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Scalar Seismic-Wave Equation Modeling by a Multisymplectic Discrete Singular Convolution Differentiator Method

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Abstract High-precision modeling of seismic-wave propagation in heterogeneous media is very important to seismological investigation. However, such modeling is one of the difficult problems in the seismological research fields. For developing methods of seismic inversion and high-resolution seismic-wave imaging, the modeling problem must be solved as perfectly as possible. Moreover, for long-term computations of seismic waves (e.g., Earth's free-oscillations modeling and seismic noise-propagation modeling), the capability of seismic modeling methods for long-time simulations is in great demand. In this paper, an alternative method for accurately and efficiently modeling seismic wave fields is presented; it is based on a multisymplectic discrete singular convolution differentiator scheme (MDSCD). This approach uses optimization and truncation to form a localized operator, which preserves the fine structure of the wave field in complex media and avoids noncausal interaction when parameter discontinuities are present in the medium. The approach presented has a structure-preserving property, which is suitable for treating questions of high-precision or long-time numerical simulations. Our numerical results indicate that this method can suppress numerical dispersion and allow for research into long-time numerical simulations of wave fields. These numerical results also show that the MDSCD method can effectively capture the inner interface without any special treatment at the discontinuity.

Introduction

High-precision seismic modeling methods become increasingly important due to practical demands for seismological research and seismic exploration. Especially, high-precision or long-time modeling of seismic-wave propagation is required when dealing with seismic-wave propagation in highly heterogeneous media, seismic-wave inversion, high-resolution seismic-wave imaging, or Earth's free-oscillations modeling and seismic noise-propagation modeling. Generally, seismic modeling methods can be classified into three categories: direct methods, integral-equation methods and ray-tracing methods. Carcione *et al.* (2002) gave a classical review of these methods. In this paper, emphasis is placed on direct methods.

Modeling seismic waves in the time domain using direct methods involves discretization of both space and time variables. The most widely used direct methods for spatial discretizations are: classical finite difference (FD) methods (Claerbout, 1985; Bayliss *et al.*, 1986; Levander, 1988), pseudospectral methods (Gazdag, 1981), and finite element methods (Ciarlet and Lions, 1991). Some optimized methods or combinations of these methods are also available, such as optimized finite difference methods (Holberg, 1987; Geller and Takeuchi, 1998; Takeuchi and Geller, 2000; Moczo *et al.*, 2002), convolution differentiator methods (Mora, 1986; Etgen, 1987; Zhou and Greenhalgh, 1992; Yomogida and Etgen, 1993), spectral element methods (Komatitsch and Tromp, 2002; Komatitsch and Vilotte, 1998), and finite volume methods (Dormy and Tarantola, 1995). Each of these methods has its merits and drawbacks. In past years, a discrete singular convolution differentiator for solving partial differential equations has been developed (Feng and Wei, 2002; Sun and Zhou, 2006). The differentiator can use optimization and truncation to form a localized operator. This is a high-precision and efficient operator to solve partial differential equations. In this paper, the discrete singular convolution differentiator will be selected for spatial differentiation.

In the past ten years, the second-order finite difference method for temporal discretizations has been widely used. Because the classical finite difference methods for temporal discretizations are not structure-preserving methods, it is extremely difficult to avoid accumulated errors in precise or long-time numerical simulations for partial differential equations using these methods. When numerically solving differential equations, some numerical algorithms can preserve the corresponding structures. This can be called the structure-preserving property of a numerical algorithm. The structure-preserving property of symplectic algorithms is well known. Theoretically, a numerical method for Hamiltonian dynamical systems can be called a symplectic algorithm if the resulting numerical solution is also a symplectic mapping. Some symplectic algorithms for partial differential equations have been developed and used, such as the Lax–Wendroff methods (Dablain, 1986; Carcione *et al.*, 2002) and Nyström methods (Qin and Zhu, 1991; Hairer *et al.*, 1993; Okunbor and Skeel, 1992; Calvo and Sanz-Serna, 1993; Tsitouras, 1999; Blanes and Moan, 2002; Lunk and Simen, 2005). Chen (2009) discussed the structure-preserving property of the Lax–Wendroff and Nyström methods in detail.

