FORWARD MODELING AND INVERSION OF
POTENTIAL FIELD DATA USING PARTIAL
DIFFERENTIAL EQUATIONS

by

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A thesis submitted to the Faculty and the Board of Trustees of the Colorado School of Mines in partial fulfillment of the requirements for the degree of Master of Science (Geophysics).

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ABSTRACT

The aim of geophysical inversion is to provide a feasible subsurface structure or distribution of physical properties of the Earth. There must be a forward modeling to predict the observations given a distribution of such properties. Standard forward modeling methods for potential fields are based on the integral equations. For large-scale or high-resolution data, however, forward models based on partial differential equations (PDE) are more efficient. These methods have been proven to be faster and less memory intensive than the standard approach. In the present work, I extend the PDE based modeling methods for both gravity and magnetics.

The gravity field from a density distribution can be computed through an indirect formulation by first solving Poisson’s equation for the gravitational potential, and then numerically differentiating the potential to obtain the field. Alternatively, given the gradient of a density distribution one may directly solve the Poisson’s equation of the gravity field, which does not require differentiation of the potential. I investigate this formulation and study its relative advantages. The direct formulation has the same degree of accuracy as the indirect formulation. Based on this result, the direct formulation can be used in inversion algorithms to recover derivatives of the density distribution as a mean to image density boundaries.

Like gravity, magnetic fields are described by Poisson’s equation. I formulate the PDE solution of the magnetic problem by including anisotropy in the forward calculation of the magnetic field. I compare the forward modeling algorithm against analytical solutions of simple bodies and against the integral equation domain solution. I find that the PDE-based forward model can accurately predict the magnetic signal of anisotropic materials.
To conclude the study, I use PDE based forward methods to invert gravity and magnetic data collected over a copper-lead zinc deposit in northern New Brunswick, Canada. The solutions are consistent with other inversion algorithms that use the standard integral equation approach. The inversion of the magnetic field is for isotropic susceptibility only. Inversion which takes into account susceptibility anisotropy requires further development of the inversion algorithm which is beyond the scope of the present work.
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ACKNOWLEDGMENTS

I would like to express my deepest gratitude to my research advisor, Professor Yaoguo Li, for his guidance, supportive encouragement, and useful critiques of my thesis work. I would also like to thank the members of my thesis committee, Professors Thomas Davis and Andrei Swidinsky, without whose knowledge and assistance this study would not have been successful. Special thanks to all members of CGEM for sharing their knowledge and ideas. I would like to express my gratitude and love to my family for their constant support throughout this time.
Gravity and magnetic fields, commonly called potential fields, have an important role in the studies of the Earth’s interior structure by sensing different physical properties of rocks; density and magnetic susceptibility respectively. This chapter provides the principal theoretical background concerning the forward model of potential fields. Then, I present a literature review of existing work and research objectives.

1.1 Theoretical background

Given a distribution of physical properties, the prediction of the variation in potential fields constitutes a forward problem. The reverse situation of determining the value of these properties using observations of the field corresponds to the inverse problem. The formulation of the forward problem contributes to the solution of the inverse problem. In potential field theory, the forward problem is typically modeled by integral equations of the first kind. The generic form is

$$\int_V G(r, r') s(r') \, dr' = F(r) \quad (1.1)$$

where $r$ is the position of the observer, $r'$ is the position of the volume element $dr$, $s(r')$ is the source, $F$ is the observed field and $G(r, r')$ is the Green’s function and represents the response of a point source. In the above equation, $F$ is unknown and $s$ and $G$ are given functions.

The forward problem can also be formulated in the partial differential equation (PDE) domain by solving Poisson’s equation

$$\nabla^2 U(r) = s(r) \quad (1.2)$$
where $U$ is a scalar potential and $s$ is a source function. The field is calculated from the gradient potential,

$$ F(r) = \nabla U(r) $$

(1.3)

In the literature one often sees $F(r) = -\nabla U(r)$. The plus or minus sign in front of equation 1.3 is a convention. Potential fields are conservatives fields, so how the source is moved from a reference point $r_{\text{ref}}$ (e.g. infinity) to $r$ is not important. Moving a test particle in the same direction as $F$ accumulates negative potential, while moving the test particle in the opposite direction as $F$ accumulates positive potential.

The forward modeling based on the integral equation requires the model to be discretized into a set of elementary volumes. The physical property is assumed constant within each volume. The field contribution from each volume is calculated using equation 1.1 and by the principle of superposition, the field at any point is approximated by summing the effects of all volumes. The limitation of this approach is that, for large data sets, and large-scale problems (i.e. more model cells), the computational cost of evaluating 1.1 can be high. In contrast, the essence of the numerical solution of the Poisson’s equation is the conversion from continuous functions and differential operators to the discrete counterparts, which converts the entire system into a sparse linear system of equations. The sparse structure of the linear solver requires significantly less storage than the dense matrices associated with the integral equation. Consequently, the computational cost of a PDE is not a strong function of the number of data points or number of model cells but instead it is controlled by the complexity of the linear solver $(A)$ used to obtain the potential May and Knepley [1, p. 5].

1.1.1 Gravity theory

The gravitational field of the Earth, $g$, is caused by its mass. If we integrate $g$ everywhere at some arbitrary surface, we obtain the flux of the gravity field. The gravitational flux is
proportional to the total mass $M$ enclose by the surface.

$$\oint_S \mathbf{g} \cdot dS = 4\pi M = 4\pi \gamma \int_V \rho \, dV$$

(1.4)

where $\gamma$ is the gravitational constant. Gravity is a conservative field, therefore

$$\mathbf{g}(\mathbf{r}) = \nabla U$$

(1.5)

Gravitational flux is a surface integral of the gravitational field over a closed surface. The surface integral is converted to volume integral using the Gauss’s theorem

$$\oint_S \mathbf{g} \cdot dS = \int_V \nabla \cdot \mathbf{g} \, dV = \int \nabla^2 U \, dV$$

(1.6)

Considering that the volume of integration is arbitrary, equations 1.4 and 1.6 yield

$$\nabla^2 U = 4\pi \gamma \rho$$

(1.7)

The potential satisfy zero Dirichlet boundary condition at infinity; that is

$$U = 0 \quad \text{at} \quad \mathbf{r} = \infty$$

(1.8)

At points external to the distribution of mass, the net flux of the gravitational field will be zero. At these points, the gravitational potential will satisfy Laplace’s equation $\nabla^2 U = 0$.

1.1.2 Magnetic theory

Magnetic surveys measure the local variation in the Earth’s magnetic field. This variation is caused by induced magnetic fields due to lateral variations in the magnetic properties of the subsurface. Unlike gravity, isolated sources and sinks of the magnetic flux $\mathbf{B}$ do not exist; the elementary source is the dipole. Most of the field at the Earth’s surface is equivalent to that of a dipole inclined at about 11° to the Earth’s spin axis. For an enclosed surface outside the region that contains the source for the magnetic potential (i.e. Earth’s core), just as many field lines enter the surface as are leaving it. Hence, the total magnetic flux is zero.

$$\oint_S \mathbf{B} \cdot dS = 0$$

(1.9)
Using Gauss’s theorem, we find that the magnetic induction is divergence free

\[ \nabla \cdot \mathbf{B} = 0 \]  

(1.10)

In the presence of matter another important quantity is the magnetic field \( \mathbf{H} \). The associated constitute relationship is

\[ \mathbf{B} = \mu \mathbf{H} \]  

(1.11)

where \( \mu \) is the magnetic permeability and is related to susceptibility, \( \kappa \) as

\[ \mu = \mu_0 (1 + \kappa) \]  

(1.12)

where \( \mu_0 \) is the permeability in free space. In analogy to gravity, the magnetic field in a source free region is the gradient of a scalar magnetic potential \( \phi \)

\[ \mathbf{H} = \nabla \phi \]  

(1.13)

Replacing equations 1.11 and 1.13 into 1.10 we obtain that indeed

\[ \nabla \cdot \mu \nabla \phi = 0 \]  

(1.14)

Note that in free space (\( \mu = \mu_0 \)), equation 1.14 reduces to Laplace equation.

\[ \nabla^2 \phi = 0 \]  

(1.15)

Unlike 1.1, forward models based on equation 1.14 are valid for materials with susceptibilities of any magnitude and are also appropriate for modeling magnetic data with demagnetization effects in which the magnetic field scale non-linearly with susceptibility.

1.2 Review of existing work

The use of gravity forward models based on equation 1.7 have so far been demonstrated to be faster and to produce more accurate results than the integral equation approach. In Cai and Wang [2], a finite element method was used to solve Poisson’s equation using Robin boundary conditions, which consist of approximating the far field gravitational attraction on the mesh boundaries. This approximation yielded a smaller error that setting \( U = 0 \) at the boundary. In contrast, Farquharson and Mosher [3] solved equation 1.7 using a finite differ-
ence discretization, where the boundaries $U = 0$ at infinity were approximated by ensuring that the model boundaries are ”far” from the density, which in their work meant six times larger than the side length of the anomaly.

On the other hand, Eldad Haber et al. [4] presented a fourth-order finite volume differential-equation solution for gravity gradiometry data. The second-order discretization leads to first order accuracy while the fourth-order discretization yields second-order accuracy. Alternatively, one may formulate Poisson’s equation directly for components of the gravity field and gravity gradient tensor, which does not require the numerical differentiation of the potential but instead it requires differentiation of the density function. This formulation was first introduced by Howell [5] and is referred to as the ”direct solution”. In Howell [5], a finite volume and finite difference method was use to compute just the vertical component of the gravity field. The direct formulation can be useful for two reasons. First, at large distances, the gravity field decays more rapidly ($1/r^2$) than the potential itself ($1/r$), so the direct solution would require a smaller mesh in order to approximate the boundary conditions. Second, it directly relates measurements of the gravity field with spatial variation of density in the subsurface.

For the magnetic problem, Lelièvre and Oldenburg [6] developed a solution of 1.14 using a finite volume discretization restricted to isotropic susceptibilities. The finite volume solution was successfully tested with inversions of synthetic data for simple bodies and inversion of field data collected over a planted UXO target.

1.3 Research objectives and thesis outline

The work in this thesis has three purposes. First, to compute gravity and gravity gradients from the Poisson’s equation which directly solves for scalar components of the gravitational field. Second, to extend the current PDE-based magnetic forward methods to include
the effect of anisotropic susceptibility. Third, to demonstrate the effectiveness of the PDE-based magnetic forward method through an inversion of a field data set.

The thesis is structured as the following. Chapter 2 present the direct solution of Poisson’s equation for scalar components of the gravitational acceleration and components of the gravity gradient tensor using a finite volume method (FVM). Chapter 3 discusses the incorporation of anisotropic susceptibility in the current finite volume solution of Poisson’s equation for magnetics. Chapter 4 discussed the use of forward methods to invert gravity and magnetic data collected over a cooper-lead zinc deposit in northern New Brunswick, Canada. The results, merits, and limitations of the thesis work are discussed in Chapter 5.
CHAPTER 2
FORWARD MODELING OF GRAVITY AND GRAVITY GRADIENTS

The gravity method is a geophysical technique that measures variations in the Earth’s gravitational field caused by variations in the density of the Earth’s subsurface. Similar to the gravity method, gravity gradiometry senses differences in the subsurface density from measurements of gravity gradients. A distribution of matter of density $\rho$ gives rise to a gravitational potential $\phi$ which satisfies Poisson’s equation $\nabla^2 \phi = -4\pi\gamma\rho$. The corresponding gravity field and gravity gradients can then be obtained from $\nabla \phi$ and $\nabla \nabla \phi$ respectively. A different approach to calculate the gravity field and gravity gradients is to start directly with Poisson’s equation for the gravity field. In this Chapter, this direct approach is described. The direct solution is achieved through a finite volume discretization.

