A fast forward algorithm for three-dimensional gravity gradient tensor using the compact difference schemes

Shuanggui Hu¹,², Kejia Pan¹ and Jingtian Tang²

¹ School of Mathematics and Statistic, Central South University, Changsha, China
² School of Geosciences and Info-Physics, Central South University, Changsha, China
E-mail: hushuanggui808@csu.edu.cn

Abstract. We propose a fast and accurate 3D large-scale forward modeling method to compute the gravity gradient tensor, in terms of a fourth-order compact finite difference scheme and the extrapolation cascadic multigrid (EXCMG) method. Firstly, the 19-point fourth-order compact finite difference scheme with unequal mesh sizes in different coordinate directions is used to discretize the governing 3D Poisson equation. The resulted symmetric positive definite linear systems are solved by the EXCMG method. Then, the second-order derivatives (gravity gradient tensor) are calculated by solving a series of tridiagonal linear systems resulting from the fourth-order compact finite difference discretization. Finally, numerical result for a cubic model with positive density is used to verify the accuracy of our presented method. It shows that our method can give nearly fourth-order accurate approximations to gravitational potential and gravity gradient tensor. The accuracy is much higher and more efficient than traditional finite difference methods.

1. Introduction
Airborne gravity gradiometry surveying methods are widely used in mineral resource exploration and environmental monitoring [1]. 3D forward modeling of airborne gravity gradient tensor plays an important role in anomaly interpretation [2]. Early studies in term of 3D gravity modeling mainly focused on the analytical methods [3,4]. The main advantage of the analytical methods may be that they are easy to implement (Li & Chouteau, 1998). However, one disadvantage of the analytical methods is relatively poor efficiency in the context of 3D large scale inversion. For instance, the complexity (degree of freedom) of these algorithms grows to \( O(M \times N) \), where \( N \) is the number of gravity data and \( M \) is the number of cells of the grid [5].

The PDE-based techniques can synthesize gravitational potential, gravity field and its gradient tensor data at a time, that is, the algorithm complexity is nearly \( O(M) \) which is independent of the amount of data [6]. The PDE-based methods mainly include the finite difference method, the finite volume method and the finite element method. The finite element and the finite volume methods can be applied to subsurface models with arbitrary geometries [7,8]. But they usually take a long calculation time and require a lot of memory. Due to easy to implement, the finite difference method is also applied to solve 3D Poisson’s equation. Farquharson & Mosher developed 3D gravity modeling method using the finite difference method and regular grids [9]. However, the traditional finite difference method needs dense grid to reach the required accuracy. And these traditional finite difference methods have only second-order calculation accuracy. However, traditional center difference approximation leads to \( O(1) \) error when computing second-order derivatives with the second-order accurate gravity potential.
To overcome the shortcoming of the finite difference methods, the compact difference schemes have been presented for evaluating spatial derivatives and solving PDE [10,11]. For instance, Spotz & Carey [12] developed a high-order compact formulation for the 3D Poisson equation. And Chavarria et al. applied this compact difference algorithm to modeling gravity gradient tensor data with second-order accuracy [13]. However, this scheme is only suitable for equal meshing in different coordinate directions. To discretize 3D Poisson equation with unequal meshing in x, y and z coordinate directions, Wang et al. presented a stable compact difference scheme with unrestricted general meshsizes in different coordinate directions [10]. The scheme has the characteristics of the fourth-order accuracy and is easier to understand in complex manipulations. But it has not yet been applied to solve geophysical problems.

In this paper, we present a fourth-order compact finite difference scheme with the EXCMG method for solving the boundary value problem of 3D gravity Poisson equation. Then, we verified the effectiveness and reliability of the proposed algorithm by testing it on a cube model with positive density. The results show that our developed method not only can reduce the computational time, but also can maintain high-order accuracy.

2. Algorithm

2.1. 3D Poisson equation and its boundary condition

According to Gauss’s law, the 3D gravity Poisson equation satisfying the boundary value problem is derived as [14]:

\[ \nabla^2 \phi(\mathbf{r}) = -4\pi G \rho(\mathbf{r}), \quad \mathbf{r} \in \Omega, \]  

(1)

where \( G = 6.674 \times 10^{-11} \text{N} \cdot \text{m}^2 / \text{kg}^2 \) represents the universal gravitational constant, \( \phi(\mathbf{r}) \) is the gravitational potential in the spatial domain and \( \rho(\mathbf{r}) \) is the residual density; \( \mathbf{r} \) is the distance vector between the mass body and the observation point \( (x_0, y_0, z_0) \); \( \Omega \) represents a three-dimensional rectangular domain.

