A new 2D/3D accurate geophysical forward modelling technique: sub-domain Chebyshev spectral method

Bing Zhou
Dept. of Geology & Geophysics
Adelaide University
bing.zhou@adelaide.edu.au

Graham Heinson
Dept. of Geology & Geophysics
Adelaide University, SA 5005
graham.heinson@adelaide.edu.au

Aixa Rivera-Rios
Dept. of Geology & Geophysics
Adelaide University, SA 5005
aixa.rivera-rios@adelaide.edu.au

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.

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 finite difference method that approximates partial derivatives in the governing equation by finite difference formulae, i.e. the fourth-order scheme and staggered grid approach, both of which are widely used for seismic wave modelling and numerical simulations of geo-electromagnetic fields (see examples, Festa & Vilotte, 2005; Streich 2009). However, due to employing a regular grid, finite difference method suffers from arbitrary free-surface topography and subsurface interfaces. It is limited to geological models whose free-surface topography and subsurface interfaces are described by stepwise curves or stepwise blocks. Though one may apply a curved coordinate system, it often requires high-order analytic functions to define the free-surface topography and subsurface interfaces.

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.

MODELLING SCHEME

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

$$\mathbf{L}(\mathbf{m}, \partial_{x_i}, \partial_{x_i x_j})\mathbf{V} = \mathbf{s}(\mathbf{r}, \mathbf{r}_s), \quad \mathbf{r}, \mathbf{r}_s \in \Omega, \qquad (1)$$

where $\mathbf{L}(.)$ is the linear differential operator that depends on the model vector $\mathbf{m}$ and partial derivatives ∂_{x_i} and $\partial_{x_i x_j}$. The vector $\mathbf{V}=\{V_\alpha\}$ (α=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 ρ and elastic moduli c_{ijkl}: $\mathbf{m}=\{\rho, c_{ijkl}\}$ for seismic modelling, or electric permittivity ε_{ij}, magnetic permeability μ_{ij} and conductivity σ_{ij}: $\mathbf{m}=\{\varepsilon_{ij}, \mu_{ij}, \sigma_{ij}\}$ for electromagnetic simulation. The right-hand side vector $\mathbf{s}(.)$ is the source vector located at $\mathbf{r}_s$ in the domain Ω.

In order to match the free-surface topography, one often employs a curved coordinates system given by

$$x_i = x_i(\xi_k), \quad (i, k = 1,2,3). \qquad (2)$$

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

$$\partial_{x_i} V_\alpha = \partial_{\xi_k} V_\alpha \partial_{x_i} \xi_k, \qquad (3)$$

$$\partial_{x_i x_j} V_\alpha = \partial_{x_i} \xi_k \partial_{\xi_k \xi_l} V_\alpha \partial_{x_j} \xi_l + \partial_{\xi_k} V_\alpha \partial_{x_i x_j} \xi_k. \qquad (4)$$

Here the summation convention of the repeated subscripts k and l. has been applied. Equations (3) and (4) may be approximated by

$$\partial_x V_\alpha \approx \overline{\mathbf{D}}_{x_i} \overline{\mathbf{V}}_\alpha, \quad \partial_{x_i x_j} V_\alpha \approx \overline{\mathbf{D}}_{x_i x_j} \overline{\mathbf{V}}_\alpha, \tag{5}$$

$$\overline{\mathbf{D}}_{x_i} = \mathbf{D}_{x_i} \overline{\xi}_k \cdot \mathbf{D}_{\xi_k}, \tag{6}$$

$$\overline{\mathbf{D}}_{x_i x_j} = \mathbf{D}_{x_i} \overline{\xi}_k \cdot \mathbf{D}_{x_j} \overline{\xi}_l \cdot \mathbf{D}_{\xi_k \xi_l} + \mathbf{D}_{x_i x_j} \overline{\xi}_k \cdot \mathbf{D}_{\xi_k}, \tag{7}$$

