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PSEUDOSPECTRAL METHOD FOR WAVE PROPAGATION SIMULATION

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ABSTRACT

The pseudospectral method is an alternative attractive finite-difference modeling method which offers high-accuracy results with substantially less computation time and memory than traditional scheme. One of the attractive characteristics of the pseudospectral method is that the differentiation of field variables are analytically calculated in the wavenumber space. Recently the advantage of the computer performance and parallel programming algorithms enable us applying the method for large scale 2-D and 3-D elastic modeling. The power of the forward modeling of 3-D elastic wavefield provides a direct means of understanding the seismic wave propagation through the use of the snapshots of the evolution of the wavefield in time and space and theoretical seismograms, to compliment the three-component observations.

KEYWORDS

Synthetic seismograms; parallel-computing; pseudospectral method; 3-D modeling.

INTRODUCTION

The pseudospectral method (*e.g.*, Kosloff and Baysal, 1982) is an alternative attractive to the other numerical techniques, such as finite-difference or finite-element method, which requires several orders of magnitude less computer memory and time than traditional schemes (*e.g.*, see Daudt *et al.*, 1989). In the pseudospectral method the spatial differentiation in the equation system are calculated analytically in the wavenumber domain. The transformation between physical and the wavenumber domain are performed efficiently by use of the fast Fourier transforms (FFT). Since only two grids per wavenumber is theoretically sufficient to treat the wavefield, total memory required for the calculation can be considerably reduced. The memory requirement for the pseudospectral method compared to the forth-order finite-difference scheme is about 1/8 and 1/64 for 2-D and 3-D modeling, respectively (*e.g.*, see Fornberg, 1987). Therefore the method has typically been applied for large scale and high-resolution forward modeling of elastic wave propagation for explosion experiments using the 2-D scheme (Kang and McMechan, 1990) and 2.5-D scheme (Furumura and Takenaka, 1996).

After Kosloff and Baysal (1982) first applied the method for the time domain solution of the seismic wavefield, very large amount of techniques such as an absorbing boundary to minimize the edge effect,

stable differentiation technique for discontinuous data and mapping technique for an accurate incorporation of curved interface have been successfully developed to apply the method for actual models. Since the pseudospectral method directly calculate the equation of motion rather than wave equation itself it is rather straightforward to incorporate seismic source by use of the equivalent body force and anelastic effect by a simple modification of the stress-strain equation (*e.g.*, Carcione, 1994). Advantage of the high-performance computers coupled with parallel programming algorithms getting gradually enables us the 3-D pseudospectral applications. Pioneering work of Reshef *et al.* (1988) who implemented the 3-D pseudospectral code onto the CRAY X/MP vector computer and parallel 3-D pseudospectral modeling developed by Furumura *et al.* (1995) may demonstrate the arrival of 3-D modeling age.

The object of the present paper is to review the numerical modeling of seismic wave propagation by the pseudospectral method with remarkable corresponding numerical techniques to incorporate the boundaries in the model as well as an efficient computing by use of the parallel computers. In the following section a brief summary of the pseudospectral calculation for the 3-D elastic wavefield will be described. Then an simple experiment for a surface wave propagation in a basin will be undertaken to show the feasibility of the parallel 3-D pseudosoectral computing.

3-D PSEUDOSPECTRAL ELASTIC MODELING

For an isotropic linear elastic medium the equation of motion in the 3-D rectangular system is given by

$$\begin{aligned}
\rho\ddot{U}_x &= \frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{xz}}{\partial z} + f_x, \\
\rho\ddot{U}_y &= \frac{\partial\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z} + f_y, \\
\rho\ddot{U}_z &= \frac{\partial\sigma_{xz}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z} + f_z,
\end{aligned} \tag{1}$$

where $\sigma_{pq} = \sigma_{pq}(x, y, z, t), (p, q = x, y, z)$ are the stress components at point (x, y, z) in time t, $f_p = f_p(x, y, z, t), (p = x, y, z)$ body force, $\ddot{U}_p = \ddot{U}_p(x, y, z, t)$ the second time derivatives of displacement (i.e. acceleration), and $\rho = \rho(x, y, z)$ the density. For marching time, the second-order finite-difference scheme is often used with a time increment intervals Δt. To keep a dispersion error, caused by the finite-difference approximation, down to an acceptable level the criterion of Daudt *et al.* (1989) of $\Delta t < 0.26\Delta r/V_P^{\max}$ is used, where $V_P^{\max}$ is the maximum P-wave velocity in the model and Δr denote the grid spacing.