In this study, the problem domain is truncated into a finite length 3D box, denoted as \( \partial \Omega \). When the boundary is far enough from the center area, we can use far-field approximated potential values as boundary values so that the computational domain is further reduced [15]:

\[ \phi(\mathbf{r}) = GM / r, \quad \mathbf{r} \in \partial \Omega, \]  

(2)

in which \( M \) is the total mass in computational domain, \( \mathbf{r} \) is the distance vector between the center \( (x_c, y_c, z_c) \) of the equivalent sphere and the point \( (x, y, z) \) on the boundary surface.

2.2. The fourth-order compact finite difference scheme

As shown in Fig. 1, we consider a cubic domain \( \Omega = [0, L_x] \times [0, L_y] \times [0, L_z] \), and discretize the domain with unequal meshsizes \( h_x, h_y \) and \( h_z \) in the \( x, y \) and \( z \) coordinate directions, respectively. Define \( N_x = L_x / h_x \), \( N_y = L_y / h_y \) and \( N_z = L_z / h_z \) as the numbers of uniform intervals along the \( x, y \) and \( z \) coordinate directions. The grid points are \( (x_i, y_j, z_k) \), with \( x_i = ih_x \), \( y_j = jh_y \) and \( z_k = kh_z \), \( i = 0, 1, \ldots, N_x \), \( j = 0, 1, \ldots, N_y \) and \( k = 0, 1, \ldots, N_z \).
Figure 1. The schematic diagram of the 19-point fourth-order compact difference scheme as shown in Eq. (3) for internal grid points.

For internal grid points, the fourth-order compact difference scheme for the 3D gravity Poisson equation as shown in Eq. (1) (Wang et al., 2006; Pan et al., 2017) can be written out explicitly,

\[
-8 \left( \frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2} \right) \phi_{i,j,k} + \left( \frac{4}{h_x^2} - \frac{1}{h_y^2} - \frac{1}{h_z^2} \right) \left( \phi_{i+1,j,k} + \phi_{i-1,j,k} \right) \\
+ \left( \frac{4}{h_x^2} - \frac{1}{h_y^2} - \frac{1}{h_z^2} \right) \left( \phi_{i,j+1,k} + \phi_{i,j-1,k} \right) + \left( \frac{4}{h_x^2} - \frac{1}{h_y^2} - \frac{1}{h_z^2} \right) \left( \phi_{i,j,k+1} + \phi_{i,j,k-1} \right) \\
+ \frac{1}{2} \left( \frac{1}{h_x^2} + \frac{1}{h_y^2} \right) \left( \phi_{i+1,j+1,k} + \phi_{i+1,j-1,k} + \phi_{i-1,j+1,k} + \phi_{i-1,j-1,k} \right) \\
+ \frac{1}{2} \left( \frac{1}{h_x^2} + \frac{1}{h_y^2} \right) \left( \phi_{i+1,j,k+1} + \phi_{i+1,j,k-1} + \phi_{i-1,j,k+1} + \phi_{i-1,j,k-1} \right) \\
+ \frac{1}{2} \left( \frac{1}{h_x^2} + \frac{1}{h_y^2} \right) \left( \phi_{i,j+1,k+1} + \phi_{i,j-1,k+1} + \phi_{i,j+1,k-1} + \phi_{i,j-1,k-1} \right) \\
= \frac{1}{2} \left( 6f_{i,j,k} + f_{i+1,j,k} + f_{i-1,j,k} + f_{i,j+1,k} + f_{i,j-1,k} + f_{i,j,k+1} + f_{i,j,k-1} \right). 
\]

On the boundary points, the values \( \phi_{i,j,k} \) can be calculated directly from the boundary condition.

At each interior grid point, there is a linear equation of the form Eq. (3). Labeling the grid points lexicographically, we obtain the sparse linear system

\[
A \psi = f
\]

where \( A \) is a sparse positive definite matrix, \( \psi \) is the solution vector, and \( f \) denotes the right-hand side vector. The coefficient matrix \( A \) is symmetric positive defining M-matrix with 19 nonzero elements in each row.