where $\mathbf{D}_{\xi_k}$ and $\mathbf{D}_{\xi_k\xi_l}$ are numerical differentiation operators, i.e. the 1st and 2nd finite-difference matrices; $\overline{\xi}_k$ and $\overline{\mathbf{V}}_\alpha$ are vectors whose components are the samples of ξ_k and $\mathbf{V}_\alpha$ at the points defined by $\mathbf{D}_{x_i}$ and $\mathbf{D}_{x_i x_j}$, 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

$$\mathbf{L}(\mathbf{m}_k, \overline{\mathbf{D}}_{x_i}^{(k)}, \overline{\mathbf{D}}_{x_i x_j}^{(k)}) \overline{\mathbf{V}}^{(k)} = \mathbf{s}(\mathbf{r}_k, \mathbf{r}_s), \ (k = 1,2,...N), \tag{8}$$

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

SUBDOMAIN SPECTRAL METHOD

As an example here, a 3D case is presented, from which one can easily obtains the 2D case by just removing the y-coordinate. The domain Ω is subdivided into subdomains $\Omega_{ijk}=[x_{i-1},x_i]\times[y_{j-1},y_j]\times[z_{k-1}(x,y),z_k(x,y)]$, for which eq. (2) is replaced with the following

$$\begin{aligned} x &= \Delta x_i \xi / 2 + \overline{x}_i, \\ y &= \Delta y_j \eta / 2 + \overline{y}_j, \\ z &= \Delta z_k(x,y) \varsigma / 2 + \overline{z}_k(x,y), \end{aligned} \tag{9}$$

where $\{\Delta x_i, \Delta y_j, \Delta z_k(x,y)\}$ and $\{\overline{x}_i, \overline{y}_j, \overline{z}_k(x,y)\}$ are the lengths and middle points of the subdomains, respectively. The function $\Delta z_k(x,y)$ 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):

$$\begin{aligned} \xi_\alpha &= \cos(\frac{N_\xi - \alpha}{N_\xi - 1})\pi, \quad (1 \le \alpha \le N_\xi), \\ \eta_\beta &= \cos(\frac{N_\eta - \beta}{N_\eta - 1})\pi, \quad (1 \le \beta \le N_\eta), \\ \varsigma_\nu &= \cos(\frac{N_\varsigma - \nu}{N_\varsigma - 1})\pi, \quad (1 \le \nu \le N_\varsigma), \end{aligned} \tag{10}$$

the operators $\mathbf{D}_{x_i}$, $\mathbf{D}_{x_i x_j}$, $\mathbf{D}_{\xi_k}$ and $\mathbf{D}_{\xi_k\xi_l}$ are obtained, as well as $\overline{\mathbf{D}}_{x_i}$ and $\overline{\mathbf{D}}_{x_i x_j}$. Here, N_ξ, N_η and N_ς are the numbers of points in the three directions of the subdomain, and they define the lengths (points) of the differentiation operators.

Apparently, 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 $\overline{\mathbf{D}}_{x_i}$ and $\overline{\mathbf{D}}_{x_i x_j}$, i.e. $\{\overline{\mathbf{D}}_{x_i}, \overline{\mathbf{D}}_{x_i x_j}\} = \{\overline{\mathbf{D}}_{x_i}^{(I)}, \overline{\mathbf{D}}_{x_i x_j}^{(I)}\}$ or $\{\overline{\mathbf{D}}_{x_i}^{(B)}, \overline{\mathbf{D}}_{x_i x_j}^{(B)}\}$, according to the two types of points: inside points (I) and boundary points (B). The operators $\{\overline{\mathbf{D}}_{x_i}^{(I)}, \overline{\mathbf{D}}_{x_i x_j}^{(I)}\}$ are the standard Chebyshev differentiation matrices and $\{\overline{\mathbf{D}}_{x_i}^{(B)}, \overline{\mathbf{D}}_{x_i x_j}^{(B)}\}$ become Lagrange differentiation matrix but use the neighbour Chebyshev points. However, no matter either $\{\overline{\mathbf{D}}_{x_i}^{(I)}, \overline{\mathbf{D}}_{x_i x_j}^{(I)}\}$ or $\{\overline{\mathbf{D}}_{x_i}^{(B)}, \overline{\mathbf{D}}_{x_i x_j}^{(B)}\}$ 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 $\overline{\mathbf{D}}_{x_i x_j}$ may be calculated by