2.1 Theory of the proposed method

Poisson’s equation for the gravity field is obtained by taking the derivative of both sides of equation 1.7

$$\nabla^2 g = -4\pi\gamma \nabla \rho$$  \hspace{1cm} (2.1)

Equation 2.1 can be split in three parts, one for each components of the gravity field

$$\nabla^2 g_x = -4\pi\gamma \frac{\partial \rho}{\partial x}$$  \hspace{1cm} (2.2a)

$$\nabla^2 g_y = -4\pi\gamma \frac{\partial \rho}{\partial y}$$  \hspace{1cm} (2.2b)

$$\nabla^2 g_z = -4\pi\gamma \frac{\partial \rho}{\partial z}$$  \hspace{1cm} (2.2c)
The rate of change of the gravity vector in all three perpendicular directions gives rise to a gravity gradient tensor,

\[
\begin{bmatrix}
T_{xx} & T_{xy} & T_{xz} \\
T_{yx} & T_{yy} & T_{yz} \\
T_{zx} & T_{zy} & T_{zz}
\end{bmatrix}
\]

\[
\begin{bmatrix}
\tau_1 \\
\tau_2 \\
\tau_3
\end{bmatrix}
\]

\[
= \begin{bmatrix}
\frac{\partial g_x}{\partial x} & \frac{\partial g_x}{\partial y} & \frac{\partial g_x}{\partial z} \\
\frac{\partial g_y}{\partial x} & \frac{\partial g_y}{\partial y} & \frac{\partial g_y}{\partial z} \\
\frac{\partial g_z}{\partial x} & \frac{\partial g_z}{\partial y} & \frac{\partial g_z}{\partial z}
\end{bmatrix}
\]  \quad (2.3)

here, \( \tau_1, \tau_2, \tau_3 \) represent the first, second and third column of the gravity gradient tensor respectively. Because the gravity gradient tensor is symmetric, its columns can be written as

\[ \tau_1 = \nabla g_x \]  \quad (2.4a)

\[ \tau_2 = \nabla g_y \]  \quad (2.4b)

\[ \tau_3 = \nabla g_z \]  \quad (2.4c)

There are numerous ways to numerically solve 2.1. To approximate the gravity field arising from a density distribution, traditional numerical solutions solve first for the gravitational potential. The region of interest is divided into many cells. Each cell is chosen small enough that the density can be assumed constant within it. Once the potential is determined the gravity field is determined by numerical differentiation of the potential. Unlike traditional numerical solution, the direct solution requires the taking the derivative of the density function. The challenge arises at the cell boundaries where the density function is not continuous and its derivative is not define at that point. This issue can be address by solving the week form of 2.1. In a week formulation of a PDE, the differentiability of the approximated function is less strict than the PDE.
2.2 Finite Volume Discretization

The finite volume method (FV) is the discretization of the weak form of a PDE expressing the conservation of quantities, such as the conservation of mass or “magnetic charge”. The weak form of a PDE is the integration of the PDE over a small volume. Thanks to the divergence theorem, the volume integrals are transformed into surface integrals. Volume integral terms describe what is stored inside the domains or added by sources, while surface integrals describe the interaction on the functions with neighboring volumes or an external environment. Weak formulation of a PDE only imposes continuity at the interfaces of the small volume and reduces the differentiability requirements on the approximation functions. The FVM involves the following steps:

- Decomposition of the problem domain into control volumes or grid design.
- Formulation of the integral form of a PDE for each control volume.
- Approximation of integrals by numerical integration.
- Approximation of function values and derivatives by interpolation with grid nodes.
- Assembling and solution of discrete algebraic system.

2.2.1 Grid design

For the discretization of the PDE, I use the right hand side coordinate system: the positive x in a northerly direction, y easterly and z axes vertically downward. The model region is discretized into \( n_x \) cells in the x-direction, \( n_y \) cells in the y-direction and \( n_z \) cells in the z-direction. The total number of cells is \( nc = n_x \times n_y \times n_z \). A single cell used in the discretization is shown in Figure 2.1. The density is assumed constant within each cell, \( \rho_n \), and the potentials are placed at the cell centers. The node coordinates in each direction are:

\[
x_i : x_1, x_2, \ldots, x_{n_x+1} \tag{2.5}
\]
\[
y_j : y_1, y_2, \ldots, y_{n_y+1} \tag{2.6}
\]
\[
z_k : z_1, z_2, \ldots, y_{n_z+1} \tag{2.7}
\]
The cell lengths in three directions are denoted respectively as

\begin{align}
  h_{x_i} &= x_{i+1} - x_i \quad (2.9) \\
  h_{y_j} &= y_{j+1} - y_j \quad (2.10) \\
  h_{z_k} &= z_{k+1} - z_k \quad (2.11)
\end{align}

The cell center coordinates in each direction are denoted

\begin{align}
  x_{i+1/2} : & x_{1+1/2}, x_{2+1/2}, \ldots, x_{n_x+1/2} \\  y_{j+1/2} : & y_{1+1/2}, y_{2+1/2}, \ldots, y_{n_y+1/2} \\  z_{k+1/2} : & z_{1+1/2}, z_{2+1/2}, \ldots, y_{n_z+1/2}
\end{align}

The distances from adjacent cell centers are denoted by

\begin{align}
  \Delta x_i &= x_{i+3/2} - x_{i+1/2} \quad (2.17) \\
  \Delta y_j &= y_{j+3/2} - y_{j+1/2} \quad (2.18) \\
  \Delta z_k &= z_{k+3/2} - z_{k+1/2} \quad (2.19)
\end{align}
The cells are numbered so that the row number changes fastest, then the column number and the layer number changes the slowest. The gravity components are assigned to the centers of cell faces. There are \((n_x + 1)n_y n_z g^x_i\) values on the x-faces (i.e. faces with normal vectors in the +x or x direction), \(n_x(n_y + 1)n_z g^y_j\) values on the y-faces and \(n_x n_y(n_z + 1) g^z_k\) values on the z-faces. This gives \(nf = (n_x + 1)n_y n_z + n_x(n_y + 1)n_z + n_x n_y(n_z + 1)\) flux values in total. The nf unknown flux values are divided into three sets

\[
\begin{align*}
  g^x_i &: g^x_1, g^x_2, \ldots, g^x_{n_x+1} \quad (2.21) \\
  g^y_j &: g^y_1, g^y_2, \ldots, g^y_{n_y+1} \quad (2.22) \\
  g^z_k &: g^z_1, g^z_2, \ldots, g^z_{n_z+1} \quad (2.23)
\end{align*}
\]

The location of the gravity field values as in Figure 2.1 implies continuity of normal \(g\) across cell interfaces (i.e. \(g_{z1} \cdot \hat{n} = g_{z2} \cdot \hat{n}\)).

### 2.2.2 Formulation and solution of integral equations

The equation to discretized are:

\[
\int_{V^D} \nabla \cdot \tau_3 dv = -4\pi \gamma \int_{V^D} \frac{\partial \rho}{\partial z} dv \quad (2.25)
\]

and

\[
\int_{V^D} \tau_3 dv = \int_{V^D} \nabla g_z dv \quad (2.26)
\]

The volumes of integration \(V^D\) are the dual grid cells defined so that \(g_z\) are at their centers (refer to Figure 2.2). The positioning of discrete variables in the dual mesh results in \(\nabla g_z\) and \(\tau_3\) being defined at the same points in space as required by equation 2.4c. Every dual cell contains cells of constant density values (the “primary mesh”) surrounding each discrete gravity field quantity. As such, this requires the addition of half of a layer of padding cell to the primary mesh, all of which have zero density. The notation of nodes, cell centers, cell lengths and distances between cell centers are the same as describe for the primary mesh. The gravity gradient values \(T^{xz}_{i+1,j+1/2,k+1/2}, T^{yz}_{i,j+1/2,k+1/2}, T^{g_z}_{i+1/2,j+1,k+1/2}\)
\( T_{yz}^{i+1/2,j+1/2,k+1/2}, T_{zz}^{i+1/2,j+1/2,k+1}, T_{zz}^{i+1/2,j+1/2,k} \) are assigned at the center of the dual cell faces.

Figure 2.2: A dual cell for the direct solution of \( g_z \)

**Discretization of the divergence**

Consider the left hand side of equation 2.25. The divergence theorem transforms the volume integral into a surface integral. The surface integral is then approximated by the midpoint rule.

\[
\int_{V_D} \nabla \cdot \boldsymbol{\tau}_3 \, dv = \int_{S_D} \boldsymbol{\tau}_3 \cdot \mathbf{n} \, dS \approx (T_{xz}^{i+1,j+1/2,k+1/2} - T_{xz}^{i,j+1/2,k+1/2}) h y_j h z_k \\
+ (T_{yz}^{i+1/2,j+1,k+1/2} - T_{yz}^{i,j+1,k+1/2}) h x_i h z_k \\
+ (T_{zz}^{i+1/2,j+1/2,k+1} - T_{zz}^{i+1/2,j+1/2,k}) h x_i h y_j
\]

(2.27)
Now consider the right hand side of 2.25. The limits of integration correspond to the centers of the primary mesh, that is where the density function has a constant value.

\[
\int_{V_{i,j,k}} \frac{\partial \rho}{\partial z} \, dv = \int_{x_{i-1/2}}^{x_{i+1/2}} dy \int_{y_{j-1/2}}^{y_{j+1/2}} dz \int_{z_{k}}^{z_{k+1}} \frac{\partial \rho}{\partial z} \, dz = \left( \rho_{i+1/2,j+1/2,k+1} - \rho_{i+1/2,j+1/2,k-1} \right) hx_i hy_j
\]

(2.28)

When all such equations (i.e. one for each dual cell) are combined, the matrix-vector equation obtained is

\[
[D_x \ D_y \ D_z] \begin{bmatrix} T_{xx} \\ T_{yx} \\ T_{zz} \end{bmatrix} = D_z m
\]

(2.29)

\[
D \ \tau_3 = D_z m
\]

(2.30)

Here, \( D \) is the divergence matrix; \( \tau_3 \) holds the unknown gravity gradient values and the vector \( m \) is a vector of length \( n_c \) that contains density values scaled by \( 4\pi\gamma \). The matrices \( D_x, D_y \) and \( D_z \) are as follows.

\[
D_x = \begin{bmatrix}
D_x & D_x & \cdots \\
D_x & D_x & \ddots \\
\vdots & \ddots & \ddots & \ddots \\
D_x & \cdots & \cdots & \cdots & D_x
\end{bmatrix}
\]

\[
D_x = \begin{pmatrix}
-hx_1^{-1} & hx_1^{-1} & hx_2^{-1} & \cdots & hx_n^{-1} \\
-hx_2^{-1} & hx_2^{-1} & hx_3^{-1} & \cdots & hx_{n+1}^{-1} \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
-hx_n^{-1} & hx_n^{-1} & hx_{n+1}^{-1} & \cdots & \cdots
\end{pmatrix}
\]

\[
D_x \text{ is } n_x \text{ by } (n_x+1) \text{. Hence, } D_x \text{ is } n_c \text{ by } n_f_x \text{ where } n_c = n_x n_y n_z \text{ and } n_f_x = (n_x+1)n_y n_z.
\]
\[ \mathbf{D}_y = \begin{bmatrix} \mathbf{D}_y \\ & \ddots \\ & & \mathbf{D}_y \end{bmatrix} \]

\[ \mathbf{D}_y = \begin{bmatrix} -h_{y_1}^{-1} & \cdots & h_{y_1}^{-1} \\ -h_{y_1}^{-1} & \ddots & \ddots \\ \vdots & \ddots & \ddots \\ -h_{y_{n_y}}^{-1} & \cdots & h_{y_{n_y}}^{-1} \end{bmatrix} \]

\[ \mathbf{D}_y \text{ is } n_x n_y \text{ by } n_x(n_y + 1). \text{ Hence, } \mathbf{D}_y \text{ is } n_c \text{ by } n_f = n_x(n_y + 1)n_z. \]

\[ \mathbf{D}_z = \begin{bmatrix} -h_{z_1}^{-1} & \cdots & h_{z_1}^{-1} \\ -h_{z_1}^{-1} & \ddots & \ddots \\ \vdots & \ddots & \ddots \\ -h_{z_{n_z}}^{-1} & \cdots & h_{z_{n_z}}^{-1} \end{bmatrix} \]

\[ \mathbf{D}_z \text{ is } n_x n_y \text{ by } n_x(n_y + 1) \text{ columns.} \]

\[ \mathbf{D}_z \text{ is } n_x n_y n_z \text{ rows.} \]

Discretization of the gradient

Equation 2.4c is first split into three parts, each corresponding to a different Cartesian direction:

\[ T_{xz} = \frac{\partial g_z}{\partial x} \]  

\[ T_{yz} = \frac{\partial g_z}{\partial y} \]
Consider 2.34a. The volume of integration for this equation runs across a cell face with normal in the x-direction so that an unknown $T_{xz}$ is at the center of the integration volume. The integral is

$$
\int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j}}^{y_{j+1}} \int_{z_{k}}^{z_{k+1}} T_{xz} dz dy dx = \int_{x_{i-1/2}}^{x_{i+1/2}} \int_{y_{j}}^{y_{j+1}} \int_{z_{k}}^{z_{k+1}} \frac{\partial g_z}{\partial x} dz dy dx
$$