In this paper, we present an alternative method for accurately and efficiently modeling seismic wave fields using a multisymplectic discrete singular convolution differentiator algorithm (MDSCD). Here, a truncated and optimized discrete singular convolution differentiator (DSCD) is used for spatial discretizations. Theoretically, the DSCD is a localized operator that can describe both the fine structure of wave fields in complex media and avoid any noncausal interaction of the propagating wavefields when parameter discontinuities are present in the medium. The operator is truncated for practical implementation. Nine-point operators on regular grids are used as a compromise between computational efficiency and accuracy. In order to improve the capability of seismic modeling methods for long-time simulations, we substitute the third-order partitioned Runge–Kutta scheme (a multisymplectic algorithm) for the second-order finite difference scheme in temporal discretizations. The MDSCD scheme is highly localized in the spatial domain and is not as accurate as global methods (e.g., the Fourier pseudospectral scheme) for approximating bandlimited periodic functions or for approximating spatial derivatives of smooth functions, though it is more suitable for treating nonbandlimited problems and for treating complex geometries (e.g., approximating spatial derivatives of discontinuous functions). For temporal discretization, the scheme presented is a third-order operator, which requires slightly more computational time than does second-order finite difference time discretization.

As an example, we apply the MDSCD to seismic scalar wave-field modeling in heterogeneous media. Our numerical results indicate that the MDSCD is suitable for large-scale numerical modeling because it effectively suppresses numerical dispersion by discretizing the wave equation when coarse grids are used. From these numerical results, we find that the MDSCD method can effectively capture the inner interface without any special treatment at the discontinuity. The numerical results also confirm that the MDSCD presented in this paper has the superior performance to solve long-time simulation problems.

Theoretical Method

Discrete Singular Convolution Differentiator

A powerfully spatial derivative operator is one of the keys to solving wave equations for strongly heterogeneous media. The most effort has been focused on developing either global methods (Fornberg, 1990; Chen, 1996; Zhao *et al.*, 2003) or localized methods (Zhou and Greenhalgh, 1992; Bayliss *et al.*, 1986; Mora, 1986; Etgen, 1987; Holberg, 1987; Levander, 1988; Yomogida and Etgen, 1993; Geller and Takeuchi, 1998; Komatitsch and Vilotte, 1998; Takeuchi and Geller, 2000; Komatitsch and Tromp, 2002; Moczo *et al.*, 2002; Yang *et al.*, 2004) for solving partial differential equations. Generally, the local methods (e.g., methods of finite difference, finite volumes, and finite elements) are highly localized in the spatial domain, yet are delocalized in their spectral domain; global methods, such as the Fourier spectral method, are highly localized in their spectral representations and localized in the spatial domain. As a consequence, global methods appear to be more accurate than local methods when they are used to approximate spatial derivatives of a smooth function. The main advantage of local methods is their flexibility for satisfying special boundary conditions and for treating complex geometries. In this paper, we select a discrete singular convolution differentiator with optimization and truncation for spatial discretizations of wave equations. This differentiator can be considered as a localized operator, though mathematical analysis (Qian, 2003) indicates that the regularized Shannon delta kernel is a local spectral kernel. Numerical analysis (Feng and Wei, 2002; Sun and Zhou, 2006) indicates that the discrete singular convolution scheme can be more accurate than global methods (e.g., the Fourier pseudospectral methods) for treating nonbandlimited problems and for treating complex geometries (e.g., approximating spatial derivatives of discontinuous functions), even if it is not as accurate as global methods for approximating bandlimited periodic functions or for approximating spatial derivatives of smooth functions.

Here, we begin by summarizing the discrete singular convolution differentiator for the spatial derivative to solve wave equations. Let $T(x-t)$ be a singular kernel and $\eta(x)$ be an element of the space of test function. A singular convolution is defined as

$$f(x) = (T * \eta)(x) = \int_{-\infty}^{\infty} T(x-t)\eta(t)dt. \qquad (1)$$

Here, singular kernels of the delta type are required:

$$T(x) = \delta^{(q)}(x), \qquad (q = 0, 1, 2, \ldots). \qquad (2)$$

The singular kernel $T(x) = \delta(x)$ is of particular importance for interpolation of surfaces and curves. Higher-order kernels $T(x) = \delta^{(q)}(x)$, where $(q = 0, 1, 2\ldots)$, are essential for numerically solving partial differential equations. However, one has to find appropriate approximations to the delta type singular kernel, which cannot be directly realized in computers. Finally, a sequence of approximations is considered as

$$\lim_{\alpha\to\alpha_0}\delta_\alpha^{(q)}(x)=\delta^{(q)}(x),\qquad q=0,1,2,\ldots,\tag{3}$$

where α is a parameter that characterizes the approximation, with α_0 being a generalized limit. Among various approximation kernels, the regularized Shannon delta kernel (Gottlieb *et al.*, 1981) is an excellent candidate. It can be written as

$$\delta_{\sigma,\Delta}(x)=\frac{\sin\frac{\pi}{\Delta}x}{\frac{\pi}{\Delta}x}\exp\left(-\frac{x^2}{2\sigma^2}\right).$$

