversion to update the model preferably in the most uncertain parts of the geological
model, instead of encouraging a certain degree of structural similarity between two geophysical inverse models. Finally, while previous work involve mostly 2D models, every step of our modelling is performed purely in 3D.

In this paper, we introduce the methodology and field application as follows. In the methodology Section, we first introduce the inversion and integration scheme and algorithm, and provide essential background information about probabilistic geological modelling. We then provide the essential background about information entropy before detailing its usage in inversion. In the ensuing section, we present a field application case focused on the Yerrida Basin (Western Australia), starting with the introduction of the geological context and modelling procedure. We then analyse the influence of local regularization conditioning on inverted models and demonstrate how it allows clearer and more reliable interpretation of the buried greenstone belts than when it is not utilized.

4.3. Modelling procedure

4.3.1. Inversion methodology

The inversion procedure we propose integrates spatially varying prior information to weight the regularization function locally (e.g., in each cell). It is implemented in an expanded version of the least-square inversion platform Tomofast-x (Martin et al. 2013, 2018), which offers the possibility to condition the regularization function (Tikhonov and Arsenin 1977) of (Li and Oldenburg 1996) locally using geological uncertainty. This is achieved by incorporating prior information into a structure-based regularization function in a fashion similar to (Brown et al. 2012; Wiik et al. 2015; Yan et al. 2017) by locally adjusting the related weight.

Solving the inversion problem regularized in this fashion consists of finding a model $m$ that minimizes the objective function $\theta$ given below:

$$\theta(d, m) = \frac{1}{2}
\left|
\begin{array}{c}
W_d(d - g(m)) \\
W_m(m - m_p)
\end{array}
\right|^2 + \frac{1}{2}
\left|
\begin{array}{c}
\nabla m
\end{array}
\right|^2 + \alpha \frac{1}{2}
\left|
\begin{array}{c}
\nabla m
\end{array}
\right|^2,$$

where $d$ relates to the geophysical measurements to be inverted, $g$ is the forward modelling operator; $m$ relates to the model being searched for, and $m_p$ is the prior model; $W_d, W_m$ and $W_H$ are diagonal weighting matrices corresponding to data noise, model weighting and gradient.
regularization, respectively. The model term is a ridge regression constraint term (Hoerl and Kennard 1970).

The structural regularization term in Equation (4.1) enforces structural constraints during inversion. Its weights are adjusted by the diagonal matrix $W_H$, which values are set accordingly with prior geological information reflecting geological uncertainty (see 4.3.3 for details). The positive free parameter $\alpha$ controls the overall weight of the regularization term; $\nabla$ is the gradient operator. Note that $\|\nabla m\|_2$ estimates the amount of structure in $m$. Note that parts of the model where $W_H = 0$ are excluded from the calculation of the structural regularization and can change freely to accommodate geophysical data.

4.3.2. Probabilistic geological modelling

Probabilistic geological modelling is performed using the Monte-Carlo Uncertainty Estimator (MCUE) method of (Pakyuz-Charrier et al. 2018), which is an uncertainty propagation method for 3D implicit geological modelling using geological rules and geological orientation measurements (foliation and interface) as inputs. The sampling algorithm perturbs orientation data by sampling probability distributions describing the uncertainty of orientation data to produce a series of unique altered models. Realizations that do not respect a series of geological rules are considered implausible and are rejected. Coupled to the 3D geological modelling engine of Geomodeller© (Calcagno et al. 2008), it produces a set of plausible geological models representing the geological model space (Lindsay et al. 2013b). The observation probabilities constituting the probabilistic geological model (PGM) are obtained, in each model cell, by calculating the relative observation frequencies of the different lithologies from the set of geological models. For the $i^{th}$ model cell of a PGM containing $L$ lithologies, vector $\psi^i = [\psi^i_{k=1}, ..., \psi^i_{k=L}]$ contains the observation probabilities of each lithology. As we show in the next subsection, the resulting PGM can be used to estimate uncertainty levels and as a source of prior information.
4.3.3. Utilisation of information entropy for local conditioning

Information entropy has recently been introduced in geological modelling by (Wellmann and Regenauer-Lieb 2012) and is gaining popularity as a measure of uncertainty in probabilistic geological modelling (Lindsay et al. 2013a, 2014; Yamamoto et al. 2014; de la Varga and Wellmann 2016; Thiele et al. 2016; Schweizer et al. 2017; Wellmann et al. 2017; de la Varga et al. 2018; Pakyuz-Charrier et al. 2018). Quoting (Schweizer et al. 2017), information entropy “quantifies the amount of missing information and hence, the uncertainty at a discrete location”.

For the $i^{th}$ model-cell, it is given as (Shannon 1948):

$$ H^i = H(\psi^i) = -\sum_{k=1}^{L} \psi_k^i \log(\psi_k^i). \tag{4.2} $$

Instead of using $H$ directly, we calculate $W_H$ utilising its normalized complementary, which reflects the degree of certainty across the model. Let us express $W_H$ as follows, for the $i^{th}$ model cell:

$$ W_H^i = \frac{\max H - H^i}{\max H - \max H} \tag{4.3} $$

The consequence of Equation (4.2) and (4.3) is that $W_H$ is minimum at interfaces and in areas poorly constrained by geological information, and equal to unity in areas where the geology is well resolved. Consequently, the conditioning process attaches small weights to the structural term of (4.1) in uncertain cells, while consistently high values will be applied to the most geologically certain cells. As a result, it enables the inversion algorithm to favour nearly constant changes in the inverted model in contiguous certain groups of cells (e.g., where $W_H \to 1$) while relaxing the regularisation constraints in the most uncertain parts (e.g., where $W_H \to 0$).

For proof-of-concept validation, we simulated an idealized case study to assess the capability of inversion using $W_H$ as per Equation (4.3) to improve inversion results compared to the non-conditioned case (e.g., with $W_H$ equal to the identity matrix). We tested the proposed methodology using synthetic geophysical data calculated from the structural geological model of the Mansfield area of (Pakyuz-Charrier et al. 2018), which we populated in the same fashion as (Giraud et al. 2017). The analysis of inverted models demonstrates the potential of the proposed inverse modelling scheme to ameliorate inversion results and to reduce interpretation uncertainty (details are given in Appendix C). Importantly, in this synthetic case, local conditioning allows geophysical
inversion to significantly improve the imaging of geologically uncertain areas. From the success of that theoretical proof-of-concept study, we are confident that our integration method can be tested here using real world data for field validation.