(2.35)

Assuming that $T_{xz}$ is constant over the integration volume leads to

$$
T_{xz}^{x_{i,j+1/2,k+1/2}} = \int_{y_{j}}^{y_{j+1}} dy \int_{z_{k}}^{z_{k+1}} dz \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial g_z}{\partial x} dx
$$

(2.36)

Dividing by the integration volume yields

$$
T_{xz}^{x_{i,j+1/2,k+1/2}} \approx \frac{g_z^{i+1/2,j+1/2,k+1/2} - g_z^{i-1/2,j+1/2,k+1/2}}{\Delta x_i}
$$

(2.37)

When 2.34b and 2.34c are discretized in a similar fashion, the following system is obtained:

$$
\begin{bmatrix}
T_{xz} \\
T_{yz} \\
T_{zz}
\end{bmatrix}
= \begin{bmatrix}
G_x \\
G_y \\
G_z
\end{bmatrix}
\begin{bmatrix}
g_x \\
g_y \\
g_z
\end{bmatrix}
$$

(2.38)

The matrices $G_x$, $G_y$ and $G_z$ are as follows:

$$
G_x = \begin{bmatrix}
G_x & \cdots & \cdots \\
G_x & \cdots & \cdots \\
G_x & \cdots & \cdots \\
\Delta x_1^{-1} & -\Delta x_1^{-1} & \Delta x_1^{-1} \\
-\Delta x_1^{-1} & \Delta x_1^{-1} & -\Delta x_1^{-1} \\
\cdots & \cdots & \cdots \\
-\Delta x_{n_x}^{-1} & \Delta x_{n_x}^{-1} & -\Delta x_{n_x}^{-1}
\end{bmatrix}
$$

(2.39)

\[ (n_x + 1) \text{ rows, } n_x \text{ columns} \]
\( G_z \) is \((n_x + 1)\) by \(n_x\). Hence, \( D_x \) is \(nf_x\) by \(nc\).

\[ G_y = \begin{bmatrix} G_y & G_y & \cdots & G_y \end{bmatrix} \]

\[ G_y = \begin{pmatrix} \Delta y_1^{-1} & \cdots & \cdots & \cdots \\ \vdots & \ddots & \ddots & \ddots \\ -\Delta y_1^{-1} & \cdots & \Delta y_1^{-1} & \cdots \\ \vdots & \ddots & \ddots & \ddots \\ -\Delta y_{n_y-1} & \cdots & \Delta y_{n_y-1} & \cdots \\ \vdots & \ddots & \ddots & \ddots \\ -\Delta y_{n_y} & \cdots & \Delta y_{n_y} & \cdots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix} \]

\[ n_x(n_y + 1) \text{ rows} \]

\[ n_xn_y \text{ columns} \]

(2.40)

\( G_y \) is \(n_x(n_y + 1)\) by \(n_xn_y\). Hence, \( G_y \) is \(nf_y\) by \(nc\).

\[ G_z = \begin{pmatrix} \Delta z_1^{-1} & \cdots & \cdots & \cdots \\ \vdots & \ddots & \ddots & \ddots \\ -\Delta z_1^{-1} & \cdots & \Delta z_1^{-1} & \cdots \\ \vdots & \ddots & \ddots & \ddots \\ -\Delta z_{n_z-1} & \cdots & \Delta z_{n_z-1} & \cdots \\ \vdots & \ddots & \ddots & \ddots \\ -\Delta z_{n_z} & \cdots & \Delta z_{n_z} & \cdots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix} \]

\[ n_xn_y(n_z + 1) \text{ rows} \]

\[ n_xn_yn_z \text{ columns} \]

(2.41)

### 2.3 Boundary conditions

There are an infinite number of functions that satisfy 2.1 and the appropriate solution is selected by specifying the appropriate boundary conditions. The potential \( \phi \) satisfies homo-
geneous Dirichlet boundary conditions at infinity. Farquharson and Mosher [3] approximated this by ensuring that the model boundaries are far from the density anomaly. Here, I use a mixed boundary condition as proposed by Cai and Wang [2]. This boundary condition uses the asymptotic behavior of $\phi$ and $\frac{\partial \phi}{\partial n}$ at large distance from the center source mass. The gravitational potential at a point $(x, y, z)$ due to a single point of mass located at $(x', y', z')$ is

$$\phi(x, y, z) = \frac{c}{\sqrt{(x - x')^2 + (y - y')^2 + (z - z')^2}} = \frac{c}{r}$$

(2.42)

where $c$ is a constant, therefore,

$$\frac{\partial \phi}{\partial n} = -\frac{c}{r^2} \hat{r} \cdot \hat{n} = -\frac{\phi}{r} \hat{r} \cdot \hat{n}$$

(2.43)

where $\hat{n}$ is the outward normal vector of the grid boundary and $\frac{\partial}{\partial n} = \hat{n} \cdot \nabla$. Equation 2.43 can be rewritten as

$$\frac{\partial \phi}{\partial n} + \left( \frac{\hat{r} \cdot \hat{n}}{r} \right) \phi = 0$$

(2.44)

Now I define a new variable $\nu = x, y, z$. The derivative of 2.43 with respect to $\nu$ yield

$$\frac{\partial}{\partial \nu} \frac{\partial \phi}{\partial n} = -\left[ \frac{2\nu}{r^2} - \frac{1}{(\hat{r} \cdot \hat{n})} \frac{\partial}{\partial \nu} (\hat{r} \cdot \hat{n}) \right] \frac{\partial \phi}{\partial n}$$

(2.45)

which has the form

$$\frac{\partial}{\partial \nu} g_n + \alpha g_n = 0$$

(2.46)

with

$$\alpha = \frac{2\nu}{r^2} - \frac{1}{(\hat{r} \cdot \hat{n})} \frac{\partial}{\partial \nu} (\hat{r} \cdot \hat{n})$$

(2.47)

For example, let us consider the case for $g_z$. A cell on a grid boundary face with normal in the $x$-direction would produce an equation of the form

$$\frac{\partial}{\partial x} g_z + \alpha g_z = 0,$$

(2.48)
with
\[ \alpha = \frac{2x}{r^2} - \frac{1}{(\hat{n} \cdot \hat{z})} \frac{\partial}{\partial x}(\hat{n} \cdot \hat{z}) = \frac{3x}{r^2}. \]  
(2.49)

Similarly, a cell on a grid boundary face with normal in the y-direction would produce an equation of the form
\[ \frac{\partial}{\partial y} g_z + \frac{3y}{r^2} g_z = 0, \]  
(2.50)
and a cell on a grid boundary face with normal on the z-direction would produce an equation of the form
\[ \frac{\partial}{\partial z} g_z + \left( \frac{3z^2}{r^2} - \frac{1}{z} \right) g_z = 0, \]  
(2.51)

The implementation of the boundary condition is presented in Appendix B.

2.4 Discrete forward modelling equation

Combining equations 2.30 and 2.38, the forward modeling systems can be written as the linear system
\[ (A + F)g_z = m_z \]  
(2.52)
where \( A = DG \) is the Laplacian operator, \( F \) is the term associated with the far field boundary condition, \( g_z \) is a vector of discrete vertical component of the gravity field, \( m_z \) is the gradient of density model and has units of kg/m^4. The solution of the linear system of equation 2.52 requires a solver from linear algebra. The solver chosen was the Conjugate Gradient method (CG).

2.5 Synthetic example

Here I consider the numerical solutions of a synthetic dense cube and compare the results from those obtained by the closed form expression of Haaz [7] and by the indirect solution as proposed by Farquharson and Mosher [3]. Figure 2.3 shows the synthetic model used throughout the example and three vertical profiles along which I calculated the data. Three uniform grids were used containing \( 12^3 \), \( 24^3 \) and \( 60^3 \) cells. These contained central, uniform,
cubic bodies of $2^3$, $4^3$ and $10^3$ cells in volume respectively. All grids have equal side length of $L = 600$ m but different cell dimensions and as such, all three central cubes are of identical side length of $H = 100$ m, to which we assigned the density contrast, $\rho = 2000$ Kg/m$^3$. The model setup is identical to that used in Farquharson and Mosher [3].

2.5.1 Discretization error

Through the synthetic example, I compare the indirect solution (i.e. the solution of the Poisson’s equation followed my numerical differentiation) and the direct solution of the vertical component of the gravity field (i.e. the solution of the Poisson’s equation directly for the gravity field) on the basis of their discretization error. The discretization error or truncation error is the error inherent in discretization which arises from the finite resolution of the domain. The order of accuracy quantifies the rate of convergence of a numerical approximation of a differential equation to the exact solution. A numerical solution to a
differential equation is said to be $n$th-order accurate if the error, $E$, is proportional to the step-size $h$ to the $n^{th}$ power LeVeque [8].

$$E(h) \propto C h^n$$  \hspace{1cm} (2.53)

The error in the vertical component of the gravity field using $L_2$ norm is

$$E_{2}^{FV} = \| g_{z}^{exact} - g_{z}^{Indirect} \|_2^2$$  \hspace{1cm} (2.54a)

$$E_{2}^{Direct} = \| g_{z}^{exact} - g_{z}^{Direct} \|_2^2$$  \hspace{1cm} (2.54b)

where $g_{z}^{exact}$ is the exact gravity computed via the analytic solution from Haaz [7] and $g_{z}^{FV-Indirect}$ and $g_{z}^{FV-Direct}$ is the gravity field approximated via the indirect and direct solution respectively along the profile $x = 250$ m (Figure 2.3). The discretization error as a function of mesh size is shown in Figure 2.7. The order of accuracy quantifies the rate of convergence of a numerical approximation to the exact solution. As seen in Figure 2.7, both, $E_{2}^{Indirect}$ and $E_{2}^{Direct}$ are proportional to the mesh resolution $h$ to the $n^{th}$ power 2. In other words, both methods produce the same errors and have the same second order convergence rate.

![Figure 2.4: $L_2$ error of the gravity field computed via the direct and indirect solutions](image-url)
Similarly, the discretization error in $T_{zz}$ as a function of the mesh resolution $h$ is shown in Figure 2.5. The indirect and direct solutions lead to first order accuracy when computing. Note that second order accuracy is achieved for cell sizes less that 10 m.

![Figure 2.5: $L_2$ error of $T_{zz}$ computed via the direct and indirect solutions.](image)

### 2.5.2 Effect of the boundary condition

Here we show the effect of the far field approximation in the boundary condition in a grid containing $60^3$ cells. Figure 2.6 and Figure 2.8 show $g_z$ and $T_{zz}$ respectively along the three profiles: $x = 150$ m, $x = 250$ m and $x = 300$ m (Figure 2.3). In Figure 2.7 and Figure 2.9, the solution with zero Dirichlet boundary condition, here denoted by FV-D and the solution with Robin boundary condition denoted by FV-R are compared with the analytical solution for a cube. As expected, the robin boundary condition yield a smaller error than using zero Dirichlet at the boundary. The improvement in the solution is more noticeable for profiles far away from the source.

To investigate the effect of the two boundary conditions to the size of the model domain, I perform another convergence test and vary the aspect ratio $L/H$, where the length of the model domain and of the central cube are denoted by $L$ and $H$ respectively. The cube
Figure 2.6: The vertical component of gravitational acceleration computed for the model and profiles shown in Figure 2.3. The values are computed by the finite-volume method using a mesh resolution $h = 10$ m mesh. The dashed dot black line indicate values calculated using $\phi = 0$ at the boundary, the solid blue line indicates values calculated using Robin type boundary condition and the dashed red line indicates the analytical solution.

Figure 2.7: The relative errors in the gravity values computed by the finite-difference method on the $h = 10$ m mesh
Figure 2.8: \( T_{zz} \) computed for the model and profiles shown in Figure 2.3. The values are computed by the finite-volume method using a mesh resolution \( h = 10 \) m mesh. The dashed dot black line indicate values calculated using \( \phi = 0 \) at the boundary, the solid blue line indicates values calculated using Robin type boundary condition and the dashed red line indicates the analytical solution.