In this formula, Δ is the grid spacing, and σ determines the width of the Gaussian envelope. For a given $\sigma\neq 0$, the limit of $\Delta\to 0$ reproduces the delta kernel (distribution). With the regularized Shannon delta kernel, a function u and its n-th order derivative can be approximated by a discrete convolution

$$u^{(q)}(x)\approx\sum_{k=\lceil x\rceil-W}^{\lceil x\rceil+W}\delta_{\sigma,\Delta}^{(q)}(x-x_k)u(x_k),\qquad q=0,1,2,\ldots,\tag{5}$$

where $\lceil x\rceil$ denotes the grid point that is closest to x, and $2W+1$ is the computational bandwidth (or effective kernel support), which is usually smaller than the computational bandwidth of the spectral method (i.e., the entire domain span). Generally, a larger W will lead to a higher accuracy. When $q=1$, the first-order derivative $d_1(x)$ can be discretized as

$$d_1(k\Delta x)=\begin{cases}\delta'_{\sigma,\Delta}(k\Delta x) & k=\pm1,\pm2,\ldots\\ 0 & k=0\end{cases},\tag{6}$$

where Δx is the grid spacing. For practical implementation, the differentiator has to be truncated as a short operator, but doing so could lead to the Gibbs phenomenon. To avoid the Gibbs phenomenon, we use a Hanning window function for truncating the differentiator:

$$w(k)=\left[2\alpha-1+2(1-\alpha)\cos^2\frac{k\pi}{2(W+2)}\right]^{\beta/2},\quad k=0,\pm1,\pm2,\ldots,W.\tag{7}$$

The constants $\alpha(0.5\leq\alpha\leq1)$ and β allow a family of different windows to be considered. A modified and practical convolutional differentiator can be denoted by

$$\hat{d}(i\Delta x)=\begin{cases}d(i\Delta x)w(i) & i=1,2,\cdots,m\\ 0 & i=0\end{cases}.\tag{8}$$

For the second-order derivative, the convolutional differentiator is written as $\hat{d}_2(i\Delta x)$.

From the discrete Fourier analysis of the discrete singular convolution (Feng and Wei, 2002; Yang *et al.*, 2002), the accuracy of the operator clearly depends on its length. The error analysis also indicates that the accuracy of the discrete singular convolution approximation to the derivative is controllable and can be better than the traditional higher-order finite difference approximation. To obtain an optimal balance between computational efficiency and accuracy of the discrete singular convolution approach, we chose nine-point explicit operators on regular grids via the discrete Fourier analysis.

The Convolutional Differentiator Expression of the Scalar Seismic-Wave Equation

Generally, the scalar equation for two-dimensional (2D) arbitrarily heterogeneous media in the time domain can be written as

$$\frac{1}{v^2}\frac{\partial^2u(x,z,t)}{\partial t^2}=\frac{\partial^2u(x,z,t)}{\partial x^2}+\frac{\partial^2u(x,z,t)}{\partial z^2}+f(x,z,t),\tag{9}$$

where u is the scalar wave field, v is the velocity of the wave, f is the body force, x and y are Cartesian coordinates, and t is the time. In the convolutional differentiator method, the spatial derivatives of u in equation (9) can be written as

$$\frac{\partial^2u(x,z,t)}{\partial x^2}=\hat{d}_1(x)*[\hat{d}_1(x)*u(x,z,t)],\tag{10}$$

where * stands for the convolution with respect to x and $\hat{d}_1(x)$ is the convolutional differentiator for the first-order derivative. Similarly, $\hat{d}_2(x)$ is the convolutional differentiator for the second-order derivative. Therefore, equation (9) can be expressed as

$$\frac{\partial^2u(x,z,t)}{\partial t^2}=v^2(x,z,t)\{\hat{d}_2(x)*u(x,z,t)+\hat{d}_2(z)*u(x,z,t)\}+f(x,z,t),\tag{11}$$

where $\hat{d}_2=\hat{d}_1*\hat{d}_1$.