The strain components $e_{pq} = e_{pq}(x, y, z, t)$, $(p, q = x, y, x)$ are calculated by the spatial differentiation of the displacement components as

$$e_{pq} = \frac{1}{2}\left(\frac{\partial U_p}{\partial q} + \frac{\partial U_q}{\partial p}\right), \tag{2}$$

which is related to the stress components through Hooke's law with the Lamé's constants $\lambda = \lambda(x, y, z)$ and $\mu = \mu(x, y, z)$ as

$$\sigma_{pq} = \lambda\,(e_{xx} + e_{yy} + e_{zz})\delta_{pq} + 2\mu\, e_{pq}, \qquad (p, q = x, y, z), \tag{3}$$

where δ_{pq} is the Kronecker delta. After the seismic disturbance of seismic point source is incorporated in the equation of (1) by use of an equivalent body force (*e.g.*, see Aki and Richards, 1980, chap. 3) the solution of the full system of eqs. from (1) to (3) is marched forward in time.

Fourier differentiation

The main attractive advantage of the pseudospectral method is that the spatial differentiations appear in the eqs. (1) and (3) are efficiently calculated by use of the FFT. In this section the characteristics of

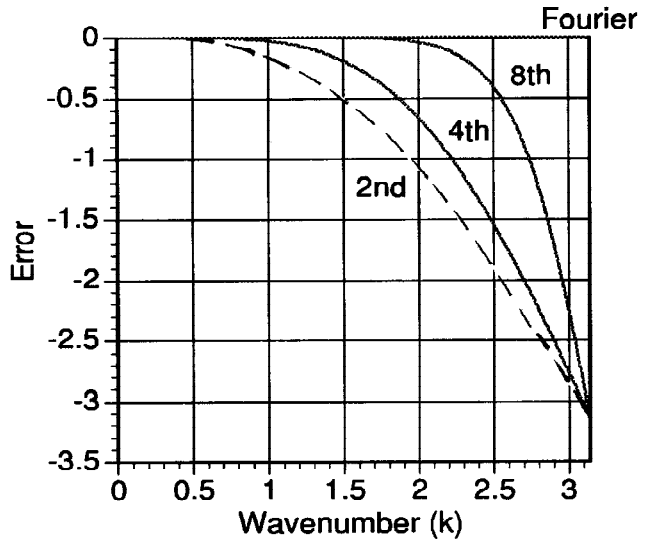

Fig. 1. Numerical error for each wavenumber produced by finite-order approximation of the differentiation: comparisons between 2-nd, 4-th, 8-th order central difference and Fourier difference (exact).

the Fourier differentiation as an infinite-order high-accuracy finite-difference scheme is compared with the traditional finite-order approximations.

The differentiation by use of the FFT is accomplished as follows; First the data to be differentiated $f(n\Delta r), (n = 0, 1, ..., N-1)$ is transformed into the wavenumber domain:

$$F(l\Delta k) = \Delta r \sum_{n=0}^{N-1} f(n\Delta r) e^{-i2\pi nl/N}, \tag{4}$$

where $F(l\Delta r); (l = 0, 1, ..., N-1); (\Delta k = 2\pi/(N\Delta r))$ represents the Fourier transform of $f(n\Delta r)$. The transformed data is then multiplying the corresponding discrete wavenumbers $i(l\Delta k)$, and the derivative is transformed back into the physical domain using an inverse FFT, that is

$$\frac{d}{dr} f(n\Delta r) = \frac{1}{N\Delta r} \sum_{l=0}^{N-1} i\,(l\Delta k)\, F(l\Delta k)\, e^{i2\pi nl/N}. \tag{5}$$