2.3. Extrapolation cascadic multigrid method with compact difference scheme

For small-scale problem, we can use the Bi-conjugate gradients stabilized method (BICGSTAB) algorithm to solve the sparse linear system as shown in Eq. (4). For large-scale problem, the Eq. (4)
forms a large sparse algebraic system. We should expect a fast convergence rate for most iterative methods used to solve this system. A popular choice is the extrapolation cascading multigrid (EXCMG) method. The advantages of the EXCMG method are extrapolation and high-order interpolation, which can produce a much better initial guess of the iterative solution on the next finer grid (Pan et al., 2017). The algorithm for solving the large sparse algebraic system with the EXCMG method is summarized as shown in Algorithm 1.

| Algorithm 1 The EXCMG method with compact difference scheme |
|-------------------------------------------------------------|
| 1: \( u_{H} \Leftarrow \text{BICGSTAB} (A_{H} u_{H} = f_{H}) \) |
| 2: \( u_{H/2} \Leftarrow \text{BICGSTAB} (A_{H/2} u_{H/2} = f_{H/2}) \) |
| 3: \( h_{i} = H_{i}/2, h_{i} = H_{i}/2, h_{i} = H_{i}/2 \) |
| 4: \( \text{for } i = 1 \text{ to } L \text{ do} \) |
| 5: \( h_{i} = h_{i}/2, h_{i} = h_{i}/2, h_{i} = h_{i}/2 \) |
| 6: \( u_{h} = \text{EXP}_{\text{mul}}(u_{2h}, u_{4h}) \) |
| 7: \( \text{while } ||A_{h} u_{h} - f_{h}||_{2} > \varepsilon \cdot ||f_{h}||_{2} \text{ do} \) |
| 8: \( u_{h} \Leftarrow \text{BICGSTAB} (A_{h}, u_{h}, f_{h}) \) |
| 9: \( \text{end while} \) |
| 10: \( u_{h} = \text{EXP}_{\text{mul}}(u_{2h}, u_{4h}) \) |
| 11: \( \text{end for} \) |

2.4. Calculation of the gravity gradient tensor

After solving Eq.(4), the gravitational potential with fourth-order accuracy can be obtained. The gravity gradient tensor can be obtained from the second-order derivatives of the gravitational potential as follows:

\[ \mathbf{T} = \nabla \nabla \phi. \]  

(5)

The gravity gradient tensor is usually obtained by numerical differentiation. Most algorithms used for geophysical applications use a second-order finite difference approximation for the discretization of differential operator (Farquharson & Mosher, 2009; Haber et al., 2014). However, traditional center difference approximation leads to \( O(1) \) error when computing second-order derivatives with the second-order accurate gravity potential. Therefore, we should develop a high-accuracy method for gravity gradient tensor modeling. Taking the second-order derivative of the gravitational potential as example, that on the top and bottom boundary surfaces are also firstly calculated using the one-side five-point difference approximation:

\[ T_{x}^{i,j,0} = \frac{1}{12h_{x}^{2}} \left( 35\phi_{i,j,0} - 104\phi_{i,j,1} + 114\phi_{i,j,2} - 56\phi_{i,j,3} + 11\phi_{i,j,4} \right), i = 0,1,\ldots,N_{x}; j = 0,1,\ldots,N_{y}, \]  

(6)

\[ T_{x}^{i,j,N_{x}} = \frac{1}{12h_{x}^{2}} \left( 35\phi_{i,j,N_{x}} - 104\phi_{i,j,N_{x} - 1} + 114\phi_{i,j,N_{x} - 2} - 56\phi_{i,j,N_{x} - 3} + 11\phi_{i,j,N_{x} - 4} \right), \]  

\[ i = 0,1,\ldots,N_{x}; j = 0,1,\ldots,N_{y}. \]  

(7)

Then, we can obtain \( T_{x}^{i,j,k} (k = 1,2,\ldots,N_{z} - 1) \) on the internal grid points by solving the following linear system resulting from the fourth-order compact FD scheme.
The above tridiagonal system can also be solved fast by the Thomas algorithm. Clearly, the other components can be obtained from similar procedures.

2.5. Algorithm instance
To evaluate the algorithm presented here, a simple density model comprising a dense cube in a zero-density background is been used. The cubic model comprises a \(100m \times 100m \times 100m\) cube of \(2000\text{kg/m}^3\) in a zero density background with \(1000m \times 1000m \times 1000m\). The origin of the coordinates is located at the center of the cube.