Discrete Seismic Scale Wave Modeling Formulas

For seismic modeling in the discrete domain, generally, the solution of the seismic scalar wave in equation (11) can be written as

$$\begin{aligned}u(m,n,t+\Delta t)&=2u(m,n,t)-u(m,n,t-\Delta t)\\&+v^2(m,n)\Delta t^2\Bigg[\Delta x\sum_{i=-mx}^{mx}\hat{d}_2(i\Delta x)u(m-i,n,t)\\&+\Delta z\sum_{j=-nz}^{nz}\hat{d}_2(j\Delta z)u(m,n-j,t)+f(m,n,t)\Bigg],\end{aligned}\tag{12}$$

where m and n are indices along the discrete x and z axes; Δx, Δz, and Δt are sampling rates along the x, z, and t axes;

and mx and nz are the half differentiator lengths in sampling number along the x and z axes. In equation (12), the second-order central FD operator is employed for temporal discretizations, and the spatial derivative operator is not based on a Taylor expansion. However, equation (12) is not a structure-preserving (symplectic) scheme, and it does not guarantee computational accuracy for high-precision and long-time simulations. To improve accuracy of the long-time modeling, a multisymplectic scheme has to be employed for temporal discretizations. Applying the discrete singular convolution differentiator to a multisymplectic partial differential equation system, a multisymplectic discrete singular convolution differentiator method can be obtained.

Applying an explicit third-order partitioned Runge–Kutta temporal discretization scheme (Iwatsu, 2009) to equation (11), we can obtain

$$\begin{aligned} &V_1 = v^n + \Delta t c_1\{L(u^n) + f(m,n,t)\}, \\ &U_1 = u^n + \Delta t d_1 V_1, \qquad V_2 = V_1 + \Delta t c_2 L(U_1), \\ &U_2 = U_1 + \Delta t d_2 V_2, \qquad v^{n+1} = V_2 + \Delta t c_3 L(U_2), \\ &u^{n+1} = U_2 + \Delta t d_3 v^{n+1}, \end{aligned} \tag{13}$$

where

$$L = v^2(m,n)\left[\Delta x \sum_{i=-mx}^{mx} \hat{d}_2(i\Delta x) + \Delta z \sum_{j=-nz}^{nz} \hat{d}_2(j\Delta z)\right],$$

$$u^{n+1} = u(m,n,t+\Delta t), \qquad c_1 = \frac{1}{12}\left(\sqrt{\frac{209}{2}} - 7\right),$$

$$c_2 = \frac{11}{12}, \qquad c_3 = \frac{1}{12}\left(8 - \sqrt{\frac{209}{2}}\right),$$

$$d_1 = \frac{2}{9}\left(1 + \sqrt{\frac{38}{11}}\right), \qquad d_2 = \frac{2}{9}\left(1 - \sqrt{\frac{38}{11}}\right),$$

$$d_3 = \frac{5}{9}.$$

Equation (13) is an explicit third-order multisymplectic discrete singular convolution differentiator scheme. Iwatsu (2009) analyzed the computational precision and stability of the third-order multisymplectic temporal discretization scheme in detail. From his analysis, it can be seen that the temporal discretization scheme described previously in this article is far superior to nonsymplectic temporal discretization schemes in terms of computational precision and stability.

Numerical Experiments

Generally, the accuracy of numerical schemes is evaluated by considering the numerical dispersion as a function of the number of grid points per wavelength. Even though the wave field in a highly heterogeneous medium is usually not known analytically, the overall performance can still be judged qualitatively. In this section, we give two numerical examples for evaluating the performance of the MDSCD approach.

We compared the numerical results obtained using MDSCD with those from the Fourier pseudospectral scheme and conventional high-order FD for a two-layered medium with a high-velocity contrast. The model consists of two different wave velocity regions separated by a rough inclined interface (Fig. 1). The model parameters were a velocity of $C_1 = 1500$ m/s for the upper layer with the source and a velocity of $C_2 = 3000$ m/s for the lower layer. The number of grid points was 256×256, the model size was 2550 m $\times$ 2550 m, and the wave source was located at $(x_s, z_s) = (1280\text{ m}, 1130\text{ m})$. The receiver was located at $(x_r, z_r) = (1280\text{ m}, 1080\text{ m})$. The spatial increments were 10 m, and the time increment was 1 ms. The interface can be considered a velocity discontinuity because the velocity contrast is very high. The source, a band-limited Ricker wavelet, is located in the upper layer and has an amplitude spectrum peak at 30 Hz and a high-frequency cut at 43 Hz.

Figure 2a is a wave-field snapshot at time 500 ms, generated by the MDSCD. The snapshots in Figure 2a and Figure 2b (the latter generated by the Fourier pseudospectral scheme) clearly show that the wavefront of the direct wave exhibits a semicircular shape at the inner interface. Other phases (e.g., the reflected, transmitted, and scattered waves from the interface) are also displayed clearly. The wavefronts are continuous and mend the velocity discontinuity in the model. From these snapshots, the wave fields simulated by MDSCD are very clear. There is hardly any grid dispersion, despite the fact that there are only 3.5 grids or less per shortest wavelength at the high-cut frequency.