Figure 2.9: The relative errors in \( T_{zz} \) computed by the finite-difference method on the 10 m mesh (relative to the values calculated using Eq. (8) of Haaz [7])
size $H$ is kept fixed at 100 m, while $L$ is increased to obtained the following aspect ratios $L/H = 4, 6, 8, 10, 12$. For this test, $g_z$ is calculated at profile $x = 150$ m and each $L/H$ yielded $h = 25$ m. The $L_2$ convergence rates are shown in Figure 2.10. We expect that $L_2$ error approaches 0 as $L/H \to \infty$. When using Dirichlet boundary conditions, the indirect solution converges faster than the direct solution. But, when using Robin boundary conditions, both, the indirect and direct solution have the same rate of convergence.

Figure 2.10: Convergence rate in $L_2$ as a function of the domain size. Indirect solution (a). Direct solution (b)
2.6 Summary

I described a method for computing gravity and gravity gradient data directly from Poisson’s equation governing the gravitational field. This equation relates the gravity anomaly to spatial derivatives of the density function and does not need the computation of the gravitational potential. We approximate the solution using a second order finite volume method with Robin boundary conditions. The finite volume forward modeling code was tested against analytical solution for a simple cubic body and against the indirect solution (i.e. the solution obtained via differentiation of the gravitational potential).
This chapter extends the PDE-based forward model for magnetic by incorporating the effect of anisotropy in magnetic susceptibility. The solution is then tested against analytical solutions for simple bodies and against solutions in the integral equation domain. To start, I present a brief overview of the principles of anisotropy in magnetic susceptibility.

### 3.1 Principles of anisotropy in magnetic susceptibility

When a substance, such as a rock, is exposed to an external magnetic field it acquires magnetization which is induced by the magnetic field. The result is a secondary field \( H_s \) that adds to the external field \( H_0 \) to form the total magnetic field \( H \). For low-amplitude magnetic fields, like the Earth’s magnetic field, the induced magnetization \( M \) is proportional to the total magnetic field

\[
M = \kappa H
\]  

where \( \kappa \) is the magnetic susceptibility. For anisotropic materials \( M \) is not in the direction of \( H \) and the magnetic susceptibility may be better described as second order tensor \( \tilde{\kappa} \). Then, equation 3.1 is written more generally as

\[
M = \tilde{\kappa} \cdot H
\]  

which can be shown in expanded form as

\[
\begin{align*}
M_x &= \kappa_{xx} H_x + \kappa_{xy} H_y + \kappa_{xz} H_z \\
M_y &= \kappa_{yx} H_x + \kappa_{yy} H_y + \kappa_{yz} H_z \\
M_z &= \kappa_{zx} H_x + \kappa_{zy} H_y + \kappa_{zz} H_z
\end{align*}
\]
The susceptibility tensor is symmetric, so the nine components in the equation above are reduced to six; that is,

$$\kappa_{xy} = \kappa_{yx}, \quad \kappa_{xz} = \kappa_{zx}, \quad \kappa_{yz} = \kappa_{zy},$$

(3.7)

Rocks for which $\kappa_{xy} = \kappa_{xz} = \kappa_{yz} = 0$ and $\kappa_{xx} = \kappa_{yy} = \kappa_{zz}$, are said to be isotropic, otherwise, rocks are said to possess an anisotropy in magnetic susceptibility. There exist a rotated Cartesian coordinate system, such that, equation 3.6 simplifies to:

$$M_x = \kappa_{xx}H_x$$

(3.8)

$$M_y = \kappa_{yy}H_y$$

(3.9)

$$M_z = \kappa_{zz}H_y$$

(3.10)

(3.11)

The components $\kappa_{xx} \leq \kappa_{yy} \leq \kappa_{zz}$ are denoted as $k_1 \leq k_y \leq k_z$ and the are called the principal susceptibilities and their directions are the principal directions.

Anisotropy in magnetic susceptibility is the directional variability in magnetic susceptibility of rocks. It arises when constituent mineral grains have a preferred orientation. The principal types of anisotropy are: magnetocristaline anisotropy which arises from the lattice alignment of crystals and shape anisotropy that emerge from the alignment of non equidimensional mineral grains Tarling and Hrouda [9]. Shape anisotropy is related with the concept of self-demagnetization. Self-demagnetization is the process in which internal magnetic fields generated inside a magnetized body, move against the magnetization direction. This internal magnetic field is called the demagnetizing field, and it works to demagnetize the body. Demagnetizing fields are strongly dependent on the magnitude of the susceptibility and on the shape of the body.
3.1.1 Geometrical representation

Consider a external magnetic field of magnitude $B_0$ and directional cosines $n_1, n_2, n_3$. The magnetization parallel to this induced field is

$$M_\parallel = H_0 k_{ij} n_i n_j, \quad i, j = 1, 2, 3,$$

where $H_0 = B_0/\mu_0$, the directional cosines are $n_i$, $n_j$ and $k_{ij}$ is the tensor of susceptibility, (i.e. $k_{ij} = k_{ji}$). The ratio of $M_\parallel$ to $H_0$ is defined as

$$K_\parallel = \frac{M_\parallel}{H_0} = k_{ij} n_i n_j$$

According to Jank [10], the components of the magnetic susceptibility tensor may be represented in 3-D space by an ellipsoid traced out by a radius vector of length

$$R = \frac{1}{\sqrt{K_\parallel}}$$

Equation 3.13 possesses principal axes that allows to write

$$K_\parallel = k_x n_1^2 + k_y n_2^2 + k_z n_3^2$$

where $k_x \geq k_y \geq k_z$ are the principal susceptibilities. To facilitate the calculation, the axes of a rectangular co-ordinate system, $x$, $y$, $z$ are identified with the principal axes of the ellipsoid of anisotropy. Defining $n_1 = x/R$, $n_2 = y/R$ and $n_3 = z/R$, equation3.15 becomes the equation of an ellipsoid.

$$1 = k_x x^2 + k_y y^2 + k_z z^2$$

Figure 3.1: Respective view of the rotational ellipsoid of anisotropy.
A perspective view of the ellipsoid is shown in Figure 3.1. The length of the semi-axes of the ellipsoid of anisotropy are \(1/\sqrt{k_x}, 1/\sqrt{k_y}, 1/\sqrt{k_z}\). The eccentricity of the anisotropy in magnetic susceptibility ellipsoid can be characterized by the relationship between the maximum to minimum principal susceptibilities. This eccentricity is referred to as the degree of anisotropy.

\[
\alpha = \frac{k_x}{k_z}
\]

By introducing new variables \(r, p, q\), instead of \(x, y, z\), for which

\[
0 \leq r, p, q \leq 1, \quad x = r/\sqrt{k_x},
\]

the equation of the ellipsoid becomes an equation of a sphere

\[
r^2 + p^2 + q^2 = 1
\]

![Figure 3.2: Direction of deflection of magnetization \(M\) from the direction of the external field \(B_0\), for a isotropic sample (a), for a rotational ellipsoid of anisotropy (b).](image)

The anisotropy of magnetic susceptibility generally changes the direction of the magnetization away from the direction of the geomagnetic field. See Figure 3.2. Jank [10] found that the magnitude of the deflection depends on the degree of anisotropy \(\alpha\) and on the direction of the magnetizing field in respect to the axes of the ellipsoid on anisotropy which
is characterized by the parameter $r$. For rotational ellipsoid of anisotropy, the magnitude of deflection is

$$
cos \theta = [(r^2 - r^4)(\alpha + 1/\alpha - 2) + 1]^{-1/2}
$$

(3.20)

Combining 3.15 and 3.18, the variable $r$ can be written as

$$
r = \frac{n_1 \sqrt{k_x}}{\sqrt{(n_1^2 k_x + n_2^2 k_y + n_3^2 k_z)}}
$$

(3.21)

Figure 3.3 shows the deflection angle as a function of the direction of the field, characterized by the quantity $r$ and the degree of anisotropy $\alpha$. The deflection is zero when the direction of the field coincides with the direction of the axis of the ellipsoid of anisotropy, $r = 0$, or $r = 1$, consistently with an isotropic body, ($\alpha = 1$). Maximum deflection occurs for $r = 1/\sqrt{2} = 0.707$ (i.e. for $\cos 45^\circ$).

Figure 3.3: Magnitude of deflection, $r$ as a function of field direction, (characterized by quantity $r$), and of the degree of anisotropy, $\alpha$, for rotational ellipsoids. (Equation 3.20)
3.2 Governing equations for magnetics

Recall the governing equation for the magnetic problem in Chapter 1.

\[ \nabla \cdot \mathbf{B} = 0 \quad (3.22a) \]

\[ \mathbf{B} = \mu \nabla \phi \quad (3.22b) \]

where \( \mu \) is the magnetic permeability and \( \mathbf{B} \) is the total magnetic field. The total magnetic field is the sum of the external field \( \mathbf{B}_0 \) and the secondary or anomalous field \( \mathbf{B}_s \). Then 3.22a and 3.22b can be decomposed to yield,

\[ \nabla \cdot (\mathbf{B}_0 + \mathbf{B}_s) = 0 \quad (3.23a) \]

\[ \mathbf{B}_0 + \mathbf{B}_s = \mu \nabla (\phi_0 + \phi_s) \quad (3.23b) \]

Combining 3.23a and 3.23b, and using \( \mu = \mu_0 (1 + \kappa) \) yields

\[ \nabla \cdot \mathbf{B}_s = 0 \quad (3.24) \]

\[ \mathbf{B}_s = \kappa \mathbf{B}_0 + \mu \nabla \phi_s \quad (3.25) \]

Combining 3.24 and 3.25 leads to the div-grad equation for the secondary potential:

\[ \nabla \cdot \mu \nabla \phi_s = -\nabla \cdot (\kappa \mathbf{B}_0) \quad (3.26) \]

In Lelièvre and Oldenburg [6] the susceptibility is treated as a scalar quantity; here I do not make that assumption and treat the susceptibility or equivalent, the magnetic permeability, as a tensor. Equation 3.26 becomes

\[ \nabla \cdot \tilde{\mu} \nabla \phi_s = -\nabla \cdot (\tilde{\kappa} \mathbf{B}_0) \quad (3.27) \]

where

\[ \tilde{\mu} = \mu_0 \left( \mathbf{I} - \tilde{\kappa} \right) \quad (3.28) \]
where \( \mu_0 \) is the magnetic permeability of free space and \( \tilde{\kappa} \) is given by

\[
\tilde{\kappa} = \begin{bmatrix}
\kappa_{xx} & \kappa_{xy} & \kappa_{xz} \\
\kappa_{yx} & \kappa_{yy} & \kappa_{yz} \\
\kappa_{zx} & \kappa_{zy} & \kappa_{zz}
\end{bmatrix}
\] (3.29)

and \( \tilde{I} \) is defined as

\[
\tilde{I} = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}
\] (3.30)

To facilitate the calculation, the axes of the rectangular co-ordinate system, \( x, y, z \), will be identified with this principal axes of anisotropy \( k_x \geq k_y \geq k_z \). In that case, the susceptibility tensor is diagonal

\[
\tilde{\kappa} = \begin{bmatrix}
k_x & 0 & 0 \\
0 & k_y & 0 \\
0 & 0 & k_z
\end{bmatrix}
\] (3.31)

### 3.2.1 Finite volume discretization

To discretize equation 3.27 I use the finite volume method in a similar way as in Lelièvre [11]. The domain is divided into many rectangular cells whose axes are parallel to the Cartesian coordinate system. A single cell used in the discretization is shown in Figure 3.4. The three principal susceptibilities \( k_x, k_y \), and \( k_z \) are assumed constants within each cell. The components of the magnetic field are placed at the center of the cell faces and the discrete potentials are located at the center of the cells. The notation of nodes, cell centers, cell lengths and distances between cell centers are the same as described in Chapter 2.

**Discretization of the divergence**

As seen in chapter 2, the finite volume method discretizes the integral form of a partial differential equation instead of the differential form. The integral of equation 3.24 over volume is

\[
\int_v \nabla \cdot \mathbf{B}_s \, dv = 0
\] (3.32)
The above integral is transformed into a surface integral using the divergence theorem. The surface integral is evaluated as magnetic fluxes at the surfaces of each cells. An important property is that the fluxes entering a given volume are identical to that leaving the adjacent volume (conservativity). When the surface integrals are approximated by numerical integration and combined all cells together, they form the following system of equations

\[ \mathbf{D} \mathbf{B}_s = \mathbf{f} \]  

(3.33)

where \( \mathbf{D} \) is the divergence operator and \( \mathbf{f} \) is a vector that contains field values from the prescribed boundary conditions. The explicit form of the operator \( \mathbf{D} \) is given in Lelièvre [11, p. 32-33].