4.4. Field validation: Yerrida Basin case study

4.4.1. Geological context and geophysical survey setup

The Yerrida Basin is located in the southern part of the Capricorn Orogen, at the northern margin of the Yilgarn Craton in Western Australia (Figure 4.1a), and extends approximately 150km N-S and 180 km E-W (Figure 4.1b). The studied area is delimited in the northwest by the Goodin Fault, which represents a faulted contact between the Yerrida Basin and the Bryah-Padbury Basin. The structures of interest in this work are: Archean greenstone belts extending north-northwest that are unconformably overlain by Paleoproterozoic sedimentary rocks the form the Yerrida Basin. Features A and B (Figure 4.1a and Figure 4.1b) indicate the interpreted position of buried Wiluna Greenstone Belt. Where the Wiluna Greenstone Belt is exposed, it is host to base and precious metal mineralisation (Williams 2009). With a relatively high positive density contrast (expected to be between 190 and 270 kg.m$^{-3}$) to the Yilgarn Craton granite-gneiss host, mafic greenstone belts A, B, and C are suitable targets for gravity inversion. Interpretations from multiple studies in the region, e.g, (Pirajno et al. 1998; Pirajno and Adamides 2000; Pirajno and Occhipinti 2000; Johnson et al. 2013) were compiled while additional geological measurements acquired in 2015, 2016 and 2017 complemented legacy data (Occhipinti et al. 2017; Olierook et al. 2018). This allowed the revision of existing models and improved our understanding of the area. This, in turn, also highlights the challenges presented by the characterization of greenstone belts A, B and C, and that further geophysical analysis through constrained inversion is a useful pathway for reducing exploration risk.

Inverted geophysical data consists of ground surveys obtained from Geoscience Australia (http://www.ga.gov.au/data-pubs). Post-processing includes spherical-cap and terrain corrections and the removal of the regional trend to obtain the complete Bouguer anomaly, which we forward model following (Boulanger and Chouteau 2001). As most data points were acquired 1 to 4 km apart, the dataset was resampled to match the geological model discretization, making up a total of 4882 measurement points. The model is discretized into 100 × 100 × 42 cells of dimensions 2.335
km $\times$ 1.875 km $\times$ 1.0475 km, down to a depth of 44 km, making up a total of 420000 cells. We utilize the integrated sensitivities technique of (Li and Oldenburg 2000; Portniaguine and Zhdanov 2002) to precondition the data term in Equation (4.1) in order to balance the decreasing sensitivity of gravity field data with depth.

Figure 4.1. Geological context and geophysical data. (a) Geological map of the area and (b) complete Bouguer anomaly. The dashed lines delineate the possible sub-basin extent of the mafic greenstone belts A, B and C.

4.4.2. Geological modelling

Geological data consists of in-situ structural measurements (interfaces and foliations) and interpretation of aeromagnetic, airborne electromagnetic, Landsat 8 and ASTER data. Legacy data from the Geological Survey of Western Australia (Pirajno and Adamides 2000) and CSIRO (Ley-Cooper et al. 2017) were used, to which about 600 data points and petrophysical measurements from recent geological field campaigns were added. Although the available petrophysical measurements are not used to derive petrophysical constraints because of the insufficient sampling of several of the modelled lithologies, they are a useful source of information to populate geological models and for interpretation.
These datasets were used jointly to build a reference geological model for MCUE simulations, after which lithologies with similar density contrasts were merged and subsequently treated as a single rock type. Uncertainty related to structural measurements was subsequently used as inputs to the MCUE perturbations (Pakyuz-Charrier et al. 2018) of the reference model to generate a collection of 500 accepted models. Information extracted from the PGM displayed in Figure 4.2 (next page). Figure 4.2a shows the lithologies with the highest probability for each cell of the PGM. The associated $W_H$ values used in inversion are shown in Figure 4.2b. The starting model for inversion, which we also use as prior model $m_p$, is equal to the mean model of the 500 plausible models generated by MCUE, is shown in Figure 4.2c.
Figure 4.2. Geological modelling results. (a) Most probable lithology in each model cell (same colour code as in Fig. 1) (b) values used for local regularization conditioning, (c) and starting model derived from PGM and prior petrophysical information). In (a), “background” refers to all the lithologies that have a density contrast equal to 0 kg m$^{-3}$. 

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4.4.3. Inversion results and analysis

Our analysis aims at determining the influence of the local conditioning of structural constraints on inversion through comparison with the non-conditioned case, all other things remaining constant.

4.4.3.1. Comparative analysis strategy

Prior to examination of the inverted models, we analyse geophysical data misfit after inversion for a fixed number of major iterations (100) of the least-square geophysical inverse solver superior to that needed for convergence of the inversion algorithm (~10 in this case). This enables us to ensure that the inversion results we compare produce, in our case, similar gravity anomalies. Our study of inverted models focuses on results obtained through usage of non-conditioned (Figure 4.3a) and conditioned regularization function (Figure 4.3b) using $W_H$ (Figure 4.2b). In addition to departures from the starting model, variations between the two cases are studied by visual comparison of Figure 4.3a and Figure 4.3b, through qualitative (Figure 4.3c) and quantitative comparative analysis (Figure 4.3d-e). Our interpretation of inversion results is complemented by metrics quantifying the differences between models. We give particular attention to model cells where the probability of mafic greenstone is superior to zero. For these cells, we classify lithologies by identifying cells with a density contrast corresponding to mafic greenstone.

4.4.3.2. Results

Data root-mean-square (RMS) error decreases during inversion from 12.46 mGal to reach 1.59 mGal and 1.53 mGal for the non-conditioned and conditioned cases, respectively. The corresponding data misfit maps show a linear correlation coefficient of 0.999 (see detailed misfit maps in Appendix C.3). This similarity illustrates that, as in many other studies, most changes related to holistic data integration in geophysical inversion occur primarily in model space, hence reducing the effect of non-uniqueness (Gallardo and Meju 2004, 2007, 2011; Abubakar et al. 2012; Gallardo et al. 2012; Gao et al. 2012; Brown et al. 2012; Jardani et al. 2013; Molodtsov et al. 2013; Moorkamp et al. 2013; Juhojuntti and Kamm 2015; Sun and Li 2016, 2017; Rittgers et al. 2016; Heincke et al. 2017; Demirel and Candansayar 2017; Guo et al. 2017; Giraud et al. 2017).
Qualitatively, comparison of Figure 4.3a and Figure 4.3b reveals that departures from the starting model (Figure 4.2c) are more significant in the most geologically uncertain areas. Quantitatively, the RMS model update for cells characterized by $0 \leq W_H < 0.05$ (most uncertain group) is equal to 40.1 $kg/m^3$ and 51.5 $kg/m^3$, for the non-conditioned and conditioned cases, respectively, whereas the same quantities are equal to 17.7 $kg/m^3$ and 16.9 $kg/m^3$ for the cells identified by $0.95 < W_H \leq 1$ (most certain group). This suggests that local regularization conditioning allows inversion to update the model preferentially in geologically uncertain areas. In turn, differences with the starting model in more geologically certain areas are reduced compared to the non-conditioned case. This effect of conditioning is corroborated by Figure 4.3c where the longest distances to the dashed line, which represents equal model update for the two studied cases, occur in geologically uncertain areas. This also translates in higher difference between model updates of the two compare cases in Figure 4.3d for lower values of $W_H$. In addition, we observe that local conditioning produces stronger density contrasts in Figure 4.3b in some of the areas where the conditioning values are higher in Figure 4.2b. Furthermore, structures in the inverted model are easier to identify when local conditioning is used. It is confirmed by global roughness measures $\|\nabla m\|_2$ equal to 3.4 $(kg/m^3)/m$ and 4 $(kg/m^3)/m$ for the non-conditioned and conditioned cases, respectively. More specifically, as shown by Figure 4.3e, this difference arise in parts of the model associated with lower $W_H$, which characterize uncertain areas, including interfaces between lithologies.

