SUMMARY

A new numerical approach, called the “sub-domain Chebyshev spectral method”, has been developed to calculate differentiations in a curved coordinate system, which may be employed for 2D/3D geophysical forward modelling. The new method utilises non-linear transformations defined by the free-surface topography and subsurface interfaces and incorporates cubic-spline interpolations to convert the global domain into subdomains, and applies Chebyshev points in the model discretisation and computation of the spatial derivatives. Such effort makes the numerical differentiations have “spectral accuracy” inside the subdomains whose boundaries match the free-surface topography and subsurface interfaces.

2D and 3D synthetic experiments have been performed with two geological models, both having different free-surface topographies and sub-surface interfaces. The computational errors of the new approach were compared with traditional finite-difference schemes, and the results show that the sub-domain Chebyshev spectral method is superior to traditional finite-difference method in its accuracy and applicable for all of the geophysical forward modelling problems.

Key words: geophysical forward modelling, numerical differentiation, Chebyshev spectral method, governing equation, numerical solution.

MODELLING SCHEME

2D/3D Geophysical forward modelling solves the governing equation as in the following form:

\[ L(\mathbf{m}, \partial_x, \partial_x) \mathbf{V} = s(\mathbf{r}, \mathbf{r}_s) \quad \mathbf{r}, \mathbf{r}_s \in \Omega. \]  

where \( L() \) is the linear differential operator that depends on the model vector \( \mathbf{m} \) and partial derivatives \( \partial_x \) and \( \partial_{xx} \). The vector \( \mathbf{V}=\{V_a\} \ (a=x,y,z) \) may be the displacement vector \( \mathbf{u} \) in seismic wave modelling, or electromagnetic field \( \mathbf{E} \) or \( \mathbf{H} \) in geo-electromagnetic simulation. The model vector \( \mathbf{m} \) comprises the density \( \rho \) and elastic moduli \( c_{ijkl} \) for seismic modelling, or electric permittivity \( \varepsilon_{r} \) magnetic permeability \( \mu_{i} \) and conductivity \( \sigma_{r} \) for electromagnetic simulation. The right-hand side vector \( s(\cdot) \) is the source vector located at \( \mathbf{r} \) in the domain \( \Omega \). In order to match the free-surface topography, one often employs a curved coordinates system given by

\[ x_i = x_i(\xi_i), \quad (i,k=1,2,3). \]  

According to the chain law, the derivatives in eq.(1) have the following forms:

\[ \partial_x V_a = \partial_{\xi_k} V_a \partial_{\xi_k} \xi_k, \]  

\[ \partial_{xx} V_a = \partial_{\xi_k} \partial_{\xi_k} V_a \partial_{\xi_k} \xi_k + \partial_{\xi_k} V_a \partial_{\xi_k} \xi_k. \]  

It is well known that the spectral method is a modern numerical differentiation technique superior to the traditional finite difference method because of the so-called spectral accuracy. It becomes a popular high accurate solver for various partial differential equations problems (Trefethen, 2000). However, the most disadvantageous aspect of the spectral method for geophysical forward modelling is the high consumption of computer memory and CPU time because standard spectral method employs global domain samples in the calculation of derivatives. This yields to a fully filling-in matrix that makes expensive computations in solving processing, particularly for a large 3D geological model.

To overcome this problem, we developed a new scheme of the spectral method, called “subdomain Chebyshev spectral method”, in which the global domain is divided into non-overlapping subdomains, and Chebyshev points are applied to discretise the subdomains of geological model and calculate the spatial derivatives of governing equations. Such manner leads to a sparse matrix and have the spectral accuracy of numerical differentiations inside the subdomains. In addition, a non-linear coordinate transform and cubic spline interpolations are introduced in the subdomains, so that the Chebyshev-pointed grid automatically matches the free-surface topography and subsurface interfaces. 2D and 3D synthetic experiments show that the new method obtains better convergences of numerical differentiations than traditional finite difference method.

INTRODUCTION

Mathematically, geophysical forward modelling seeks the numerical solution of a partial differential equation (called the governing equation), subject to a Dirichlet or Neumann boundary condition. The simplest traditional solver is the fourth-order scheme and staggered grid approach, both of which are widely used for seismic wave modelling and electromagnetic simulation. The right-hand side vector \( s(\cdot) \) is the source vector located at \( \mathbf{r} \) in the domain \( \Omega \). In order to match the free-surface topography, one often employs a curved coordinates system given by

\[ x_i = x_i(\xi_i), \quad (i,k=1,2,3). \]  

According to the chain law, the derivatives in eq.(1) have the following forms:

\[ \partial_x V_a = \partial_{\xi_k} V_a \partial_{\xi_k} \xi_k, \]  

\[ \partial_{xx} V_a = \partial_{\xi_k} \partial_{\xi_k} V_a \partial_{\xi_k} \xi_k + \partial_{\xi_k} V_a \partial_{\xi_k} \xi_k. \]  