**Discretization of the gradient**

When the non-diagonal elements of \( \tilde{\kappa} \) equal zero, 3.25 can be split into three parts, one for each Cartesian direction. The following governing equations are obtained:

\[ B_x = k_x B_{0x} + \mu_1 \frac{\partial \varphi_x}{\partial x} \]  

(3.34a)
\[ B_y = k_y B_{0x} + \mu_y \frac{\partial \varphi_s}{\partial y} \quad (3.34b) \]

\[ B_z = k_z B_{0z} + \mu_z \frac{\partial \varphi_s}{\partial z} \quad (3.34c) \]

In order to obtained harmonic averages in \( \mu_x, \mu_y \) and \( \mu_z \) when discretized, equations 3.25 should be rearrange into the more rough equations Lelièvre [11, p. 33-35].

\[ \mu_x^{-1} B_s = \left( \frac{1}{\mu_0} - \frac{1}{\mu_x} \right) B_0 + \frac{\partial \varphi_s}{\partial x} \quad (3.35a) \]

\[ \mu_y^{-1} B_s = \left( \frac{1}{\mu_0} - \frac{1}{\mu_y} \right) B_0 + \frac{\partial \varphi_s}{\partial y} \quad (3.35b) \]

\[ \mu_z^{-1} B_s = \left( \frac{1}{\mu_0} - \frac{1}{\mu_z} \right) B_0 + \frac{\partial \varphi_s}{\partial z} \quad (3.35c) \]

Consider 3.35a. The finite volume applied to 3.35a is

\[ \int \mu_x^{-1} B_{sx} \, dv = \int \left[ \left( \frac{1}{\mu_0} - \frac{1}{\mu_x} \right) B_{0x} + \frac{\partial \varphi_s}{\partial x} \right] \, dv \quad (3.36) \]

when numerical integration (i.e. mid point approximation), one for each grid cell are combined, the following matrix vector equation is obtained.

\[ M^{-1}_x B_x = (\mu_0 I - M^{-1}_x) B_{0x} + G_x \varphi_s \quad (3.37) \]

where \( M_x \) is a diagonal matrix whose elements are harmonic average values of susceptibility, \( G_x \) is the gradient with respect to \( x \) operator and \( I \) is the identity matrix of appropriate size. When 3.35b and 3.35c are discretized in a similar way, the following equation are obtained

\[ M^{-1}_y B_y = (\mu_0 I - M^{-1}_y) B_{0x} + G_x \varphi_s \quad (3.38) \]
Explicit forms of the differential operators $G_x$, $G_y$, $G_z$, $M_x$, $M_y$, $M_z$ are given in Lelièvre [11, p. 42-43]. Combination of equations 3.37 to 3.39 yield

$$B_s = (\mu_0^{-1}M - I)B_0 + G\phi_s$$  \hspace{1cm} (3.40)

where,

$\phi_s$ is the unknown discrete potential values.

$D = [D_x D_y D_z]$ is the divergence matrix.

$G = [G_x G_y G_z]^T$ is the gradient matrix.

$B_0 = [B_{0x} B_{0y} B_{0z}]^T$ is a vector of primary field values.

$M$ is diagonal matrix containing harmonic average of permeability values.

$$M = \begin{bmatrix} M_x^{-1} & 0 & 0 \\ 0 & M_y^{-1} & 0 \\ 0 & 0 & M_z^{-1} \end{bmatrix}$$ \hspace{1cm} (3.41)

In Lelièvre and Oldenburg [6], the matrices $M_x$, $M_y$ and $M_z$ contain harmonically averaged $\mu$ values. Here, $M_x$, $M_y$ and $M_z$ contain harmonically averaged $\mu_x$, $\mu_y$ and $\mu_z$ values respectively.

### 3.2.2 Solution of the discrete forward modeling equations

Equation 3.33 and 3.40 can be written as a linear of linear systems

$$A(m)\phi_s = q(m),$$ \hspace{1cm} (3.42)

where

$$A(m) = DM(m)G$$ \hspace{1cm} (3.43)

and

$$q(m) = -D(\mu_0^{-1}M - I)B_0$$ \hspace{1cm} (3.44)
The matrix $A$ is squared, non-symmetric and in general not positive definite. For the numerical solution I choose the Bi-Conjugate Gradient Stabilized method (BiCGStab). Once $\varphi_s$ is determined, the data of interest (i.e. certain flux components at specified locations) are calculated as

$$d_{\text{pred}} = Q B_s$$  \hspace{1cm} (3.45)

where $B_s$ is the secondary field given by 3.40 and $Q$ is a matrix that interpolates for specific flux quantities at specified measurement positions.

3.3 Testing the forward model for anisotropy

In this section the finite volume solutions were compared to analytical solutions and to the slower, more memory intensive full integral equation domain solution. To validate the method two tests were performed. First, total magnetic anomaly profiles are calculated above simple anisotropic prism for different degrees of anisotropy. For the prism, the main effect of anisotropy is the rotation of the magnetization direction away from the inducing field direction. The second test calculate the total magnetic anomaly profiles are calculated above an anisotropic vertical dike.

3.3.1 Anisotropic prism

The synthetic model consists of a uniform grids containing $55^3$ cells. This contained a central, uniform, anisotropic cube of $5^3$ cells in volume. The grid and the central cube have physical dimensions of 33 m and 3 m respectively. The external magnetic field has magnitude of 54000 nT, declination $D = 0$ and inclination $I = 45^\circ$. The numerical solution is validated using the analytical magnetic field due to an anisotropic prism. The analytical magnetic field response of a rectangular prism oriented parallel to the $x, y, z$ axes is presented in Appendix C.
Profiles of the total magnetic anomaly 3 m above the center of the prism (i.e. data 1 in Figure 3.5) are shown in Figure 3.6 for $\alpha = 1$, $\alpha = 2$ and $\alpha = 3$. Figure 3.7 show differences respect to the analytical solution. The maximum differences from the finite volume and Integral solution correspond to 15% and 5% relative errors respectively. The inaccuracies in the finite volume solution in this test are severe. The major two source of errors are: the level of discretization and the boundary condition approximation. The discretization is such that the anisotropic cubic is modelled with $5^3$ cells. The solution is expected to increase accuracy with increasingly refined discretization. The inaccuracy in the finite volume solution also results from inaccuracies in the prescribed boundary conditions. Here, the Neumann boundary condition ($\mathbf{B} = \mathbf{B}_0$ at the boundary) is approximated by ensuring that the model boundaries are “far” from the susceptible anomaly, which in this test constituted using a model domain with side lengths eleven times larger than the side length of the anomaly ($L/H = 11$). To increase accuracy the grid can always be enlarged in order to move the boundary further from the susceptible material.
Figure 3.6: Total field anomaly along a profile in the x-direction at a height of 12m above the center of the prism for average susceptibility $\kappa = 1$ and degree of anisotropy $\alpha = 1$ (blue), $\alpha = 2$ (red), $\alpha = 3$ (black).

Figure 3.7: Differences ($\Delta T_{\text{Int.Sol}} - \Delta T_{\text{analytic}}$) (left) and ($\Delta T_{\text{FV}} - \Delta T_{\text{analytic}}$) (right) for the profiles shown in figure Figure 3.6
3.3.2 Anisotropic dike

As an illustration, Figure 3.8 shows total magnetic $\Delta T$ profiles over a dike structure, indicating the differences in anomalies produced by isotropic susceptibility and anisotropic susceptibility ($\alpha = 2.5$). The regional geomagnetic field intensity is 54,000 nT and the field direction is declination of 0°, and inclination of 90°. Solid curves represent pure induced magnetisation with isotropic susceptibility $\kappa = 0.5653$ SI, dashed curves represent induced magnetisation with anisotropy $k_\parallel = 0.942SI; k_\perp = 0.377SI \alpha = 2.5$.

Recall section 3.1.1 that for a given degree of anisotropy, $\alpha$, the angle, $\theta$, between the inducing field and the principal direction of anisotropy, $k_1, k_2, k_3$. There is no dip error, when the field is parallel to principal axes of anisotropy. However, the magnitude of the total magnetic anomaly is significantly less when the field is normal to the axis along which the susceptibility is larger. Assuming a degree of anisotropy of 2.5, the maximum deflection of induced magnetization towards the z-axis is about 25° when the inducing field is 30°, Figure 3.9. error in interpreted dip depends on the angle.

3.4 Summary

This chapter considers magnetic anisotropy and how this phenomena is introduced into the modeling methods. We just consider the simpler case in which the coordinate axes are parallel to the three mutually perpendicular principal susceptibility values. We perform various in order to asses the accuracy of the forward modeling algorithm. The tests consisted in modeling the magnetic response over simple bodies and compared them to analytical solutions and to the slower, more memory intensive full integral equation domain solution. The test have shown a good agreement between numerical solutions and calculated values of deflection angle and apparent susceptibility. In addition, we have shown that an interpretation of the magnetic signal that ignores anisotropy will lead to errors in interpreted dips.
Figure 3.8: north-south total magnetic anomaly profile over a vertical dike, showing the effects of anisotropy. The regional geomagnetic field intensity is 54,000 nT and the field direction is declination of 0°, and inclination of 90° (top); 0° (center); 30° (bottom). Solid curves represent pure induced magnetisation with isotropic susceptibility $k = 0.5653 SI$, dashed curves represent induced magnetisation with anisotropy $k_\parallel = 0.942; k_\perp = 0.377 SI, \alpha = 2.5.$
In this chapter I use the forward modeling algorithms described in previous chapters to invert field gravity and magnetic data. The inversion results are then compared with those obtained with forward models based on the integral equation.

4.1 Solution of the forward problem

In this section I summarize the PDE-based forward model. Recall from chapters 2 and 3 that the forward problem can be written as a linear system of equations

\[ A(m)u = q(m) \]  

where \( u \) is the unknown scalar potential, \( m \) is the model of physical properties (e.g. density or magnetic susceptibility) and \( A(m) \) is a differential operator defined on each mesh. Once \( u \) is determined, the data of interest is calculated through a linear operation, which will be written as

\[ d_{\text{fwd}} = F[m] = Q[C(m)A^{-1}(m)q(m) + b(m)] \]

where \( F \) is the forward operator, \( Q \) is an interpolation matrix that performs linear interpolations from the grid-located values onto the measurement locations. The matrix \( C \) and vector \( b \) convert the potentials into the field values throughout the discrete grid.

4.2 Tikhonov Regularization

To compute \( m \) from 4.2 is a not well posed problem and its solution requires regularization. The goal is to compute the minimizer, \( m \), for the model objective function \( \varphi \)

\[
\text{minimize} \quad \varphi(m) = \varphi_d(m) + \beta \varphi_m(m) \\
\text{subjected to} \quad m_{\text{low}} \leq m \leq m_{\text{high}}
\]  

(4.3)  

(4.4)
where $\phi_m$ is the model objective and $\phi_d$ is the data misfit and $\beta > 0$ is the regularization parameter, which controls the strength of regularization.

### 4.2.1 The data misfit

The data misfit measures the residual between the data, $d^{\text{obs}}$, and the theoretical predictions of the forward problem, $F(m)$. We assume that the relationship between observed and predicted data is:

$$d^{\text{obs}} = F(m) + \epsilon$$

(4.5)

where $\epsilon$ is the measurement errors. The data misfit is defined as:

$$\phi_d = \sum_{i=1}^{N} \left( \frac{d^{\text{obs}}_i - d^{\text{fwd}}_i}{\sigma_i} \right)^2 = \| W_d(d^{\text{obs}} - F(m)) \|_2^2$$

(4.6)

where $\sigma_i$ is the standard deviation associated with the $i^{th}$ data point. Assuming that the noise in measurements is independent and normally distributed with zero mean and standard deviation $\sigma$, $\phi_d$ in equation 4.6 is a chi-squared variable with expected value $N$. Therefore, to prevent over-fitting, an appropriated value for the data misfit is $N$.