The recovered greenstone belts are shown in Figure 4.3a and Figure 4.3b. In Figure 4.3b, the extension of recovered mafic greenstone belts is significantly different than when geological uncertainty is not accounted for (Figure 4.3a). In particular, belt A is significantly larger in Figure 4.3b than in Figure 4.3a ($2.4 \times 10^2$ km$^3$ vs $4.6 \times 10^2$ km$^3$). Similarly, the extent of belt C is increased overall (volume of $5.3 \times 10^2$ km$^3$ vs $14 \times 10^2$ km$^3$), while its different portions reconnect; the northern half is also significantly shallower and broader than in Figure 4.2a and Figure 4.3a. It appears that belt A remains thinner and shallower (Figure 4.3b) than suggested by the preferred lithology volume (Figure 4.2a). While similar geometries for belt B are recovered in Figure 4.3a and Figure 4.3b, they both differ from Figure 4.2a as only the eastern part is preserved. Note that it is larger in Figure 4.3b, with a volume 40% higher than in Figure 4.3a. As discussed in the next subsection,
these differences have a significan impact on the interpretation of inversions results and are important to understand the influence of local conditioning on inversion.

Figure 4.3. Comparison of inversion results. (a) inverted models with non-conditioned regularization, and (b) using local conditioning, (c) cross-plot between the absolute difference with the starting model, (d) difference in model updates $\delta \| \Delta m \| = \| m_{\text{cond}} - m_{\text{nocond}} \|_2$ as a function of values of $W_H$ and (e) difference in model roughness $\delta \| \nabla m \| = \| \nabla m_{\text{cond}} \|_2 - \| \nabla m_{\text{nocond}} \|_2$ as a function of values of $W_H$. Model cells labelled A, B and C are interpreted as mafic greenstone belts.

4.4.4. Interpretation

Note that, in contrast to the differences between inversion results highlighted above for belts A and C, differences between the inverted models in the north-eastern part of the model and the
different interpretations of belt B (Figure 4.3a and Figure 4.3b) are small. This shows that locally conditioned regularization does not enforce changes in the inverted model everywhere geological uncertainty is high as uncertainty is only a reflection of potential errors. Rather, this indicates that in such cases, the guiding effect of such regularization will be exerted provided that it does not prevent the data term in $\theta(d, m)$ as per Equation (4.1) from decreasing. This also confirms that geophysical data is the main driver of the model updates in geologically uncertain areas. Instead of smooth departures from the starting model to match geophysical data regardless of geological considerations, local regularization constraints allow inversion to account for the probabilistic geological modelling of the area and for geological uncertainty. It can therefore provide results that conform better to known geology.

In consequence, by confronting a probabilistic geological model encapsulating all MCUE realizations with geophysical measurements in an inversion scheme favouring model updates in the most geologically uncertain areas, inversion complements probabilistic geological modelling in that it guides and refines the interpretation of the geoscientific data in the area.

Geophysical inversion using uncertainty information (Figure 4.2b) confirms the presence of high density anomalies that we interpret to be geological the mafic components of the greenstone as suggested by MCUE in several portions of the model. It also adjusts the outline and geometry of belts A, B and C to obtain a model honouring geological uncertainty information. In particular, mafic greenstone A and B may be smaller than the extent suggested by the PGM, and mafic greenstone C shallower than anticipated. Inversion results interpretation also reveal that greenstone B might be extended further to the east than indicated by the preferred lithology volume (Figure 4.2a) and that greenstone C may be thinner in its central part.

4.5. Concluding remarks

We have introduced a new integration scheme for the inversion of gravity data that utilizes a measure of geological uncertainty to calculate locally-conditioned gradient regularization constraints. Contrarily to previous work, this approach enables the integration of probabilistic geological modeling in geophysical inversion in the absence of petrophysical information sufficient to the calculation of petrophysical constraints. It uses geophysical measurements to optimize the
inverse problem by updating the physical property model preferably in geologically uncertain parts of the studied area during what we called *uncertainty-guided inversion*. This therefore partly mitigates inversion’s non-uniqueness through the addition of constraints encouraging inversion to produce models that account for geological uncertainty across the entire inverted volume. We have demonstrated that it can be used collaboratively with geological modelling efficiently through field application in the Yerrida Basin. Inversion results show that our integration methodology has the capability to refine the recovered physical property model and interpretations in portions of the model where geological uncertainty is high. Another advantage of the proposed technique pertains to its time and cost-effectiveness as our workflow utilizes the PGM resulting from geological modelling and requires the same parameterization as non-conditioned inversion.

In the Yerrida Basin study area, application of the proposed methodology provided the effective delineation of the greenstone belts by quantitatively integrating geological measurements and geophysical data. Our findings suggest that some of the greenstone belts covered by the basin might be shallower than previously anticipated and occupy smaller volumes. This is particularly pronounced in the North-East (belt C) where the resulting model is in agreement with the shallowest cases allowed by the PGM. Likewise, in the South (belt A), only the shallowest part of the mafic greenstone body can be resolved, while the south-eastern (belt B) greenstone belt appears to be limited in extension to the eastern part of the volume where it is the preferred lithology in the PGM. In such cases, this can also indicate that these greenstone bodies might be too thin to be imaged by gravity data. These results have implications for the geological knowledge of the southern Capricorn Orogen as they indicate reduced (compared to the preferred lithology volume) mafic greenstone volumes under the Yerrida Basin on one hand, and decreased cover thickness on the other hand, thereby opening the door to updates in the geological interpretation of the history of the Yerrida Basin and potential new undercover exploration prospects.

Future research include the utilization of local petrophysical constraints of (Giraud et al. 2017) in the uncertainty-guided inversion scheme we presented, as well as its application to weight the cross-gradient term of (Gallardo and Meju 2003) in joint inversion schemes. With this last respect, uncertainty-guided inversion can be assisted in the most uncertain parts of the model by guided inversion (in the sense of (Brown et al. 2012)) or through cross-gradient joint inversion.
4.6. Code and data availability


4.7. Acknowledgements

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4.8. Chapter 4 References


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Chapter 5

Concluding remarks and perspectives

“It is only by combining the information furnished by all the Geo-Sciences that we can hope to determine ‘truth’, that is to say, to find the picture that sets out all the known facts in the best arrangement and that therefore has the highest degree of probability.”