From the preceding comparison of Figure 2a and Figure 2b, it can be seen that the MDSCD scheme is as

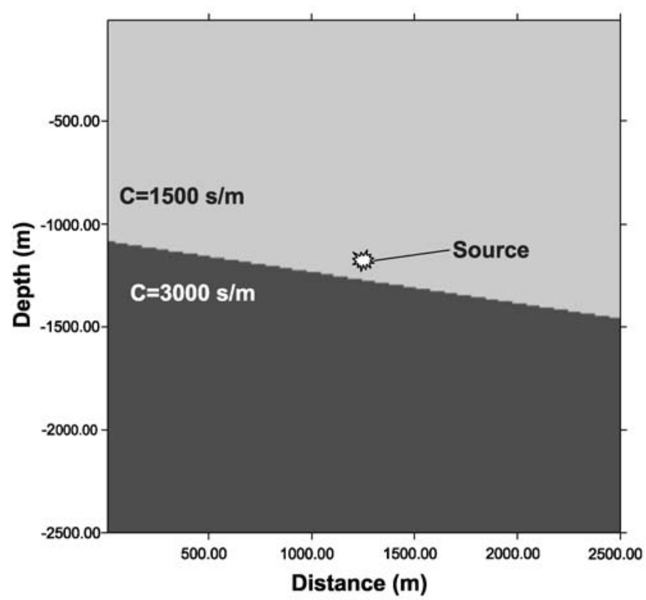

Figure 1. Two-layered medium model: configuration and parameters.

accurate as the Fourier pseudospectral scheme for short-time simulations and for treating uncomplicated geometries.

Comparing the wave-field snapshot generated by the MDSCD (Fig. 2a) with the conventional high-order FD (Fig. 2c), one can see that there is hardly any evidence of numerical dispersion in the MDSCD approach, whereas numerical dispersion (i.e., periodic oscillation waveforms after the head wave) is obviously present when using the conventional high-order FD method. A similar phenomenon also appears when comparing the synthetic seismograms (Fig. 3a for the MDSCD, Fig. 3b for the Fourier pseudospectral scheme, and Fig. 3c for the conventional high-order FD). Note that the number of grid points (or sampling interval) is consistent among the three methods. Although the accuracy of the conventional high-order finite difference can be improved by heavy oversampling along the spatial axes, more computational resources would naturally be required. Therefore, both the MDSCD and the Fourier pseudospectral scheme are suitable for large-scale numerical modeling with coarse spatial grids.

Based on these results, we conclude that the convolutional operator designed here is accurate to about 3.5 grids or less per shortest wavelength. Also, the MDSCD method effectively captures the inner interface without any special treatment at the discontinuity.

To examine the long-time performance of the MDSCD scheme, we compared the numerical results computed by MDSCD with those from a Fourier pseudospectral scheme for a 2D homogeneous medium model. The model parameter is a velocity of $C = 3000$ m/s. The number of grid points was