### 4.2.2 Model objective function

The purpose of the regularization functional is to allow the incorporation of a priori information about the desired solution $m$. The standard regularization functional is

$$\phi_m = \alpha_s \int_R W_s \{ W_r (m - m_{\text{ref}}) \}^2 + \alpha_x \int_R W_x \left\{ \frac{d}{dx} [W_r (m - m_{\text{ref}})] \right\}^2 + \alpha_y \int_R W_y \left\{ \frac{d}{dy} [W_r (m - m_{\text{ref}})] \right\}^2 + \alpha_z \int_R W_z \left\{ \frac{d}{dz} [W_r (m - m_{\text{ref}})] \right\}^2$$

(4.7)

where $R$ is the region occupied by the model; $\alpha_s, \alpha_x, \alpha_z$ are coefficients specifying the relative importance of the various terms; $m$ is the model of subsurface density contrast; $m_{\text{ref}}$ is the reference model; $W_s, W_x, W_y, W_z$ are spatially dependent weighting functions; and $W_r$ is a depth weighting function.
The first term of 4.7 is the "smallest" term. It controls the closeness of the model \( m \) with respect to the reference \( m_{\text{ref}} \). It ensures the recovered model is compatible with the a priori geological information. The remaining terms smooth the model differences over several cells in \( x, y \) and \( z \) directions. The weighting functions \( W_x, W_y, \) and \( W_z \) are relative and can be designed to enhance or attenuate structures in various regions in the model domain. Values of one indicate moderately smoothness and values less than one promote roughness. Explicit forms of the model weighting matrices can be found in Li and Oldenburg [12].

4.2.3 Depth Weighting

Depth weighting is very important in potential field inversion as it counteracts the natural decay with distance from the source of potential fields. The typical form for the depth weighting function comes from Li and Oldenburg [12]

\[
W(z) = (z + z_0)^{-\xi}
\]

where \( z \) below the surface and \( z_0 \) depends upon the observation height and cell size. For magnetic data \( \xi = 3 \), and for gravity \( \xi = 2 \). Any potential field data collected above the Earth’s surface can be fitted with either smaller values (density, magnetic susceptibility) at the surface or with larger values at depth. Without depth weighting, any inversion would prefer the near surface option. When depth weighting is applied, the inversion places the anomaly at depth. The discrete form of the depth weighting matrix is

\[
W_r = \text{diag}[(z + z_0)^{-\xi/2}]
\]

Here, \( z \) is a vector containing the \( z \)-coordinates of the centers of each model cell. This depth weighting function will always be applied twice in the model objective function and the effective weighting is then consistent with 4.8.

4.3 The regularization parameter

The regularization parameter \( \beta \) represents the trade-off between fitting the data and the smoothness of the estimate model. The determination of the proper value of \( \beta \) depends
on the standard deviation of the noise $\sigma$. The L-curve is a convenient graphical tool for displaying the trade-off between the size of the misfit and model objective function as the regularization parameter varies. The appropriate $\beta$ value is chosen as one corresponding to the elbow of the L-curve.

4.3.1 Bound constrains

For the majority of inverse problems the model parameters are constrained to be in a given range. The most common method to impose bound constrains in inversion of potential field data is the "logarithm barrier method" Li and Oldenburg [12]. A second regularization parameter $\lambda$ is introduced and the total objective function is modified by adding a logarithmic barrier term that gets large as the model parameters approach zero

$$\varphi = \varphi_d + \beta \varphi_m - \lambda B(m) \quad (4.10)$$

where

$$B(m) = \sum_{i=1}^{nc} \ln(m_i) \quad (4.11)$$

The minimization of $\varphi$ for a fix regularization parameter $\beta$ starts with a large $\lambda$ and gradually reduce its value using previous solutions as a starting point.

4.4 Discrete form of the model objective function

The general form of the model objective function with positive constrain is

$$\varphi = \| W_d(F[m] - d^{obs}) \|^2 + \beta \| W_m(m - m_{ref}) \|^2 \quad (4.12)$$

where

$m$ : model vector.

$m_{ref}$ : reference model.

$W_m$ : model weighting matrix.

$W_d$ : data weighting matrix.

$F[m]$ : forward operator.
4.5 Gauss-Newton Method and line search

The aim is to find the model that minimize the objective function 4.12. To minimize $\varphi$ we set its gradient to zero. Solving $\nabla \varphi = 0$ is a non linear problem and its solution requires an iterative method. We use the Gauss Newton method (GN). The GN method locally expand $\varphi$ to second order using Taylor expansions about a perturbation $\delta \mathbf{m}$

$$
\varphi(\mathbf{m} + \delta \mathbf{m}) = \varphi(\mathbf{m}) + \mathbf{g}^T \delta \mathbf{m} + \frac{1}{2} \delta \mathbf{m}^T \mathbf{H} \delta \mathbf{m} + \ldots
$$

where $\mathbf{g}$ is the gradient vector,

$$
\mathbf{g} = \mathbf{J}^T(\mathbf{m}) \mathbf{W}_d^T \mathbf{W}_d (\mathbf{F}[\mathbf{m}] - \mathbf{d}^{\text{obs}}) + \beta \mathbf{W}_m^T \mathbf{W}_m (\mathbf{m} - \mathbf{m}_{\text{ref}}) - \lambda \mathbf{X}^{-1}(\mathbf{m}) \mathbf{e},
$$

and $\mathbf{H}$ is the hessian matrix

$$
\mathbf{H} = (\nabla \mathbf{J})^T(\mathbf{m}) \mathbf{W}_d^T \mathbf{W}_d (\mathbf{F}[\mathbf{m}] - \mathbf{d}^{\text{obs}}) \mathbf{J}^T(\mathbf{m}) \mathbf{W}_d^T \mathbf{W}_d \mathbf{J} + \beta \mathbf{W}_m^T \mathbf{W}_m (\mathbf{m} - \mathbf{m}_{\text{ref}})
$$

In the above equations $\mathbf{X} = \text{diag}(\mathbf{m}_1, \ldots, \mathbf{m}_2)$, $\mathbf{e} = \{1, \ldots, 1\}$ and $\mathbf{J}$ is the sensitivity matrix, whose calculation is covered in the next section. For a minimum we require that $\nabla \varphi = 0$, and from equation 4.13 we obtain

$$
\nabla \varphi = \frac{\varphi(\mathbf{m} + \delta \mathbf{m}) - \varphi(\mathbf{m})}{\delta \mathbf{m}} = \mathbf{g} + \mathbf{H} \delta \mathbf{m} = 0,
$$

then the perturbation $\delta \mathbf{m}$ is computed as the solution of

$$
\mathbf{H} \delta \mathbf{m} = -\mathbf{g}.
$$

This gives the iterative update

$$
\mathbf{m} = \mathbf{m} + \delta \mathbf{m}
$$

Provided that $\mathbf{H}$ is positive definite, the solution $\delta \mathbf{m}$ is guaranteed to be a downhill direction. Rather than immediately update the model, it is better to perform line search to ensure global convergence.

$$
\mathbf{m} = \mathbf{m} + \alpha \delta \mathbf{m}
$$
If the problem size is large and the Hessian matrix is dense then it may be infeasible to compute it directly. The Gauss-Newton method avoid this problem by approximate the Hessian as

\[ H \approx J^T(m)W_d^T W_d J + \beta W_m^T W_m (m - m_{\text{ref}}) \] (4.20)

### 4.6 The global non-linear procedure

The method developed in the previous section is for solving the non linear problem for a particular regularization parameter \( \beta \). The problem is that we don’t know the appropriated value of the regularization parameter. There is many approaches to solve this problem..... In this thesis work, I adopt continuation or cooling method cite. Cooling strategy distinguishes two iteration procedures: an outer iteration to find the optimum regularization parameter \( \beta \) and inner iteration that solves a Gauss-Newton problem for a specific \( \beta \). The first outer iteration is with a large value of \( \beta \) for which the quadratic term \( \| W(m - m_{\text{ref}}) \|^2 \) dominates, then, gradually reduces \( \beta \) and solve a new Gauss Newton problem with the solution for the previous \( \beta \). The algorithm is terminated when the data misfit is close enough to the target misfit. The target misfit is discussed in section 4.2.1.

### 4.7 Sensitivity computation

The sensitivity matrix \( J \) is defined as

\[ J = \frac{\partial d_{\text{fwd}}(m)}{\partial m} \] (4.21)

As expressed by its name, the sensitivity matrix indicates the sensitivity of the fields with respects to changes in the model. The derivative of equation 4.2 is expanded using the chain rule.

\[ J = Q \frac{\partial}{\partial m} [C(m)\phi(m) + b(m)] \]
\[ = Q \left\{ C(m) \frac{\partial \phi}{\partial m} + \frac{\partial}{\partial m} [C(m)\phi]_{\phi} + \frac{\partial b}{\partial m} \right\} \] (4.22)
where the subscript after the bracketed term being differentiated is used to indicate that
the specified quantity is treated as a constant in the differentiation.

### 4.7.1 Sensitivity for gravity

From the results in chapter 2, the forward model can be written as

\[
d_{fwd} = Q[GU] = Q[GA^{-1}m]
\] (4.23)

here \(m\) is the model of density values scaled by \(4\pi\gamma\). According to equation 4.22, the matrix \(C\) and the vector \(b\) reduce to:

\[
A = DG \\
C = G \\
b = 0
\]

replacing 4.24 in 4.22 yield to

\[
J_g = QGA^{-1}
\] (4.24)

### 4.7.2 Sensitivity for magnetics

Recall chapter 3 the forward modeling equation for the secondary flux can be written as:

\[
DM(m)Gu = (\mu_0^{-1}M(m) - I)B_0
\] (4.25a)

\[
d_{fwd} = QB_s = Q[M(m)Gu(m) + (\mu_0^{-1}M(m) - I)B_0]
\] (4.25b)

here is \(u\) is the secondary potential and \(m\) is the model of susceptibility values. Comparing
with 4.22 the following definitions are made
\[ C(m) = M(m)G \]
\[ A(m) = DM(m)G \]
\[ q(m) = g(m) - D(\mu^{-1}M(m) - I)B_0 \]
\[ \phi(m) = A^{-1}(m)q(m) \]
\[ b(m) = (\mu_0^{-1}M(m) - I)B_0 \]  (4.26)

which expanded and evaluated gives ([6]):

\[
J_B = QMG A^{-1}[-DMM \text{diag}(w)Y \text{diag}((m + 1)^{-2})] \\
+ QMM \text{diag}(w)Y \text{diag}((m + 1)^{-2})]
\]  (4.27)

From 4.24 and 4.27 we see that to compute the sensitivities one requires to compute the inverse of the forward problem matrix \( A \). This may make the computation of the sensitivities difficult if not impossible. Fortunately the iterative algorithm used to solve equation 4.17, just requires the computation of the products of the sensitivity \( J \) and its transposes times a vector \( v \). Thus the matrix \( J \) never needs to be constructed. By careful choice of multiplication order, \( Jv \) and \( J^Tv \) can be computed avoiding any matrix-matrix multiplications. In the case of the magnetics, the computation of \( J_Bx \) and \( J_B^Tx \) requires eleven sparse matrix-vector multiplications and one vector dot product. While in the case of gravity, the computation of \( J_gx \) and \( J_g^Tx \) just requires three matrix-vector multiplications. The complication of this approach is that a system equivalent to a linearized forward problem needs to be computed at each iteration.

The computation of \( J_g \) via equation 4.24 is tested against a finite difference approach. The test uses a small model consisting of \( 33^3 \) cubic cell of 100 m of dimension with a central dense cell of 1 g/cm\(^3\). The observation location is at the center of the grid. We compute the vertical component of gravity field data 200 m above the center of this cube. The number of data is \( N = 121 \). The sensitivity matrix calculated for the single-cell is a column vector of length \( N \). I calculate the sensitivity through two methods; a finite difference approach and
Figure 4.1: The analytic solution for $J$ (top). The finite difference solution for $J$ (middle). The difference between the finite difference and analytic solution for $J$ (bottom). Units are [mGal/g/cm$^3$].
a analytical approach by calculating $J_gv$ for a vector with a single element of 1. The test is similar to that presented in Lelièvre [11, p. 147] for the magnetic sensitivity matrix. In Figure 4.1, both solutions are displayed as a data map. As expected, the difference between these two maps is near zero.

### 4.8 Inversion of survey data above a cooper-lead-zinc deposit

Here, I invert total flux magnitude survey data and vertical gravity data collected over copper-lead-zinc deposit. The Health Steel Stratmat is located in northern New Brunswick, Canada.