$$\overline{\mathbf{D}}_{x_i x_j} = (\overline{\mathbf{D}}_{x_i} \overline{\mathbf{D}}_{x_j} + \overline{\mathbf{D}}_{x_j} \overline{\mathbf{D}}_{x_i}) / 2, \tag{11}$$

instead of eq. (7). This equation shows that the high order derivatives $\mathbf{D}_{x_i x_j} \overline{\xi}_k$ are not necessary.

As mentioned in the previous section, replacing $\{\overline{\mathbf{D}}_{x_i}^{(I)}, \overline{\mathbf{D}}_{x_i x_j}^{(I)}\}$ and $\{\overline{\mathbf{D}}_{x_i}^{(B)}, \overline{\mathbf{D}}_{x_i x_j}^{(B)}\}$ 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:

$$\text{2D}: \quad u(x,z) = \cos(2\pi x/85)\cos(2\pi z/95), \tag{12}$$

$$\text{3D}: \quad u(x,y,z) = \sin(2\pi x/85)\cos(2\pi y/85)\sin(2\pi z/95), \tag{13}$$

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 $\partial_{x_i}\mathbf{u}$ and $\partial_{x_i x_j}\mathbf{u}$, which can be used as

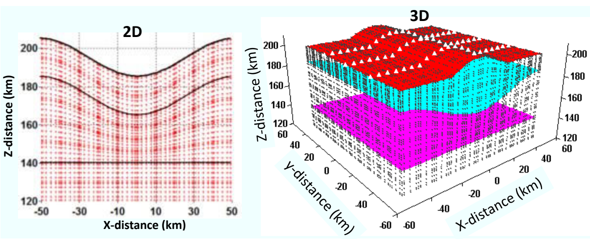

Figure 1. Synthetic models for subdomain Chebyshev differentiation experiments.

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 approaches (FDM0, FDM1, FDM2). Here, the number "0" stands for the curved coordinate system of the Lagrange interpolations for $\Delta z_k(x,y)$. The integers "1" and "2" represent the high order differentiation operator $\overline{\mathbf{D}}_{x_i x_j}$ computed by eq. (7) and (11) respectively, and incorporated the cubic spline interpolations for $\Delta z_k(x,y)$. Each scheme was performed with different lengths (starting from 3 to 10 points) of the differentiation operators. Figure 2 gives the 2D results calculated by the seven-point subdomain Chebyshev spectral method, and Figure 3 shows the convergence curves of the averaged absolute relative errors of the five schemes.

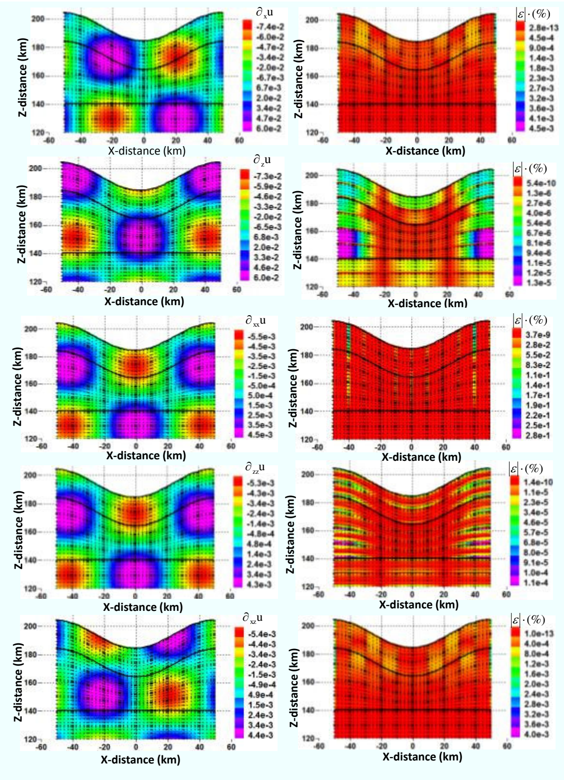

Figure 2. 2D subdomain Chebyshev differentiation results and the absolute relative errors.