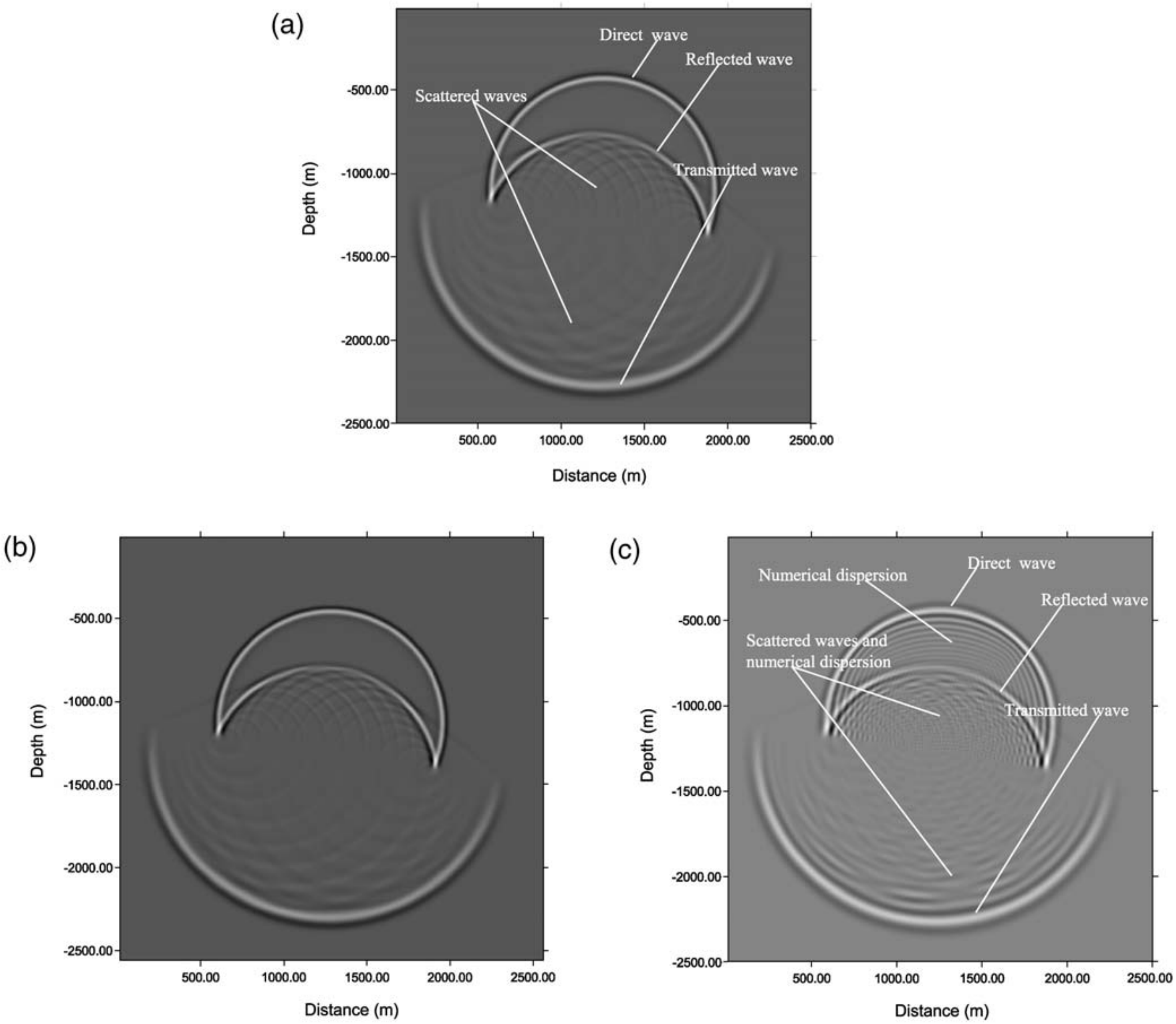

Figure 2. Snapshots of seismic wave fields (a) in a two-layered medium model at time 500 ms, generated by MDSCD, (b) using the Fourier pseudospectral method, and (c) the conventional high-order FD method.

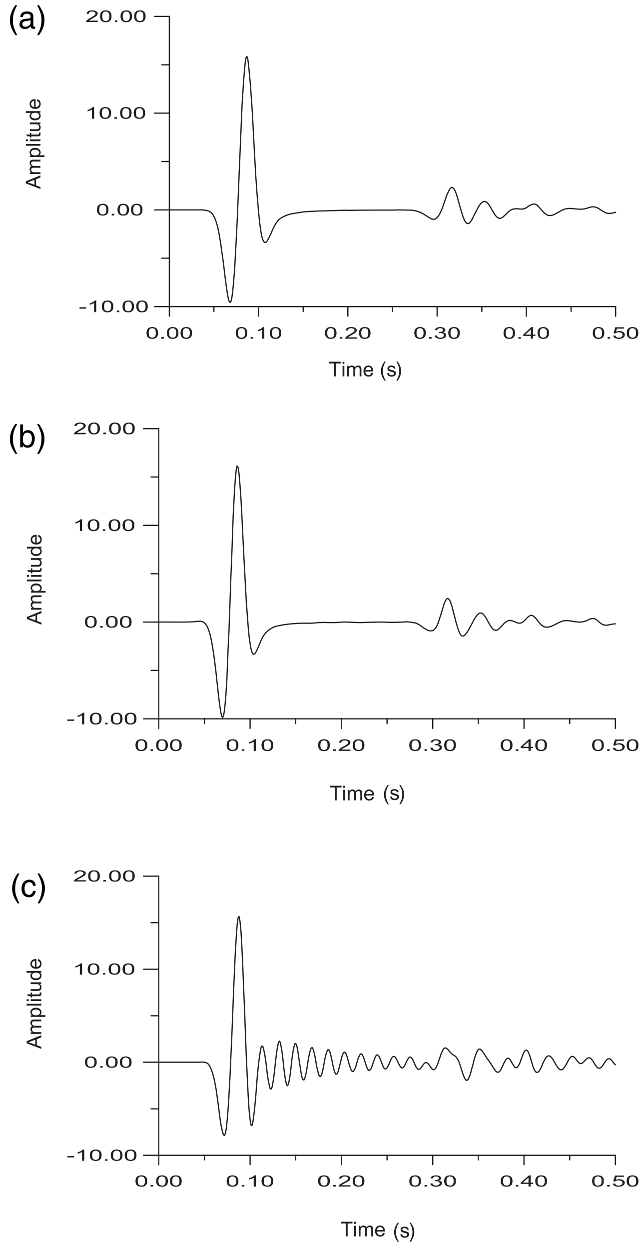

Figure 3. Comparison of synthetic seismograms for (a) a two-layered medium model generated by the MDSCD, (b) the Fourier pseudospectral method, and (c) the conventional high-order FD method.