- Alfred Wegener, 1915, Die Entstehung der Kontinente und Ozeane (The Origin of Continents and Oceans)

5.1. Consolidated conclusion of the presented research

We have developed and introduced a new holistic inversion workflow that can integrate probabilistic geological modeling, petrophysical measurements and geophysical data. The workflow’s strength lies in its flexibility and can accommodate different types and combinations of prior information and data. Through the development and application of this workflow, this PhD project has explored new areas of research and extended existing methodologies. As we have seen in the previous Chapters, any combination of gravity data and/or magnetic data can be inverted using constraints encapsulating information from probabilistic geological modeling and/or petrophysical measurements, in 2D or in 3D. The efficacy of the workflow has been evaluated using both synthetic and field data and the work presented has shown that integrating different data types can help reducing uncertainty and interpretation ambiguity.
Using a series of metrics, we have studied how petrophysical and geological uncertainty propagates into and influences geophysical inversion results. Through this, we have investigated a relatively unexplored area of inversion and integrated studies by simulating a series of realistic uncertainty levels in prior information. Our results reveal that in the general holistic framework we propose, the main control on the inverse model’s geological features is geological information, while petrophysical influence is somewhat restricted to enhancing model resolution. We have also shown that quantitative geological interpretation is a powerful tool that can be used to constrain further geological modeling as it can reveal uncertain areas or alternative geological configurations.

To overcome difficulties related to suitable petrophysical measurements or the lack thereof, we introduced a methodology exploiting probabilistic geological modeling to constrain inversion in the absence of petrophysical information. We have applied part of the proposed general workflow to the inversion of gravity data by utilising a measure of geological uncertainty to calculate locally-conditioned gradient regularisation constraints. We have demonstrated that this strategy can be used collaboratively with geological modelling efficiently to improve imaging of geologically uncertain areas using synthetic data derived from the Mansfield area and applied to the Yerrida Basin case study to image the underlying Yilgarn Craton greenstones. For these cases, inversion results show that our integration methodology has the capability to refine the recovered physical property model and interpretations in portions of the models where geological uncertainty is high. In the Yerrida Basin study area, application of the proposed methodology allowed the re-interpretation of the geology of the area.

Another aspect of the proposed inversion approach is that it relies only on the results of separate, standalone modeling. Therefore, it requires only limited resources to be implemented in cases where petrophysical and/or geological measurements have been modeled beforehand. The proposed methodology thus constitutes a useful tool for re-interpretation or reprocessing studies in both brownfields and greenfields regions. In addition, memory requirement for 3D real world scenarios remain tractable. The addition of local petrophysical or gradient constraints requires the allocation of an array the size of the model. Inversions for two dimensional or small three-dimensional problem (up to approximately ~50000 model cells) can be modeled in a matter of second to minutes using a laptop computer. The implementation of the proposed methodology is
highly scalable and there is no limit as to the size of the problem (e.g., number of data points and model cells) provided that sufficient computational power is available.

From a geological perspective, the integrated inversion schemes we present are more consistent and easier to interpret than traditional, non-holistic approaches where integration plays a lesser role in the modeling process. The different examples shown in this thesis hence provide an argument in favor of data integration towards the characterisation of unique Earth subsurface models. Our results support the claim that robust incorporation of measurements of different nature and disciplines in geophysical inversion reduces non-uniqueness and interpretation uncertainty. Practically, our findings demonstrate that the methodology presented in this thesis can be used to support better-informed decision making in exploration scenarios through quantitative evaluation of results.

Lastly, a noteworthy aspect of this thesis is that the work is presented in sufficient details to be reproduced by informed scientists, the importance of which is highlighted by (Baker 2016; Gil et al. 2016; Larcombe and Ridd 2018). It can be used by geoscientists working on the similar problems for teaching, training or benchmark purposes as field and synthetic data shown in Chapter 2, 3 and 4 are available online.

5.2. Discussion and future work

5.2.1. Limitations of the presented work and potential mitigation

Although the utilisation of MCUE with petrophysical data in inversion holds the potential to improve results greatly (Chapter 2, 3, and 4), inversion may be affected by biases or unaccounted uncertainty propagating from the input into the constraints derived from non-geophysical data. For instance, PGMs derived from MCUE where one or more lithologies have not been sampled may misestimate uncertainty in some areas. Likewise, if one or more lithologies have not been sampled by petrophysical measurements, it is possible that petrophysical constraints will guide inversion towards a model satisfying biased petrophysical statistics or that will not converge properly altogether. In such cases, geoscientists are provided with the evidence that petrophysical and geological data contain information about different rock units if the number of lithologies sampled by petrophysics differs from that present in the geological model. Such observation could
be useful, however, to highlight a lack of knowledge about the area or to suggest future exploration effort.

The formulation of the distributions sought to represent the statistics of petrophysical measurements may suffer from the limitations presented by the usage of Gaussian distributions. The Gaussian approximation of such statistics suffers from obvious pitfalls when, for instance, the magnetic susceptibility of a particular rock type follows a bi-modal or log-normal law. The simplest mitigation strategy is to offer the possibility to choose from a range of distributions when calculating the statistics of the petrophysical measurements. Another option, which is more general and robust solution, consists of the usage of non-parametric distributions. This requires, however, substantial modifications of the current version of Tomofast-x.

The topological analysis performed in this thesis relies only on the analysis of adjacency relationship, which constitute the simplest relationship between two bodies in space. Although it is a good first-order indicator about the spatial relationships between lithologies, it is insufficient to fully characterise the geological relationship between the different geological structures. Techniques enabling the recognition of complex geological relationships between rock units are necessary improve our understanding of inverted models further.

5.2.2. Continuation of the presented research

The flexibility of the integration framework introduced here permits the further integration of datasets. One can, for instance, with limited additional coding effort, utilise any 3D attributes and representations of the subsurface to constrain joint inversion in the same fashion as geological uncertainty is used in Chapter 4. In addition, the local conditioning technique presented in Chapter 2 can be extended, for example, to the utilisation of locally varying normal distributions’ parameters (e.g., center values, standard deviations) constrained by geochemical data or lateral facies variation modeling. Besides extensions of the existing methodology, potential applications of the workflow as per Figure 2.1 can be explored. That is, a number of combinations between datatypes and integration approaches can be tested (see Figure 5.1). This includes, for instance, but is not limited to, usage of electromagnetic (e.g., controlled-source electromagnetism and magnetotellurics) or seismic models to constrain gravity or magnetics in the same fashion as in
Chapter 4, which can be used in conjunction with the petrophysical constraints used in Chapter 2 and 3.

Future developments of the methodology introduced here may include the investigation of a workflow not limited to a static feedforward approach where geological models and geophysical inversion results are simply fed to the next stage of the workflow. For instance, an interactive workflow between geophysical inversion as presented in this thesis and the MCUE technique proposed by (Pakyuz-Charrier et al. 2018) could be developed. Various ways can be devised, but the easiest and most straightforward one is to identify the geological model recovered from inversion results that is closest to a geological model sampled by MCUE. This can in turn be used as a reference model for further MCUE simulations to be re-input to inversion.