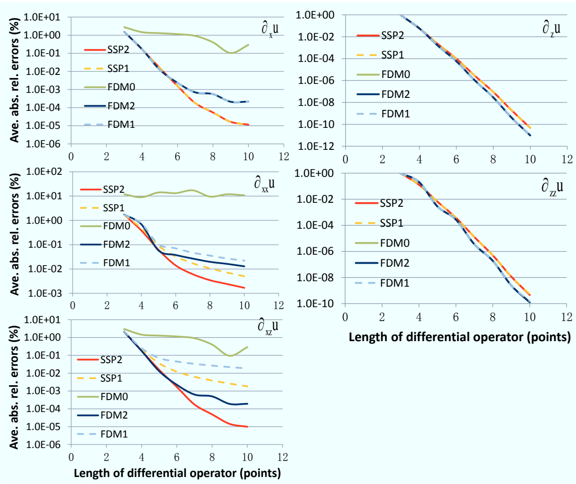

Figure 3. Convergence curves of the averaged absolutely relative errors of five differentiation schemes.

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.

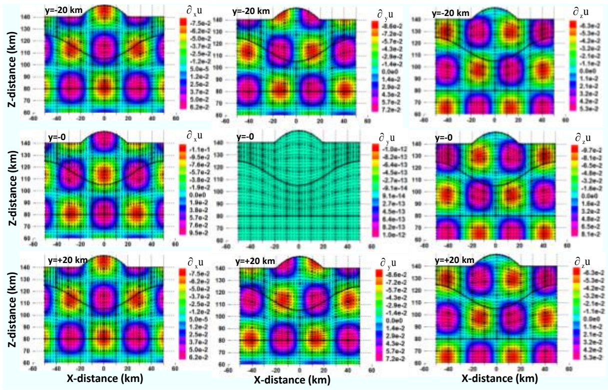

Figure 4. The 3D first derivatives calculated by the subdomain Chebyshev spectral method.

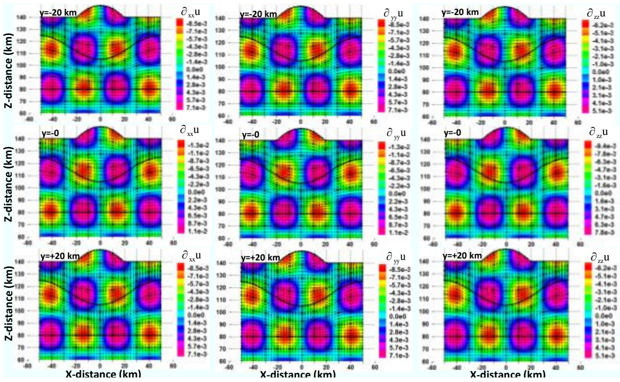

Figure 5. The 3D secondary derivatives obtained by the subdomain Chebyshev spectral method.

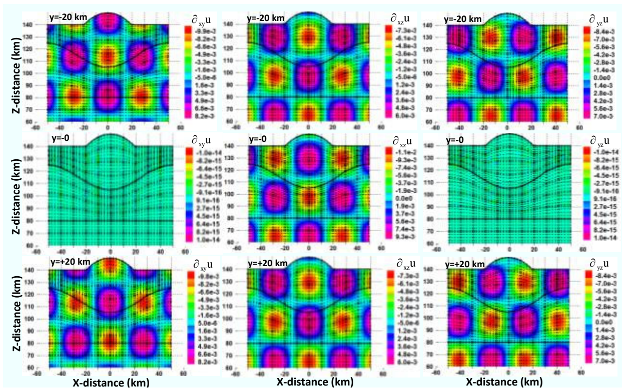

Figure 6. The 3D secondary mixed derivatives calculated by subdomain Chebyshev spectral method.