The inducing flux in the region had a strength of 56000 nT and it is inclined 72° to the horizontal and declined -22°. The survey covers an area of 1000 m × 1000 m in a region of smooth topography. See Figure 4.2. The survey parameters are summarized in Table 4.1. The vertical gravity anomaly and the total magnetic anomaly data are shown in Figure 4.3. The main feature is a high gravity and low magnetic responses with peak around (10500N, 12800E). The high gravity and low magnetic responses are typical signatures of sulfide minerals such as chalcopyrite, sphalerite and galena. The mesh used in the inversion
Figure 4.3: (a) Observed vertical component of the gravity field. (b) Observed total magnetic data is displayed in Figure 4.4; it is three times larger than the area cover by the data and it is split in two regions; an inactive region which contains the outer free-space padding region that remain fixed during the inversion and an active region which contains all the cells with unknown density/susceptibility values. The grid contained cubic cells of 25 m dimension in the inner portion with increased dimensions in the padding cells. The total number of grid cells was $n_c = 60 \times 60 \times 28 = 100800$.

<table>
<thead>
<tr>
<th>Survey parameters</th>
<th>N° stations</th>
<th>area ($m^2$)</th>
<th>$\Delta x$ (m)</th>
<th>$\Delta y$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>gravity</td>
<td>443</td>
<td>$1000 \times 975$</td>
<td>25</td>
<td>100</td>
</tr>
<tr>
<td>magnetics</td>
<td>779</td>
<td>$1000 \times 900$</td>
<td>25</td>
<td>50</td>
</tr>
</tbody>
</table>

For the gravity and magnetic inversion, the alpha parameter values are $\alpha_s = 0.001$ and $\alpha_x = \alpha_y = \alpha_z = 1$. All spatial weighting functions are constant throughout the grid. The initial model is also constant over the active region with a value of 0.01 g/cm$^3$ for the gravity inversion and 0.01 SI units for the total magnetic field inversion. I use a reference model of constant zero-valued. The boundary conditions were calculated without the far field approximation (i.e. $F = 0$).
A comparison between the inversion results using the PDE-based forward solution and those using the integral-based forward solution are shown from Figure 4.5 to Figure 4.10. Figure 4.5, Figure 4.7 and Figure 4.8 show a perspective view, South-North and West-East cross-sections of the recovered density model respectively. The cross-sections would bisect the ore body. Both inversion results (i.e. using the PDE-based and Integral-based forward solution) are structurally similar. However, the density anomaly recovered by the PDE-based solution is more concentrated and present greater values. Figure 4.6, Figure 4.9 and Figure 4.10 show a perspective view, South-North and West-East cross-sections of the recovered susceptibility model respectively. In these case the structure is different. The PDE-based solution recovered anomalies at greater depths. To this respect, the depth weighting function introduced into the inversion has a stronger effect in the PDE-based solution. The inversion results shouldn’t be identical because I neglected forward modeling errors. The finite volume method suffer from inaccuracy due to finite discretization and this source of inaccuracy has less effect in the integral solution. Furthermore, the FVM solutions suffer
from inaccuracy due to the boundary condition approximation and the integral solution does not.

Figure 4.5: Perspective view of the recovered density model using the integral equation based forward model (top) and PDE-based forward model (bottom). Density units is \( [\text{g/cm}^3] \)
Figure 4.6: Perspective view of the recovered susceptibility model using the integral equation based forward model (top) and PDE-based forward model (bottom)
Figure 4.7: South - North cross section at $y = 12855$ m. (a) PDE-based forward model (b) Integral-based forward model. Density anomaly [g/cm$^3$]

Figure 4.8: South - North cross section at $x = 10425$ m. (a) PDE-based forward model (b) Integral-based forward model. Density anomaly [g/cm$^3$]
Figure 4.9: South - North cross section at $y = 12855$ m. (a) PDE-based forward model (b) Integral-based forward model. Susceptibility in SI units.

Figure 4.10: South - North cross section at $x = 10425$ m (a) PDE-based forward model (b) Integral-based forward model. Susceptibility in SI units
The standard deviations assigned to the data are defined as in section 4.3. For the gravity inversion, the estimate standard deviation of the noise is \( \sigma = 0.06 \text{ g/cm}^3 \). The target misfit is \( N = 434 \) and the misfit obtained is \( 459 = 1.04N \); corresponding to a \( \beta \) value of 0.06. The observed data, \( g_{z}^{\text{obs}} \), predicted data, \( g_{z}^{\text{pre}} \) and differences (\( g_{z}^{\text{obs}} - g_{z}^{\text{pre}} \)) are displayed in Figure 4.11. For the total magnetic field inversion, the estimate standard deviation of the noise is 10 nT. The target misfit was \( N = 779 \) and the misfit obtained was \( 785 = 1.01N \), corresponding to a \( \beta \) value of 0.001.

For a comparison of the predicted using the PDE-based against the integral-based forward solutions consider Figure 4.11 and Figure 4.12. These figures shows the predicted data and the difference values (\( d_{\text{obs}} - d_{\text{pre}} \)). In both cases the observed data has been fit less well around the positive and negative peak values. Furthermore, the amplitude of the difference values using the PDE-based forward solution is close to (i.e. within an order of magnitude of) the amplitude of the errors using the integral-based forward solution. This is a favorable result because we are seeking a model that reproduces \( d_{\text{fwd}} \) and that should be the same no matter what method we use to solve the forward problem.

Figure 4.13 shows the behavior of the data misfit and model objective function for the inversion of the total magnetic data. The initial value was \( \beta = 1 \times 10^4 \) (i.e at iteration 0 in Figure 4.13) has high \( \phi_{d} \) and low \( \phi_{m} \) values. As the iterations continue \( \phi_{d} \) and \( \phi_{m} \) settle to limiting values for the initial \( \beta \). At iteration 10 the model objective function was changing slowly enough for the algorithm to break from inner iterative process (i.e model iteration at a constant \( \beta \)). At this point the value of \( \beta \) was reduce and the minimization continue. This process is repeated until \( \phi_{d} \) is close enough to the target misfit and the inversion algorithm quit.
Figure 4.11: Maps for various data quantities associated with the gravity inversion. The predicted data, $g_{z}^{\text{pre}}$, using integral-based and PDE-based forward models are shown in (a) and (b) respectively. Differences, $(g_{z}^{\text{obs}} - g_{z}^{\text{pre}})$, using integral-based and PDE-based forward at (c) and (d) respectively.
Figure 4.12: Maps for various data quantities associated with the magnetic inversion. The predicted data, $\Delta T^{pre}$, using integral-based and PDE-based forward models are shown in (a) and (b) respectively. Differences, $(\Delta T^{obs} - \Delta T^{pre})$, using integral-based and PDE-based forward at (c) and (d) respectively.
Figure 4.13: Values of the data misfit (a), model objective function (b). The circle values are those at the beginning of each outer iteration (i.e. the initial values for each value of $\beta$).

Figure 4.14 shows the Tikhonov curve for the gravity inversion. The curve characteristics are as expected; $\phi_m$ increases with increasing $\beta$ and $\phi_d$ decreases with increasing $\beta$. The target misfit is $f_d^* = 435$ corresponding to a beta value of $\beta = 0.002$.

Figure 4.14: L-curve for the gravity inversion.
4.9 Summary

I use a finite-volume forward modeling approach to invert gravity and magnetic data. The magnetic inverse problem is non linear and when positivity constrains are imposed the gravity inverse problem is also non linear. I solve the problem using a Gauss-Newton approach in which the sensitivities are never explicitly formed and only sparse discrete operators are stored. I demonstrate the applicability of the method by inverting 773 magnetic data and 443 gravity data on a mesh consisting of 100800 cells. The results are consistent with inversion results based on integral equation-based forward model.
CHAPTER 5
CONCLUSIONS

The goal of this research was to extend the current partial differential equations (PDE)-based forward modeling methods of gravity and magnetostatics by incorporating gravity gradiometry data and the effect of anisotropy in magnetic susceptibility respectively. This chapter reviews the main conclusions regarding the extensions in the forward models and their incorporation in the inversion of field data. Moreover, possible improvements are considered for future research.

Gravity Field: I developed a solution of Poisson’s equation for scalar components of the gravity field and gravity gradient tensor. I referred to this approach as the “direct formulation” (Chapter 2). The direct solution was compared to the fields obtained from the solution of the traditional Poisson’s equation for the gravitational potential, which were referred to the “indirect solution”. The governing equation of both approaches were solved using the finite volume method with Robin boundary conditions. The numerical solutions were validated using analytic closed form solutions for a prism; relative errors were less than 1 % and, as expected, accuracy improved with refined discretization. The motivation of a direct solution was to approximate the gravity field with the same accuracy as the indirect solution using a smaller mesh extend. Since the gravity field decays faster (1/r^2) than the potential (1/r), for a given mesh size, the far field approximation at the boundaries is closer to the true field for the direct solution. However, the direct solution is not more accurate. Solving Poisson’s equation for gravity requires approximating the derivatives of density distribution at cell faces and that approximation reduces the precision of the solution. In addition, the direct solution is more complicated to implement as it requires a dual cell scheme for the finite volume discretization. Nevertheless, the direct solution can be used in an inversion algorithm
to recover the gradient of the density instead of a density distribution.

**Anisotropy in magnetic susceptibility:** I have successfully incorporated anisotropy in magnetic susceptibility into the current PDE-based forward modeling methods for source free magneto-statics (Chapter 3). The governing equations were solved using the finite volume method (FVM) with Neumann boundary conditions. The numerical solution has also been validated with a known analytical solutions from a prim and also with results that comes from the theoretical framework of the ellipsoid of anisotropy. Anisotropy causes a reduction in the amplitude of the magnetic response and causes the magnetization vector to deflect directly towards the axis of maximum susceptibility. The magnitude of the deflection depends on the degree of anisotropy and on the direction of the external field with respect to the principal axes of anisotropy. All numerical solutions substantiated these theoretical conclusions; for a moderate level of discretization the errors were below 15 %.

**Inversion:** I used the PDE-based forward algorithms to invert potential field data collected over a copper-lead-zinc deposit in the Stratmat mine site (Chapter 4). The magnetic inversion is for isotropic susceptibility only and the gravity inversion uses the “indirect solution” (i.e. the solution Poisson’s equation for the gravitational potential). The survey consists of 443 gravity and 779 magnetic data points. The subsurface was discretized using an irregular rectilinear grid of $10^5$ cells. The inverse problem was formulated as an optimization problem in which the sensitivities are never explicitly formed and only discrete operators are stored. When comparing the recovered models using the PDE-based inversion against the integral-based inversion, the density models are structurally similar, however, the PDE-based magnetic inversion recovered additional structure not prominent in the integral based recovered model. Furthermore the PDE-based inversion places the anomalies at greater depths. To this respect, the
depth weighting function has a stronger effect in the PDE-based solution. While the susceptibility models recover similar features, this illustration is meant to show the PDE vs. integral inversion applied to field data. Interpretation of the two models should be based on geologic knowledge and is outside the scope of this work.

5.1 Future research

Real world problem: For cases where realistic scenarios are considered, future research directions may take advantage from the state-of-the-art in the field of numerical solution of partial differential equations. Mainly four techniques can be included in the PDE based-forward model of potential fields, namely: unstructured grids, adaptivity, multi-grid methods and parallelism. Structured grids generally lead to accurate and fast solvers. However, for situations where the complexity of the domain is such that a structured requires a very large number of cells, unstructured grids are advantageous [13]. Adaptive grid refinement provides a local enhancement of resolution of the total solution with a minimum number of grid points Haber et al. [14]. Multigrid methods are well known for being the fastest numerical methods for solving elliptical PDEs [15]. Finally, the methods above mentioned can be parallelized to take advantage of modern computational resources and maximize the speed of the algorithms. The improvements suggested above can make feasible the solutions of larger and more complicated inverse problems than the case studies considered in the present thesis.

Accuracy: Accuracy is important because we want the numerical solution be closer to the true value. In the present work, the flux integrals are approximated using the midpoint rule, which lead to convergence at a rate $O(h^2)$ for gravity components and $O(h)$ for gravity gradients. To improve accuracy in the solution, higher order finite volume method are necessary [4].
APPENDIX A - INTEGRAL EQUATION SOLUTION

In this appendix, we present a full solution for arbitrary distributions of anisotropic susceptibility developed in the integral equation domain. The 3-D distribution is approximated by small rectangular; by summing the effect of the total number of prism, the magnetic field of the whole body is evaluated. This solution uses analytical expressions for each prismatic cell and is appropriated for modeling the response of or complicated distributions. Thus, the integral equation provides a method of comparison against the finite volume solutions.