The analytical solution and the numerical solution from our algorithm for uniform grid on \(161 \times 161 \times 161\) mesh are shown in Fig. 2. The differences between the analytical solution (Li & Chouteau 1998) and the numerical solution from our algorithm are also shown in these figures. From Fig. 2, we find that the maximum absolute errors on plane \(h = 100m\) for gravitational potential \(\phi\) is \(1.59 \times 10^{-9} \text{m}^2 \text{s}^{-2}\). The high accurate gravitational potential guarantees to obtain high accurate gravity gradient tensor. The maximum absolute errors for the principal diagonal components of the gravity gradient data \(T_{xx}, T_{yy}\) and \(T_{zz}\) are \(1.25 \times 10^{-7}E\), \(1.25 \times 10^{-4}E\) and \(1.98 \times 10^{-5}E\). It is clear that the differences of the calculation results between our developed algorithm and the analytical solution are quite small. And the maximum absolute errors occurred at the interface of the anomaly and the background medium. From Tab. 1, we further see that the numerical gravitational potential \(\phi\) is a fourth-order approximation to the exact solution in \(L^\infty\)-norms. And the gravity gradient tensor is also nearly fourth-order approximation, which is two orders higher than that of the central difference method.

![Figure 2](image-url)

**Figure 2.** Comparison between numerical solution calculated by our compact finite difference solution and analytical solution (Li & Chouteau, 1998) for the principal diagonal components of gravity gradient tensor of the cubic model on the plane of \(h = 100m\).
The computation time is fundamentally dependent on the number of the cubic cells. The machine used has six processors of 2.60GHz Intel Core i7 and 16GB memory in total. Tab. 2 shows the computation time with different numbers of the cells. We can find the EXCMG method is three times faster than the BICGSTAB method. For tens of millions of grids, the EXCMG only takes a minute and a half.

Table 1. The errors and convergence orders of $U_h$, $T_{xx}h$, $T_{yy}$ and $T_{zz}h$ caused by the synthetic cubic model in $L^\infty$-norms for the numerical results using our proposed algorithm and the finite difference algorithm.

| Type   | Cell number | $\|U_h-U\|_c$ | Order | $\|T_{xx}h-T_{xx}\|_c$ | Order | $\|T_{yy}h-T_{yy}\|_c$ | Order | $\|T_{zz}h-T_{zz}\|_c$ | Order |
|--------|-------------|---------------|-------|------------------------|-------|------------------------|-------|------------------------|-------|
| Compact| 40×40×40    | 2.95E-07      |       | 1.96E-02               |       | 1.96E-02               |       | 1.31E-01               |       |
|        | 80×80×80    | 1.85E-08      | 3.99  | 1.83E-03               | 3.42  | 1.83E-03               | 3.42  | 3.29E-03               | 5.32  |
|        | 160×160×160 | 1.59E-09      | 3.55  | 1.25E-04               | 3.87  | 1.25E-04               | 3.87  | 1.98E-04               | 4.05  |
| Central| 40×40×40    | 5.54E-06      |       | 2.41E-01               |       | 2.41E-01               |       | 3.30E-01               |       |
|        | 80×80×80    | 1.54E-06      | 1.84  | 1.00E-01               | 1.27  | 1.00E-01               | 1.27  | 1.23E-01               | 1.42  |
|        | 160×160×160 | 3.91E-07      | 1.98  | 2.69E-02               | 1.90  | 2.69E-02               | 1.90  | 3.27E-02               | 1.91  |

Table 2. The computational time of our proposed method for modeling the gravity gradient tensor caused by the cubic model using the BICGSTAB method and the EXCMG method.

| Cell size   | BICGSTAB | EXCMG | |
|-------------|----------|-------|---|
|             | iteration | residual | time | iteration | residual | time |
| 128×128×128 | 52.0      | 5.8e-09 | 24.87 | 24.5      | 9.3e-09  | 11.94 |
| 256×256×256 | 87.5      | 7.7e-09 | 338.23| 23.5      | 9.0e-09  | 104.03|

3. Conclusion

We have introduced a novel accurate and fast algorithm for modeling of the gravity gradient tensor using the compact difference schemes and the EXCMG method. For the gravitational potential, the 19-point fourth-order compact finite difference scheme was applied to derive the 3D gravity Poisson equation into a symmetric positive definite linear system, which was solved by the EXCMG method. In order to guarantee the correctness of the second derivatives of the gravitational potential, a series of cheap tridiagonal linear systems resulting from the fourth-order compact finite difference discretization are applied to overcome the disadvantages of traditional PDE algorithm. At last, we tested the accuracy and efficiency of our method by applying it to the assessment of the gravity gradient tensor for a cubic model. The testing result demonstrates that our newly presented algorithm had nearly fourth-order convergence accuracy which is much higher than the traditional PDE method. Besides, the EXCMG can greatly improve the calculation efficiency.

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