256×256, the model size was 5100 m $\times$ 5100 m, and the wave source was located at $(x_s, z_s) = (2550\ \text{m}, 2550\ \text{m})$. The spatial increments were 20 m, and the time increment was 2 ms. The source, a bandlimited Ricker wavelet has an amplitude spectrum peak at 25 Hz.

Figure 4a–c show wave-field snapshots generated by the MDSCD scheme after 400, 2000, and 5000 time steps, respectively. Similarly, Figure 4d–f display wave-field snapshots generated by the Fourier pseudospectral scheme after 400, 2000, and 5000 time steps, respectively. From Figure 4a and Figure 4d, it is apparent that the wavefront curves generated by the two schemes after 400 time steps are quite clear. For short-time numerical simulations, therefore, they have similar performance in the same case. For long-time numerical simulations, however, the aforementioned two schemes perform quite differently and have different error growth. After 2000 times steps, the MDSCD scheme has slightly numerical dispersion, whereas the Fourier pseudospectral scheme suffers obvious numerical dispersion. After 5000 time steps, the wavefront curves computed by the MDSCD scheme are still clearly seen. At this time, however, the wavefront curves computed by the Fourier pseudospectral scheme have blurred seriously. The CPUs (Core 2 Duo 2.53 GHz) time for the MDSCD scheme and the Fourier pseudospectral scheme are 685.2813 s and 560.5625 s, respectively. This comparison indicates that the two schemes perform very differently for long-time computation, and the MDSCD scheme is very suitable for long-time simulation.

Conclusions

In this paper, a novel approach for a seismic scalar wave equation with variable coefficients modeling has been presented, which is based on an explicit third-order multisymplectic discrete singular convolution differentiator scheme (MDSCD). For temporal discretizations, the MDSCD method is a structure-preserving scheme. In theory, it is suitable for long-time simulations. For spatial discretizations, nine-point operators on regular grids are designed for optimizing the computational efficiency and accuracy of the presented approach. The nine-point MDSCD is a localized operator that can describe the local properties of complicated wave fields and avoid noncausal interaction of the propagating wave field when parameter discontinuities are present in the medium. This approach is therefore suitable for large-scale numerical modeling because it effectively suppresses numerical dispersion by discretizing the wave equations when coarse grids are used. Because the MDSCD approach is equivalent to an optimized FD method in nature, it is suitable to any type of absorbing or transmitted boundary condition that is suitable for conventional FD methods.

In this paper, the numerical experiments focus on comparison of the MDSCD scheme with the Fourier pseudospectral scheme. The Fourier pseudospectral method is accurate and efficient for smooth functions (e.g., problems associated with smooth heterogeneous media), but a global operator is used when taking the Fourier transform that can lead to nonlocal interactions between globally distant points. This is inconsistent with physical phenomena where interactions occur through local wave motion. In theory, the MDSCD scheme is highly localized in the spatial domain and is not as accurate as global methods (e.g., the Fourier pseudospectral scheme) for approximating bandlimited periodic functions or for approximating spatial derivatives of smooth functions, though it is more suitable for treating nonbandlimited problems and for treating complex geometries (e.g., approximating spatial derivatives of discontinuous