Furthermore, there remains the hybridisation between MCUE, which samples the geological model space, and the deterministic inversion scheme used here. In this regard, EPC 2018 utilises a
clustering technique to classify geological models sampled during MCUE into groups called archetypes. These can be treated as independent PGMs to run a series of inversions constrained in the same fashion as presented in Chapter 3 or Chapter 4, thereby effectively utilising constrained geophysical inversion to accept or reject geological archetypes. This can subsequently be used to refine the corresponding geological scenarios before (re)interpretation (or to be re-input into MCUE and subsequently to inversion for further refinement). Posterior analysis of inversion results should, in such case, include more thorough topological analysis (e.g., that identifies more types of relationships between geological units) of inversion results to allow comprehensive characterisation of inversion outcomes. This could be achieved through utilisation of deep learning algorithms or specifically trained neural networks to identify more informative Egenhofer relationships (see Section 4.3.2).

The main additions to the presented workflow that we suggest and which would not require extensive coding effort are highlighted in green in Figure 5.1.

### 5.2.3. Further research directions

A prerequisite to the topological analysis (Chapter 3) is the recovery of lithologies from inverted models (Chapter 3 and 4). The process which was used identifies the most probable lithology from the inverted model. It does not address, however, uncertainty or indetermination in the assignment of lithologies to model cells. Consequently, a possible extension of the presented research is to develop techniques accounting for uncertainty during the process matching inverted properties with lithologies. For instance, one can think of the combined usage of the statistical framework describing petrophysical measurements (e.g., mixture models) with the probabilistic description of geology (e.g., the lithologies’ observation probability) to calculate local uncertainty indicators (e.g., Shannon’s entropy) and to estimate the degree of indetermination of said recovered lithologies. In this way, both petrophysical and geological uncertainty could be accounted for in the posterior analysis, in particular during the identification of lithologies from inversion results. This could be complemented by a sensitivity analysis of different parts of the model to variations in the measurements (translated by the Jacobian matrix as per equation 2.2). This follows (Bauer et al. 2003) to ‘add model resolution in the parameter space’ as proposed by (Paasche 2016). Results would thus allow better-informed analysis and reliable scenario generation.
A different research direction that could push the integration of geology and geophysics further is the development of a methodology utilising the geological potential used in the implicit geological modelling used by MCUE directly in geophysical inversion. We can envisage the possibility to integrate said geological potential in inversion such that it be considered simultaneously to petrophysical information and geophysical data. Such methodology would achieve integration between geological and geophysical data at a deeper level than current methodologies. This is because MCUE acts as a proxy between geological data and geophysical inversion permitting the indirect integration of geological field measurements into geophysical inversion through a PGM. The utilisation of geological potential directly in geophysical inversion would therefore integrate geological modeling and geophysical inversion at a more fundamental level through the combined use of the physical principles these modeling processes rely upon. Considering uncertainty, this would remove the propagation of discretization and modeling uncertainty from MCUE into inversion.

5.3. Chapter 5 references

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Appendices

Appendix A

A.1 Front page of first-authored publications

The following pages of this appendix show the first page of published material I am the lead author of as it appears in the literature. This appendix first shows the journal articles (2), organised in chronological order. Following this, it shows the conference abstracts and conference papers organised in chronological order.
Uncertainty reduction through geologically conditioned petrophysical constraints in joint inversion

Jérémie Giraud1, Evren Pakyz-Charrier1, Mark Jessell1, Mark Lindsay1, Roland Martin2, and Vitaliy Ogarko1

ABSTRACT

We have developed a joint geophysical inversion workflow that aims to improve subsurface imaging and decrease uncertainty by integrating petrophysical and geologic data. In this framework, probabilistic geologic modeling is used as a source of information to condition the petrophysical constraints spatially and to derive starting models. The workflow then uses petrophysical measurements to constrain the values retrieved by geophysical joint inversion. The different sources of constraints are integrated into a least-squares framework to capture and integrate information related to geophysical, petrophysical, and geologic data. This allows us to quantitatively calibrate posterior statistical indicators. To test this workflow, using a simplified real field data, we have generated a set of geologic models, which we used to derive a probabilistic geologic model. In this synthetic case study, we found that the integration of geologic information and petrophysical constraints in geophysical joint inversion could reduce uncertainty and improve imaging. In particular, the use of petrophysical constraints retrieves sharper boundaries and better reproduces the statistics of the observed petrophysical measurements. The integration of probabilistic geologic modeling permits more accurate retrieval of model parameters, and it better constrains the solution while still satisfying the statistics derived from geologic data. The analysis of statistical indicators at each step of the workflow indicates that (1) the inversion methodology is effective when applied to complex geology and (2) the integration of prior information and constraints from geology and petrophysics significantly improves the inversion results while decreasing uncertainty. Finally, the analysis of uncertainty to the integration of the conditioned petrophysical constraints also indicates that, for this example, the best results are obtained for joint inversion using petrophysical constraints spatially conditioned by geologic modeling.

INTRODUCTION

Over the past 15 years, significant research efforts have been directed toward the integration and use of the complementarity between different geophysical data sets in geophysical exploration to better constrain the properties of the subsurface (see Gallow and Meul [2011], Györi et al. [2013], and Moorkamp et al. [2016] for more information about the different joint-inversion approaches in exploration geophysics). The main interest of joint inversion is to use and combine the strengths of different geophysical techniques to reduce the effect of nonuniqueness and uncertainty with respect to single-domain inversions (Vanoff and Japp, 1975). One of the motivations for developing these techniques is that the exploration of natural resources is becoming increasingly challenging. Hydrocarbon discoveries are becoming rarer and smaller (Connors, 2015), and economic mineral deposits are also shrinking (Scheidt, 2010), whereas prospects are being found at increasing depths (Scheidt, 2014). Geophysical joint inversion is one of the tools used to mitigate the risk of inaccurate interpretation of geophysical data in exploration scenarios (Rabin et al., 2006).

The usual approach in performing geophysical joint inversion is to jointly invert data sets of two or more geophysical methods using...
Integration of geological uncertainty into geophysical inversion by means of local gradient regularization

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Abstract. We introduce a workflow integrating geological uncertainty information in order to constrain gravity inversions. We test and apply this approach to data from the Yerrida Basin (Western Australia), where we focus on prospective greenstone belts beneath sedimentary cover. Geological uncertainty information is extracted from the results of a probabilistic geological modelling process using geological field data and their uncertainty as input. It is utilized to locally adjust the weights of a minimum-structure gradient-based regularization function constraining geophysical inversion. Our results demonstrate that this technique allows geophysical inversion to update the model preferentially in geologically less certain areas. It also indicates that inverted models are consistent with both the probabilistic geological model and geophysical data of the area, reducing interpretation uncertainty. The interpretation of inverted models finally reveals that the recovered greenstone belts may be shallower and thinner than previously thought.