22nd International Geophysical Conference and Exhibition, 26-29 February 2012 - Brisbane, Australia
Here the summation convention of the repeated subscripts k and l has been applied. Equations (3) and (4) may be approximated by

\[
\frac{\partial \mathbf{u}_a}{\partial x} \approx \mathbf{D}_{x} \mathbf{u}_a, \quad \frac{\partial \mathbf{u}_a}{\partial y} \approx \mathbf{D}_{y} \mathbf{u}_a, \quad \frac{\partial \mathbf{u}_a}{\partial z} \approx \mathbf{D}_{z} \mathbf{u}_a, \quad (5)
\]

where \( \mathbf{D}_x, \mathbf{D}_y \), and \( \mathbf{D}_z \) are numerical differentiation operators, i.e. the 1st and 2nd finite-difference matrices; \( \xi_k \) and \( \eta_l \) are vectors whose components are the samples of \( \xi_k \) and \( \eta_l \) at the points defined by \( \mathbf{D}_x \) and \( \mathbf{D}_{xk} \), which can be obtained from eq. (2).

Substituting eq. (5) for eq. (1) and applying the governing equation to each point \( \mathbf{r}_k \in \Omega \), one obtains 3N linear equations

\[
L(\mathbf{m}_k, \mathbf{D}_{xk}^{(k)}, \mathbf{D}_{yk}^{(k)}, \mathbf{D}_{zk}^{(k)}) \mathbf{V}^{(k)} = s(\mathbf{r}_k, \mathbf{r}_l), \quad (k = 1, 2, ..., N), \quad (8)
\]

which involves 3N unknowns of \( \mathbf{V}^{(k)} = (\mathbf{V}_x^{(k)}, \mathbf{V}_y^{(k)}, \mathbf{V}_z^{(k)}) \). Solving eq. (8) subject to a Dirichlet or Neumann boundary condition, one obtains the numerical solutions of \( \mathbf{V}^{(k)} \). Therefore, the key step of the geophysical forward modelling is to find accurate numerical differentiation operators \( \{\mathbf{D}_{xk}^{(k)}, \mathbf{D}_{yk}^{(k)}, \mathbf{D}_{zk}^{(k)}\} \). 

**SUBDOMAIN SPECTRAL METHOD**

As an example here, a 3D case is presented, from which one can easily obtain the 2D case by just removing the y-coordinate. The domain \( \Omega \) is subdivided into subdomains \( \Omega_{ik} = \{x_i, x_l, y_j, y_l, z_k, z_l\} \), for which eq. (2) is replaced with the following

\[
x = \Delta x \xi / 2 + \xi, \quad y = \Delta y \eta / 2 + \eta, \quad z = \Delta z \zeta / 2 + \zeta(x, y), \quad (9)
\]

where \( \Delta x, \Delta y, \Delta z \) are the lengths and middle points of the subdomains, respectively. The function \( \Delta x \Delta y \Delta z \) must be differentiable in the \((x, y)\)-plane and therefore approximated by cubic spline interpolations (Helmuth, 2006). Applying eq. (9) and the Chebyshev differentiation matrix based on the points in the subdomain (Trefethen, 2000):

\[
\xi = \cos(\frac{N_y - \alpha}{N_y - 1} \pi), \quad (1 \leq \alpha \leq N_y), \quad (10)
\]

the operators \( \mathbf{D}_x, \mathbf{D}_{xk}, \mathbf{D}_y, \) and \( \mathbf{D}_{yk} \) are obtained, as well as \( \mathbf{D}_{xk}, \mathbf{D}_{yk} \). Here, \( N_x, N_y, \) and \( N_z \) are the numbers of points in the three directions of the subdomain, and they define the lengths (points) of the differentiation operators.

Apparent, such numerical differentiation operators have the spectral accuracies at the points inside subdomains, but cannot be applied to the points on subdomain boundaries because of possible multiple values. However, for the boundary points, the operators may be replaced with differentiations of Lagrange interpolations defined by the neighbours of the Chebyshev points. Consequently, we have two versions of the differentiation operators \( \mathbf{D}_x \) and \( \mathbf{D}_{xk} \), i.e. \( \{\mathbf{D}_x, \mathbf{D}_{xk}\} = \{\mathbf{D}_x^{(1)}, \mathbf{D}_x^{(2)}\} \) or \( \{\mathbf{D}_x^{(B)}, \mathbf{D}_{xk}^{(B)}\} \), according to the two types of points: inside points (I) and boundary points (B). The operators \( \{\mathbf{D}_x^{(B)}, \mathbf{D}_x^{(1)}\} \) are the standard Chebyshev differentiation matrices and \( \{\mathbf{D}_x^{(B)}, \mathbf{D}_{xk}^{(B)}\} \) become Lagrange differentiation matrix but use the neighbour Chebyshev points. However, no matter either \( \{\mathbf{D}_x^{(B)}, \mathbf{D}_x^{(1)}\} \) or \( \{\mathbf{D}_x^{(B)}, \mathbf{D}_{xk}^{(B)}\} \) is substituted into eq. (5), it will be called the “subdomain Chebyshev spectral method”, because both are based on the Chebyshev points in the subdomains. The only difference is the spatial arrangements of the Chebyshev points for the differentiation operators.