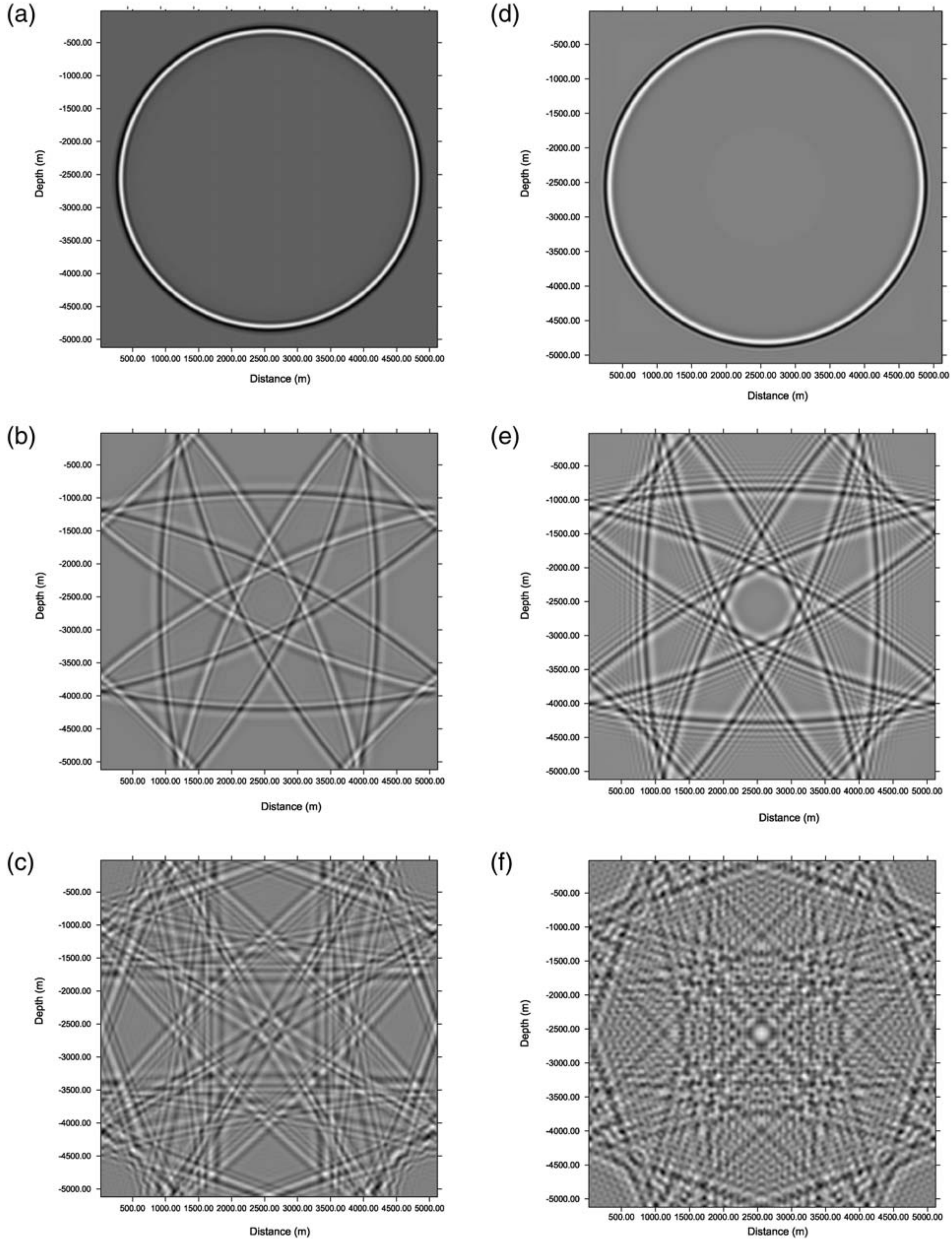

Figure 4. Snapshots of seismic wave fields in a 2D homogeneous medium model generated by MDSCD after (a) 400 time steps, (b) 2000 time steps, and (c) 5000 time steps. Snapshots of seismic wave fields in the same medium model generated by the Fourier pseudospectral method after (d) 400 time steps, (e) 2000 time steps, and (f) 5000 time steps.

functions). For temporal discretization, the scheme presented is a third-order operator, which requires slightly more computational time than second-order finite difference time discretization for long-time simulations.

From the simulation results in this paper, it has been shown that the MDSCD method can effectively capture the inner interface without any special treatment at the discontinuity; therefore, it can simulate seismic waves in complicated geometries and highly heterogeneous media without any additional treatment. The MDSCD allows us to use a coarse grid, that is, fewer samples per wavelength, to achieve the same accuracy in modeling waves and is similar to that obtained by conventional FD schemes on a finely-sampled grid. The numerical experiments also demonstrate the remarkable ability of the MDSCD for long-time simulation. The results here hold promise not only for future seismic-wave studies but also for any geophysical study that requires high-precision numerical solution (or long-time simulations) of partial differential equations with variable coefficients. Although the new method is only applied to the 2D scalar wave-field calculation for heterogeneous models and to long-time simulation of the 2D scalar wave field in this paper, it can be readily extended to 3D scalar wave-field calculations. For elastic wave-field calculations, the modification and extension of the new method will be described in a later paper.

Data and Resources

No data were used in this paper. All plots were made using the Surface Mapping System, version Surfer32 (available at http://www.freedownloadmanager.org/downloads/surfer-32-program-302675.html) and the 2D Graphing System, version GRAF4WIN (available at http://vetusware.com/download/Grapher%201.06/?id=6185). (The programs were last accessed January 2011.)

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