1 Introduction

The integrated interpretation of multiple data types and disciplines in geophysical exploration is a powerful approach to mitigating the limitations inherent to each of the datasets. For instance, gravity data, which has poor horizontal resolution, can be integrated with seismic inversion to mitigate the poor lateral resolution of seismic inversion (Lelièvre et al., 2012). Likewise, geological modelling and geophysical inversions are routinely performed in the same area to obtain a subsurface model consistent with geological and geophysical measurements (Guillen et al., 2008; Lelièvre and Farquharson, 2016; Peers et al., 2017; Williams, 2008). When sufficient prior information is available, petrophysical constraints can be derived for inversion (Lelièvre et al., 2012; Paasche and Trouwqicie, 2007), and integrated with geological modelling to derive local constraints (Giraul et al., 2017). However, in exploration scenarios, this might be impractical as the available petrophysical information may be insufficient to allow us to derive such constraints (Dentith and Mudie, 2014). In such cases, when more than one
Uncertainty reduction of gravity and magnetic inversion through the integration of petrophysical constraints and geological data

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We introduce and test a workflow that integrates petrophysical constraints and geological data in geophysical inversion to decrease the uncertainty and non-uniqueness of the results. We show that the integration of geological information and petrophysical constraints in geophysical inversion can improve inversion results in terms of both uncertainty reduction and resolution. This workflow uses statistical petrophysical properties to constrain the values retrieved by the geophysical inversion and geological prior information to decrease the effect of non-uniqueness. Surface geological data are used to generate geological models as a source of geometrical prior information. Petrophysical measurements are used to derive the statistical laws used for the petrophysical constraints. We integrate the different sources of information in a Bayesian framework, which will take into account these states of information. This permits us to quantify the posterior state of knowledge, the reduction of the uncertainty and to calculate the influence of prior information.

To quantify the influence of petrophysical constraints and geological data we compare results obtained with several levels of constraints. We start by inverting data without petrophysical constraints and geological prior information. Then, we add petrophysical constraints before using geological prior information.

The results of the inversion are characterized using fixed-point statistics. Various indicators such as model and data misfits, resolution matrices and statistical fit to the petrophysical data are calculated. The resolution matrices are used to plot sensitivity maps. We calculate the posterior covariance matrices to estimate the uncertainty of the model.

This workflow was first tested using very simple synthetic datasets before using a subset of the Mansfield area data (Victoria, Australia). The geological model is derived from geological field data. We simulate petrophysical properties based on field measurements and standard values obtained from the literature. Finally, we ran the different inversions on gravity and magnetic data generated using this model.

As a result, the use of petrophysical constraints permits us to retrieve sharper boundaries while prior structural information from geology on the shallow lithologies permits to retrieve the contacts more accurately. The integration of the different constraints provides a better-resolved model, with reduced uncertainties such as improved posterior covariance and resolution matrices. The analysis of the sensitivity to and resolution indicators using geological a priori information and petrophysical constraints shows complementarity between the resolution matrices. Moreover, the comparison of the posterior covariance matrices (diagonal and non-diagonal elements) shows that when geological prior information and petrophysical constraints are used together higher values coincide with poorly resolved lithologies. This is not always the case when either only geological prior information or no constraints are used. However, the improvement of the inversion results due to the constraints and prior information are more pronounced on gravity inversion than on magnetic inversion.
The influence of geoscience integration in post-processing lithological reconstruction

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After running a series of increasingly integrated and constrained single domain and joint geophysical inversions integrating geology, petrophysics and geophysics, we applied tools allowing to reconstruct lithological models from inversion results. To assess the capability of the inversions to retrieve accurate lithological models, we applied our workflow to a synthetic case study using geological field data. The comparison of the reconstructed lithological models shows that integration of geophysical and petrophysical measurements alone does not suffice to recover a realistic lithological model retaining the essential geological features. This investigation also shows that the retrieval of an accurate lithological model is possible only when statistical geological modelling and petrophysical measurements are integrated in geophysical inversion, and that best matching models are obtained when geophysical inversions are run jointly.

Introduction
Recent advances in geophysics include improvements of the optimisation algorithms and the increase in integration efforts. However, only a few authors tackled the problem of inferring geology from geophysical inversion (see Sun and Li 2016 and references therein). In this work we apply a method for retrieving lithologies a posteriori (in a similar fashion to Sun and Li 2013), and compare the lithological models obtained for increasingly integrated inversions. This work builds on previous work from Giraud et al. 2017, who integrate geological, petrophysical and geophysical data in joint inversion. Here, we perform a further validation of this integrated inversion workflow, through the comparison of the lithological models reconstructed from the results of increasingly integrated geophysical inversion of gravity and magnetic data.

Integrated geophysical inversion and statistical geological modelling
As it accounts for uncertainties in both the input data and constraints, we formulate the inverse problem using a Bayesian inversion approach. The inverted models which we apply the lithological reconstruction to are obtained from: (a) non-constrained single domain inversion; (b)
Geophysical joint inversion using statistical petrophysical constraints and prior information

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SUMMARY

We introduce and test a workflow that integrates petrophysical constraints and geological data in joint geophysical inversion in order to decrease the uncertainty of the result. This workflow uses statistical petrophysical properties to constrain the results retrieved by the geophysical inversion and geological prior information to decrease the effect of non-uniqueness. We integrate the different sources of information in a Bayesian framework, which takes into account the state of information. This permits us to quantify the posterior state of knowledge, the reduction of the uncertainty and to calculate the influence of prior information using quality indicators based on fixed-point statistics. This workflow was first tested using simple synthetic datasets that validate the method and assess the robustness of the workflow. As a result, the use of petrophysical constraints permits us to retrieve sharper boundaries, while prior structural information from geology permits to retrieve the geometry more accurately. Overall, the integration of the different constraints provides a model, with reduced uncertainties and better resolved parameters.

Key words: geoscience integration, joint inversion, uncertainty, petrophysical constraints, prior information.

INTRODUCTION

Context and motivations

In recent years, the integration of different geophysical techniques has been of growing importance in natural resources exploration and production due to the necessity to 1) exploit the complementarity between methods in increasingly challenging scenarios and 2) reduce the risk of costly development of low-productivity deposits and reservoirs. Previous studies have developed joint inversion techniques focusing on structural constraints to enforce structural similarity between the different models (Gallardo and Mejía, 2003; Colombo and Di Stefano, 2007). Others studies focused on the use of constitutive petrophysical laws to link the different domains (Gao et al., 2012).

More recently, San and Li (2012, 2013) have introduced clustering algorithms as a means to enforce similarities between values in the inverted model and petrophysical data. Zhang and Kervi (2013) show the integration of petrophysical clustering and geological data in joint inversion. However, even if the objective of the approaches quoted above is to obtain better constrained models, as mentioned by Reid et al. (2013), little work has been done to quantify the uncertainty or the resolving power of these techniques. In this abstract we present a workflow integrating single domain and constrained joint inversion procedures to accurately assess uncertainty changes.

We constrain the joint inversions using petrophysical constraints in the same spirit as the clustering approaches introduced by San and Li (2012), but also further the method by integrating prior geological information. We formulate the problem in a Bayesian framework in order to quantify the posterior uncertainties and confidence levels in the result. The approach we follow allow for the inversion to produce results that are statistically consistent with petrophysical measurements. Before using the algorithm on complex, realistic cases we tested and validated the workflow using a synthetic model. As a result, the use of petrophysical constraints in joint geophysical inversion permits us to retrieve petrophysical properties accurately while honouring geophysical data. Moreover, the integration of petrophysical constraints and the use of geological prior information increases the level of confidence in the results. Therefore, we conclude that integration of petrophysical, geological and geophysical information reduces uncertainty.