Note that the second order differentiation operator \( \mathbf{D}_{xk}^{(B)} \) may be calculated by

\[
\mathbf{D}_{xk}^{(B)} = (\mathbf{D}_x - \mathbf{D}_{xk}) / 2, \quad (11)
\]

instead of eq. (7). This equation shows that the high order derivatives \( \mathbf{D}_x \mathbf{D}_{xk} \) are not necessary.

As mentioned in the previous section, replacing \( \{\mathbf{D}_x^{(B)}, \mathbf{D}_x^{(1)}\} \) and \( \{\mathbf{D}_x^{(B)}, \mathbf{D}_{xk}^{(B)}\} \) with the finite difference operators, the geophysical forward modelling scheme becomes the traditional finite difference method that has the same form of eq. (8). So, a comparison of the subdomain Chebyshev spectral method with the finite difference approach can be easily made.

**NUMERICAL EXPERIMENTS**

To investigate the accuracy of the subdomain Chebyshev spectral method and compare it with some other methods, i.e. analytic and finite difference methods, two synthetic models were designed. Figure 1 gives the models involving 2D and 3D cases. The following testing functions:

\[
2D: \quad u(x, z) = \cos(2\pi/85) \cos(2\pi/95), \quad (12)
\]

\[
3D: \quad u(x, y, z) = \sin(2\pi/85) \cos(2\pi/85) \sin(2\pi/95), \quad (13)
\]

were chosen as field quantities for the two models, both of which have different free-surface topography and subsurface interfaces. Differentiating eq. (12) and (13), one may obtains the analytic derivatives \( \hat{u}_x \) and \( \hat{u}_z \), which can be used as the true solutions of the subdomain Chebyshev spectral method and any other numerical approach, i.e. finite difference approach. Five numerical differentiation schemes were implemented, which include two subdomain Chebyshev spectral methods (SSP1 and SSP2) and three finite difference

![Figure 1. Synthetic models for subdomain Chebyshev differentiation experiments.](image-url)
approaches (FDM0, FDM1, FDM2). Here, the number “0” stands for the curved coordinate system of the Lagrange interpolations for $\Delta z(x,y)$. The integers “1” and “2” represent the high order differentiation operator $D_{\Delta z}$, computed by eq. (7) and (11) respectively, and incorporated the cubic spline interpolations for $\Delta z(x,y)$. Each scheme was performed with different lengths (starting from 3 to 10 points) of the differentiation operators. Figure 2 gives the 2D results for $\Delta z(x,y)$ and the absolute relative errors. Figure 3 shows the convergence curves of the averaged absolute relative errors of the five schemes.

Figure 2. 2D subdomain Chebyshev differentiation results and the absolute relative errors.

Figure 4, 5 and 6 are the 3D results obtained with the seven-point subdomain Chebyshev spectral method. Figure 7, 8 and 9 are the averaged absolute relative errors of the results shown in Figure 4, 5 and 6. From the 2D and 3D results, one can see that the two subdomain Chebyshev spectral methods (SSP1 and SSP2) yield to accurate derivatives whose maximum relative errors are less than 0.28%, and much better than the finite difference methods when the lengths of the differentiation operators are larger than six points. Accordingly, the subdomain Chebyshev spectral method is a new solver for geophysical forward modelling problem.

Figure 4. The 3D first derivatives calculated by the subdomain Chebyshev spectral method.

Figure 5. The 3D secondary derivatives obtained by the subdomain Chebyshev spectral method.

Figure 6. The 3D secondary mixed derivatives calculated by subdomain Chebyshev spectral method.
Conclusively, the subdomain Chebyshev spectral schemes, SSP1 and SSP2, may be applicable for geophysical forward modelling in a complex geological model.

Figure 10. Convergence curves of four numerical differentiation schemes.

ACKNOWLEDGMENTS

This work was supported by the Australian Research Council.

REFERENCES


Helmuth, S., 2006, Two dimensional spline interpolation algorithms, University of Odenburg, Oldenburg, Germany.

Streich, R., 2009, 3D finite-difference frequency-domain modeling of controlled-source electromagnetic data: Direct solution and optimization for high accuracy: Geophysics, 74, F95-F105


CONCLUSIONS

A 2D/3D subdomain Chebyshev spectral method has been developed for numerical differentiations, which may be employed in solving the governing equation of the geophysical forward modelling. Synthetic experiments show that the subdomain Chebyshev spectral method is superior to the finite difference approach in the accuracy of approximation of field quantity derivatives. Particularly, the scheme SSP2 does not need to calculate the high-order derivatives of the transformed coordinates and the high order differentiation operators are obtained by multiplications of the first order differentiation operators.

Figure 7. Absolute relative errors of the first derivatives shown in Figure 4.

Figure 8. Absolute relative errors of the secondary derivatives shown in Figure 5.

Figure 9. Absolute relative errors of the secondary mixed derivatives shown in Figure 6.