A.1 Full solution of the magnetic problem

In the presence of a external field such as the geomagnetic field, many rocks and minerals are magnetized by induction and cause small variations or ”anomalies” in the Earth’s main field. At each observation location the effective field is the vectorial sum of the external field \(H_0\) and the secondary field, \(H_s\)

\[
H = H_0 + H_s
\]  

(A.1)

The secondary field is given by [16]

\[
H_s = \frac{1}{4\pi} \int_{V} M(q) \cdot \nabla \nabla \frac{1}{|r - q|} dq
\]  

(A.2)

where \(M\) is the induce magnetization within the material, \(r\) represents the position of the observer and \(q\) represents the position of the volume element \(dv\). When the material is isotropic, linear and contains no remanent magnetization, the corresponding equation for the effective magnetization is given by

\[
M = \kappa H_0 + \kappa \left[ \frac{1}{4\pi} \int_{V} M(q) \cdot \nabla \nabla \frac{1}{|r - q|} dq \right]
\]  

(A.3)

If we approximate the magnetic material as an assemblage of \(nc\) small prismatic cells and assume a uniform magnetization \(M\) all over each cell, the above equation A.3 can be written
in terms of components,

\[ M_i^p = \kappa^p H_{0i} + \kappa^p \sum_{u=1}^{nc} \left[ \sum_{k=1}^{3} T_{ik}^{pu} M_k^u \right] \]  

(A.4)

where

\[ T_{ik} = \int_V \nabla \nabla \frac{1}{|r - q|} \]  

(A.5)

Analytical expression for the various \( T_{ik} \) components for the case of a rectangular prism are given in [17]. For the case when there is anisotropic susceptibility the above equation A.4 becomes

\[ M_i^p = \kappa^p_{ij} \left( H_{0j} + \sum_{u=1}^{nc} \left[ \sum_{k=1}^{3} T_{jk}^{pu} M_k^u \right] \right) \]  

(A.6)

A.6 represent a linear system of 3n equations of with 3n unknowns which can written in a matrix-vector form as

\[ \mathbf{m} = \mathbf{K}(\mathbf{H}_0 + \mathbf{Tm}) \]  

(A.7)

where

\[ \mathbf{K} = \begin{pmatrix} K_{xx} & K_{xx} & K_{xx} \\ K_{xx} & K_{yy} & K_{xx} \\ K_{xx} & K_{xx} & K_{zz} \end{pmatrix} \]  

with \[ \mathbf{K}_{xx} = \begin{pmatrix} \kappa_{xx} \\ \vdots \end{pmatrix} \]  

(A.8)

\[ \mathbf{H}_0 = \begin{pmatrix} H_{0x} \\ H_{0x} \\ H_{xx} \end{pmatrix} \]  

(A.9)

\[ \mathbf{T} = \begin{pmatrix} T_{xx} & T_{xx} & T_{xx} \\ T_{xx} & T_{yy} & T_{xx} \\ T_{xx} & T_{xx} & T_{zz} \end{pmatrix} \]  

(A.10)

\( \mathbf{K} \) is a 3nc by 3nc matrix with the susceptibilities components, \( \mathbf{H}_0 \) is a length 3nc vector formed by repeating each component of the inducing field nc times and stacking and \( \mathbf{T} \) is a 3nc by 3nc full matrix. .... A.7 can be rearranged into an equation of the form

\[ (\mathbf{I} - \mathbf{KT}) \mathbf{m} = \mathbf{KH}_0 \]  

(A.11)
which has the form $Ax = b$ and can be solve using iterative method form linear algebra.

If we assumes the observation location in free space the magnetic flux is calculated as

$$B = \mu_0 Tm$$  \hspace{1cm} \text{(A.12)}

The solution of the system in A.11 for the magnetizations requires many operations and for large scale problems the full matrix $T$ requires considerable construction time and memory.
APPENDIX B - BOUNDARY CONDITIONS IMPLEMENTATION

In this appendix I show how I implement Robin boundary condition. Let us consider a one-dimensional problem and refer the discretized line in Figure B.1.

The equations to discretize is

\[
\frac{d^2 \phi}{dx^2} = -4\pi\gamma\rho \tag{B.1}
\]

and is subject to the following Robin boundary conditions

\[
\frac{\partial \phi}{\partial x} + \alpha \phi = 0 \tag{B.2}
\]

The boundary conditions are used to define \( \phi \) at cell faces that constitute the grid boundary. First, we write \( \phi \) as a finite difference including a ghost cell, \( \phi_0 \).

\[
\frac{\phi_1 - \phi_0}{\Delta x_0} + \alpha \phi(x_1) = 0 \tag{B.3}
\]

Then we average over cells \( \phi_0 \) and \( \phi_1 \) to find the intermediate value.

\[
\phi(x_1) = \frac{\phi_0 + \phi_1}{2} \tag{B.4}
\]

The dependence on ghost cell, \( \phi_0 \), can be eliminated via substitution into equation B.3.

\[
\phi_0 = \frac{(2 + \alpha \Delta x_0)}{(2 - \alpha \Delta x_0)} \phi_1 \tag{B.5}
\]
B.1 Finite volume discretization

Discretization of the divergence

\[ \int_{x_i}^{x_{i+1}} \frac{d\phi}{dx} dx \approx g_{i+1} - g_i = -4\pi\gamma \rho_i h_i \]  \hspace{1cm} (B.6)

Dividing by the length of the cell yields

\[ h_i^{-1} g_{i+1} - h_i^{-1} g_i = -4\pi\gamma \rho_i, \quad i = 1, \ldots, n \]  \hspace{1cm} (B.7)

The corresponding matrix-vector equation is

\[
\begin{pmatrix}
- h_1^{-1} & h_1^{-1} & & & \\
- h_2^{-1} & h_2^{-1} & & & \\
& & \ddots & & \\
- h_n^{-1} & h_n^{-1} & & & \\
\end{pmatrix}
\begin{pmatrix}
g_1 \\
g_2 \\
\vdots \\
g_n \\
g_{n+1}
\end{pmatrix}
= 4\pi\gamma
\begin{pmatrix}
\rho_1 \\
\rho_2 \\
\vdots \\
\rho_n
\end{pmatrix}
\]  \hspace{1cm} (B.8)

Discretization of the gradient

\[ \int_{x-1/2}^{x+1/2} g dx = \int_{x-1/2}^{x+1/2} \frac{d\phi}{dx} dx \]  \hspace{1cm} (B.9a)

\[ g_i \Delta x_{i-1} = \phi_i - \phi_{i-1} \]  \hspace{1cm} (B.9b)

\[ g_i = \Delta x_{i-1}^{-1} \phi_i - \Delta x_{i-1}^{-1} \phi_{i-1}, \quad i = 1, \ldots, n \]  \hspace{1cm} (B.9c)

A cell on a grid boundary would produce an equation of the form
\[ g_1 = \Delta x_0^{-1} \phi_1 - \Delta x_0^{-1} \phi_0 \]  
\quad (B.10)

Assuming \( \Delta x_0 = \Delta x_1 \) and replacing \( \phi_0 \) by equation B.5

\[ g_1 = \Delta x_1^{-1} \phi_1 - \Delta x_1^{-1} \frac{(2 + \alpha \Delta x_1)}{(2 - \alpha \Delta x_1)} \phi_1 \]  
\quad (B.11)

The corresponding matrix-vector equation is

\[
\begin{bmatrix}
  g_1 \\
g_2 \\
  \vdots \\
g_n \\
g_{n+1}
\end{bmatrix} =
\begin{bmatrix}
  \Delta x_1^{-1} & \Delta x_1^{-1} \\
  -\Delta x_1^{-1} & \Delta x_1^{-1} \\
  \vdots & \vdots \\
  -\Delta x_n^{-1} & \Delta x_n^{-1} \\
  -\Delta x_n^{-1} & -\Delta x_n^{-1}
\end{bmatrix}
\begin{bmatrix}
  \phi_1 \\
  \phi_2 \\
  \vdots \\
  \phi_n
\end{bmatrix} +
\begin{bmatrix}
  -c_1 \Delta x_1^{-1} \\
  0 \\
  \vdots \\
  0 \\
  c_n \Delta x_n^{-1}
\end{bmatrix}
\begin{bmatrix}
  \phi_1 \\
  \phi_2 \\
  \vdots \\
  \phi_n
\end{bmatrix}
\]
\quad (B.12)

where

\[ c_1 = \frac{(2 + \alpha \Delta x_1)}{(2 - \alpha \Delta x_1)} \quad \text{and} \quad c_n = \frac{(2 + \alpha \Delta x_n)}{(2 - \alpha \Delta x_n)} \]  
\quad (B.13)

To summarize, the discrete equations are

\[ Dg = m \]  
\quad (B.14)

\[ g = (G + C)u \]  
\quad (B.15)

which combine yield

\[ (DG + DC)u = m \]  
\quad (B.16)

\[ (A + F)u = m \]  
\quad (B.17)
APPENDIX C - ANISOTROPIC PRISM

The magnetic field due to a rectangular prism was derived by Bhattacharyya [18] starting with

\[ \mathbf{B} = \frac{\mu_0}{4\pi} \nabla P \int_R \mathbf{M} \cdot \nabla_Q \frac{1}{r} dv \]  \hspace{1cm} (C.1)

where \( \mu_0 \) is the magnetic permeability of free space, \( \mathbf{M} \) is the magnetization, and \( r \) is the distance from the observation point \( P \) to the element \( dv \) of the body located at point \( Q \). Each prism is oriented parallel to the \( x \), \( y \) and \( z \) axes and has magnetization

\[ \mathbf{M} = \mathbf{K} \cdot \mathbf{H}_0 \]  \hspace{1cm} (C.2)

Where \( \mathbf{H}_0 = \mathbf{B}_0/\mu_0 \) and \( \mathbf{K} \) is referred as the apparent susceptibility [19]. If the axis of symmetry of the body are parallel to its principal direction of anisotropy, and if the principal susceptibilities \( k_x \), \( k_y \), and \( k_z \) are parallel to the \( x \), \( y \), and \( z \) axes the components of the apparent susceptibility are

\[ K_i = \frac{k_i}{1 + N_i k_i}, \quad (i = x, y, z) \]  \hspace{1cm} (C.3)

where \( N_i \) are the demagnetization factors. For a cube, \( N_x = N_y = N_z = 1/3 \). Then, equation C.2 simplifies to

\[ M_x = K_x B_{0x}/\mu_0 \]  \hspace{1cm} (C.4a)

\[ M_y = K_y B_{0y}/\mu_0 \]  \hspace{1cm} (C.4b)

\[ M_z = K_z B_{0z}/\mu_0 \]  \hspace{1cm} (C.4c)
The dimensions of the prism are given by \( x_1 \leq x \leq x_2, \ y_1 \leq y \leq y_2 \) and \( z_1 \leq z \leq \infty \). If the external field has \( B_0 \) and direction \( \hat{B}_0 = (\hat{B}_{0x}, \hat{B}_{0y}, \hat{B}_{0z}) \), then the total magnetic anomaly observed at the origin is given by Blakely [16],

\[
\Delta T = \frac{\mu_0}{4\pi} M \left[ \frac{c_{23}}{2} \log \left( \frac{r - x'}{r + x'} \right) + \frac{c_{13}}{2} \log \left( \frac{r - y'}{r + y'} \right) - c_{12} \log (r + z_1) \right. \\
- \hat{M}_x \hat{B}_{0x} \tan \left( \frac{x' y'}{x'^2 + rz_1 + z_1^2} \right) - \hat{M}_y \hat{B}_{0y} \tan \left( \frac{x' y'}{r^2 + rz_1 + x'^2} \right) \\
\left. + \hat{M}_z \hat{B}_{0z} \tan \left( \frac{x' y'}{r z_1} \right) \right] \bigg|_{x' = x_1, \ y' = y_1} \bigg|_{x' = x_2, \ y' = y_2} \tag{C.5}
\]

where

\[
M = \sqrt{M_x^2 + M_y^2 + M_z^2} \\
c_{12} = \hat{M}_z \hat{B}_{0y} + \hat{M}_y \hat{B}_{0z} \\
c_{13} = \hat{M}_x \hat{B}_{0y} + \hat{M}_y \hat{B}_{0x} \\
c_{23} = \hat{M}_x \hat{B}_{0z} + \hat{M}_z \hat{B}_{0x} \\
r^2 = x^2 + y^2 + z_1^2 \tag{C.6}
\]

In order to calculate the total magnetic anomaly due to a prism with top at \( z_1 = z_t \) and bottom at \( z_1 = z_b \) equation C.5 needs to be evaluated twice, once for \( z_t \) and magnetization \( M \) and once for \( z_b \) and magnetization \( -M \).
REFERENCES CITED