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Integrated geophysical joint inversion using petrophysical constraints and geological modelling

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Summary

We introduce and test a workflow that integrates petrophysical constraints and geological data in geophysical inversion in order to decrease the effect of non-uniqueness and to improve imaging. This workflow uses petrophysical measurements to constrain the values retrieved by geophysical inversion. Geological modelling is used to define petrophysical constraints spatially and to provide starting models. We integrate the different sources of information in a Bayesian framework that quantitatively unifies geological modelling, petrophysical measurements, and geological data. It accounts for the levels of prior knowledge related to the various sources of information. Inversion modifies the model accordingly to honor the different datasets. This methodology was tested using synthetic dataset in order to validate the methodology and to assess its robustness for gravity and magnetic data. The results showed that the use of petrophysical constraints during inversion increase constrains in inverted models. Prior structural information from geological modelling allows for better retrieval of the geometry of geological structure. Overall, the integration of the different constraints reduce model misfit and provides geologically consistent geometries.

Introduction

In recent years, the integration of data from diverse geoscientific disciplines has gained importance in resource exploration and production. Increasingly challenging scenarios require us to take advantage of the synergies offered by this diversity and to reduce the risk of costly development of non-economic deposits and reservoirs. Geology is used as a means to constrain geophysical inversion and techniques for the joint inversion of several datasets have been developed.

Previous studies have developed joint inversion techniques focusing on structural constraints to enforce structural similarity between the different models (Gallardo and Mejia, 2003; Colonobe and De Stefano, 2007). Others studies focused on the use of constitutive petrophysical laws to link the different domains (Gao et al., 2012). More recently, Sun and Li (2012, 2013) have introduced clustering algorithms as a means to enforce similarities between values in the inverted model and petrophysical data. Zhang and Revi (2015) integrate geology as a source of prior information for joint inversion. However, while these approaches take advantage of the links between the different disciplines, integration can be pushed further. In this abstract we introduce and test a workflow where statistical geological modelling is combined with petrophysical data to constrain geophysical inversion.

We apply the workflow to gravity and magnetic inversion, both of which are known to be affected by non-uniqueness. We constrain the joint inversion using petrophysical information in a similar way to the clustering approach introduced by Sun and Li (2012) and further the method by integrating prior geological information. Conditioned petrophysical constraints are generated using surface measurements and geological modelling. The quantitative use of geology to constrain geophysical inversion is inspired from concepts developed by Bosch (1999). We formulate the problem in a Bayesian framework to account for the uncertainty carried by petrophysical measurements, geological models and geological data. In this framework we use geometrical statistical geological modelling to generate a probabilistic petrophysical model.

In the joint inversion workflow constrained single domain inversions are performed first. The petrophysical constraints we apply can either be conditioned by geological modelling or derived from petrophysical measurements only. The results of single domain inversions are then used as a source of prior information for joint inversion. Running single inversion first is useful to obtain improved starting models for joint inversion and to constrain it further. The petrophysical constraints are calculated in the same way for joint inversion and single domain inversion. The workflow results in one model set obtained from single domain inversion (intermediate results) and one model set obtained from joint inversion (final result).

The workflow as applied to gravity and magnetic data is summarised in Figure 1.

Figure 1: integrated joint inversion workflow: illustration of the interaction between single domain inversion, geological modelling and petrophysical data as sources of information. (1) and (2) are the two sets of constrained inversion results the workflow provides. (1) relates to single domain inversion, (2) relates to joint inversion.
Impact of uncertain geology in constrained geophysical inversion

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SUMMARY

The integration of geological modelling, petrophysics and geophysics in a single inversion scheme is a complex and powerful strategy for solving challenges faced in geoscientific resource exploration. Probabilistic geological modelling and geophysical inversion are non-linear processes that show various degrees of sensitivity to uncertainty in input measurements. Using field geological measurements from the Mansfield area (Victoria, Australia) and synthetic geophysical data, we present a synthetic case study investigating the impact of geological uncertainty on constrained joint geophysical inversion. We investigate the influence of uncertain geological models on geologically constrained inversion through a sensitivity analysis to uncertainty in orientation data. Probabilistic geological models used to define constraints for geophysical joint inversion are obtained through a Monte-Carlo based uncertainty estimation (MCUE) method. We simulate a broad range of possible cases through a parameter sweep on uncertainty levels in geological models to provide a reference for practitioners. The analysis and comparison of the results at varying uncertainty levels show that results can be grouped into two main categories: The highest uncertainty levels, significant portions of the models retain the characteristic features of geologically unconstrained inversions. Meanwhile, below a threshold in uncertainty level, inversion benefits from the interaction of geophysical data and geologically conditioned constraints. In such cases, inverted models are improved compared to both the geological model alone and geologically unconstrained inversion. The conclusion of this work is that knowledge of this threshold is critical for the interpretation of results and decision making because it indicates whether the datasets provide enough information to take advantage of the complementarities between geological modelling and geophysical inversion. Knowledge of this threshold can also support decision making pertaining to inversion strategies and geological field data collection.

Key words: inversion, geophysical integration, sensitivity analysis, geological modelling

INTRODUCTION

In the past decade, the integration of different geophysical techniques has been of growing importance in geophysical resource exploration due to the need to exploit complementarities between exploration techniques in increasingly challenging scenarios. Previous studies have focused on joint inversion techniques using constraints enforcing structural similarity between the different models (Galard and Mejia, 2003; Colomb and De Stefano, 2007), or the use of constitutive petrophysical laws to link the different domains (Gao et al., 2012). More recently, Sun and Li (2012, 2016) have introduced clustering algorithms as a means of enforcing similarities between the inverted model and prior geophysical data. Zhang and Revil (2015), and more recently Biondi et al. (2017) and Giraud et al. (2016 and 2017) integrate petrophysics and geology in joint inversion and demonstrate the advantages of integration and joint inversion. However, even if the goal of the aforementioned methods is to obtain better-constrained models, little work has been done to quantify the impact of uncertainty in non-geophysical sources of information used to derive constraints accounting for geological information (Reid et al., 2013).

In this extended abstract, we present a study of the sensitivity of integrated geophysical inversion to uncertainty in geological measurements. Using quality and similarity indicators, we characterize the response of inverted models to varying geological uncertainty. Knowledge of the dependency of constrained inversion to the uncertainty of input geological data is key to guide geoscientists during inverse modelling interpretation, survey design or project management. In this study, we first introduce the inverse modelling approach in three steps: (i) the objective function, (ii) how the probabilistic geological model (PGM) is obtained and (iii) how it is used to condition petrophysical constraints. In the second section, we introduce our synthetic case study. The third and last section presents and illustrates the findings of the study.