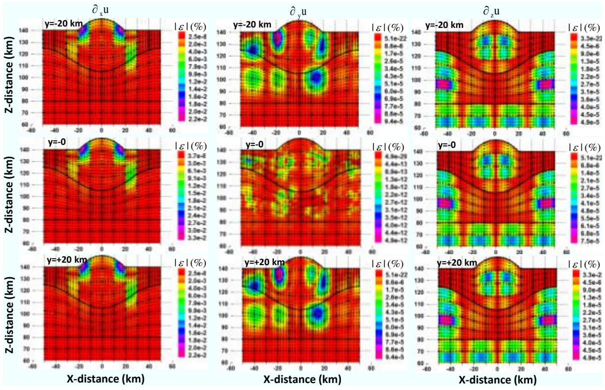

Figure 7. Absolute relative errors of the first derivatives shown in Figure.4.

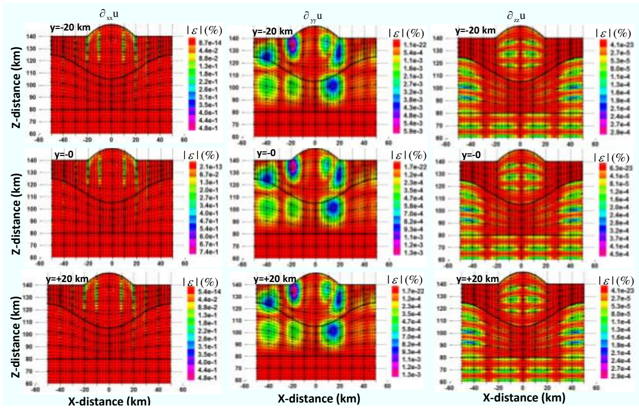

Figure 8. Absolute relative errors of the secondary derivatives shown in Figure 5.

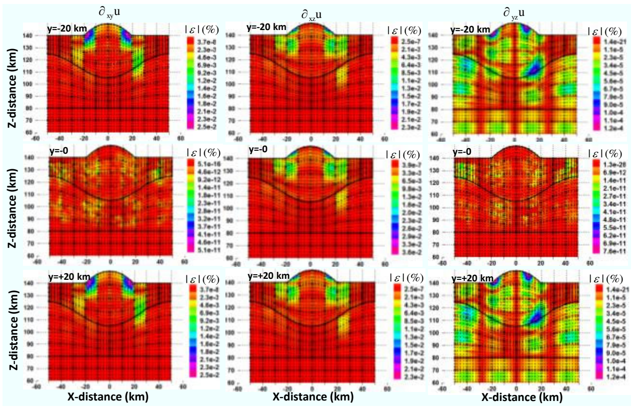

Figure 9. Absolute relative errors of the secondary mixed derivatives shown in Figure 6.

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. The subdomain Chebyshev spectral schemes, SSP1 and SSP2, may be applicable for geophysical forward modelling in a complex geological model.

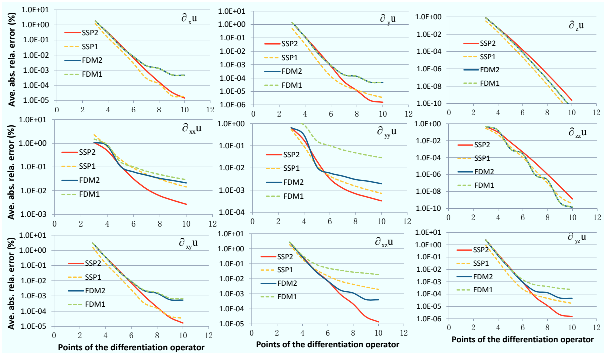

Figure 10. Convergence curves of four numerical differentiation schemes.

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