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Inverse Problem Resolution Using Geologically Conditioned Gradient-Based Regularization – Application to the Yerrida Bas

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Summary

The qualitative integration of geological and geophysical data is a useful approach to constrain inversion that aims to improve interpretation and to reduce the geophysical data misfit. Here, we introduce an inversion approach that incorporates probabilistic geological information into geophysical inversion in the absence of the data necessary to derive petrophysical constraints. We develop the local conditioning of a minimum-gradient regularization function that utilizes statistical information from a Probabilistic Geological Model (PGM) which is derived from Monte-Carlo simulations perturbing field geological measurements. The use of the PGM allows us to support model updates in geologically uncertain areas while promoting consistent changes in well-constrained portions of the model. The methodology is applied using dip, strike and orientation measurements and gravity data acquired in the Yerrida Basin. The results obtained are characterised by (i) higher density contrast and inverted models that are easier to interpret and, (ii) an improved geophysical data fit. We conclude that by allowing inversion to update the model more freely in geologically uncertain areas, our methodology is capable of focusing inversion and to reduce interpretation uncertainty.
Appendix B

B.1 L-surfaces for hyperparameter estimation

Figure B 1. L-surfaces for hyperparameter estimation.

B.2 Complete set of inversion results

Density contrast

Figure B 2. Set of inverted density contrast models.
Magnetic susceptibility

Figure B 3. Set of inverted magnetic susceptibility models.

Differences between true and inverted density contrast

Figure B 4. Set of calculated differences between true and inverted density contrast models.
Differences between true and inverted magnetic susceptibility

Figure B 5. Set of calculated differences between true and inverted magnetic susceptibility models.

Recovered lithological models

Figure B 6. Set of retrieved lithological models.
Appendix C

This Appendix introduces the proof-of-concept of the method proposed in Chapter 4 through an idealized case study illustrating the potential of the proposed inverse modelling scheme to ameliorate inversion results and to reduce interpretation uncertainty. We use the same 3D density contrast model as (Giraud et al. 2017), which is obtained using the structural framework and PGM of (Pakyuz-Charrier et al. 2018). The short presentation of the model below and the analysis of results provides essential information and support about the proof-of-concept of the methodology used in the paper.

C.1 Synthetic survey setup

The 3D unperturbed geological model was generated from contact (interface points) and surface orientation (foliations) field measurements collected in the Mansfield area (Victoria, Australia). It presents a Carboniferous mudstone-sandstone basin oriented N170, abutting a faulted contact with a folded ultramafic basement to the South-West. Model complexity was artificially increased through the addition of a North-South fault and of a mafic intrusion.

The reference density contrast model (Figure C1a) was obtained assigning density contrasts consistently with the structural setting of the unperturbed model, assuming a flat topography. Density contrasts of 0 and 100 kg.m$^{-3}$ were assigned to the upper and lower basin lithotypes, respectively. Mafic rocks were assigned a density contrast of 200 kg.m$^{-3}$ while the density contrast of the ultramafic basement was set to 300 kg.m$^{-3}$.

MCUE perturbations of the reference model were performed using standard measurement uncertainty values recommended by metrological studies as reported by (Allmendinger, Siron, and Scott 2017; Novakova and Pavlis 2017) generating a series of 300 models subsequently combined into a PGM. The resulting volume representing the $W_H$ values calculated from this PGM in each cell of the model as per Equation (4.3) is show in Figure C1b.
Figure C1. Reference model and $W_H$ values used for local regularization conditioning. (a) Unperturbed reference model with density contrast value, (b) uncertainty values used for local regularization conditioning.

C.2 Comparison of inversion results

To assess the impact of local conditioning of the regularization function, we compare inversions using non-conditioned (Figure C2a) and locally conditioned (Figure C2b) regularization function, respectively. Please note that, simulating the absence of prior petrophysical information, a homogenous starting model set to 0 kg.m$^{-3}$ was used in both cases.
Besides qualitative visual comparison of the models, we interpret inversion results through the commonly used model and data root-mean-square error (RMSE). We evaluate the geometrical similarity between inverted and true model through the Bravais-Pearson correlation (also often called ‘linear correlation coefficient’) between their gradients (Table C1).

Comparison of the reference model (Figure C1a) with inversion results in Figure C2a and Figure C2b shows that while the structures in shallowest part of the model are well retrieved in both cases, it appears that they are considerably better recovered through usage of conditioned regularization overall (Figure C2b). The guiding effect of $\mathbf{W}_H$ is visible in Figure C2b where the main structures at depth follow the general features of the conditioning volume (Figure C1b). Moreover, in order to minimize the conditioned regularization constraint simultaneously to data misfit, inversion was driven to accommodate inverted model values (Figure C2b) such that they are closer to the causative model (Figure C1a) than without conditioning (Figure C2a). This leads to reduced model RMSE on one hand, and data RMSE on the other hand (Table C1). This reduction in data RMSE can also be explained by the relaxation of the constraints in several
portions of the model, thus increasing the degree of liberty to accommodate the model towards lower data misfit. Importantly, the Bravais-Pearson correlation between the inverted and reference model gradients is nearly three times higher when information from information entropy is used, which indicates that local conditioning of the regularization function also allows for significantly better retrieval of the causative bodies’ (e.g., true model) structural features.

From these observations, we conclude that the application of the local conditioning scheme can fulfill the objectives of data integration in inversion as it is capable to recover models that are closer to the causative bodies and easier to interpret, while potentially providing reduced data misfit.

Table C1. Indicators for comparison of inversion results in terms of model, data, and structure.

<table>
<thead>
<tr>
<th></th>
<th>Model RMSE (kg.m³)</th>
<th>Data RMSE (m.s²)</th>
<th>Bravais-Pearson correlation between gradients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-conditioned</td>
<td>74.66</td>
<td>2.38 × 10⁻⁹</td>
<td>0.18</td>
</tr>
<tr>
<td>conditioned</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>regularization</td>
<td>53.05</td>
<td>7.44 × 10⁻¹⁰</td>
<td>0.53</td>
</tr>
</tbody>
</table>

C.3 Data misfit maps from inversion in the Yerrida Basin

Figure C3 below relates to the analysis of data misfit in Section 4.4.3.1 through the plot of the data misfit maps for the non-conditioned and conditioned cases (Figure C3d and Figure C3h, respectively). It is complemented by the corresponding plots of starting (Figure C3a and Figure C3e), observed (Figure C3b and Figure C3f), and calculated data (Figure C3c and Figure C3h). Note that Figure C3c and Figure C3g show little visual differences, and that Figure C3d and Figure C3h exhibit similar features while showing limited coherent signal.
Figure C3. Comparison of input and output geophysical data. (a) and (e) show data calculated from the starting model, (b) and (f) input measurements, (c) and (g) data calculated from the inverted model, and (d) and (h) the absolute value of the difference of the misfit between the observed and calculated data. (a)-(d) (e.g., first line) and (e)-(h) (e.g., second line) correspond to the non-conditioned and conditioned cases, respectively.