This is usually called as N-th order (or infinite-order) differentiation scheme. While a second-order central finite-difference scheme, which is equivalent to multiplying the $i\sin(l\Delta k)$ in the wavenumber space (see, Huntley, 1989), that is

$$\frac{d}{dr} f(n\Delta r) = \frac{1}{N\Delta r} \sum_{l=0}^{N-1} i\,\sin(l\Delta k)\, F(l\Delta k)\, e^{i2\pi nl/N}. \tag{6}$$

The derivatives by the lower-order approximations clearly involve errors in large wavenumbers. Figure 1 comparing the numerical errors produced by 2nd, 4-th and 8-th order central difference formula with an exact result by the Fourier differentiation. Clearly significant energy extinction in large wavenumbers producing large problems especially by use of lower-order approximations. On the other hands the analytical differentiation in the pseudospectral calculation allows all wavenumber to propagate in the model, and in consequence high-frequency noise appeared in the calculation and gradually enlarged with large time steps sometimes cause an oscillation noise on the waveform .

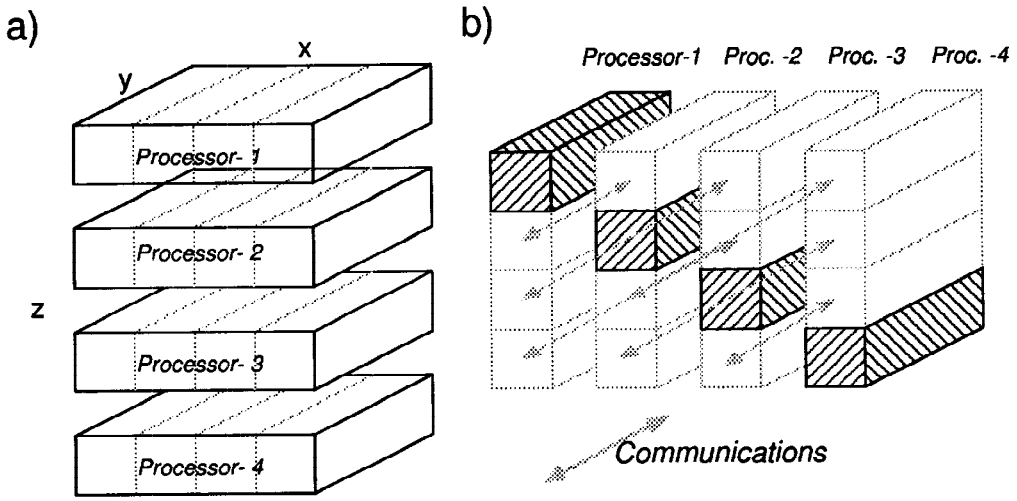

Fig. 2. Example for domain decomposition of the 3-D wavefield with four processors. (a) for horizontal (x, z) differentiations, (b) for vertical (z) differentiation with communication between processors.

Boundary condition

Boundary conditions such as free-surface and absorbing boundary (or equivalently non-reflecting boundary) are required for applying the pseudospectral method to practical applications of bounded model.

The free-surface boundary is simply incorporated in the modeling by specifying zero values on the stress components above the upper side of the surface. A number of zeros prepared prior to the differentiation are then removed immediately after the calculation to reduce the total computational memory. Since the large discontinuity in the wavefield along the free-surface sometimes cause unstable oscillations, an stable differentiation technique for discontinuous data "Symmetric differentiation" (Furumura and Takenaka, 1995) is usually applied for the vertical (z) differentiation of the displacement components.

An wraparound noise produced by the periodic boundary conditions implicitly involved in the FFT is efficiently reduced by tapering approach (Cerjan *et al.*, 1985) or by use of a warparound elimination technique based on an anti-periodic extension of the wavefield (Furumura and Takenaka, 1995).

PARALLEL 3-D PSEUDOSPECTRAL CALCULATION

For the 3-D modeling the spatial differentiation by means of the Fourier transform is carried out along x, y and z directions of the 3-D variables, which expends more than 50 % of the total pseudospectral computation time. It should be noted that enormous FFTs are used in the 3-D modeling, for example, in the case of 128^3 model with a time step of 1000 needs more than six hundred million 1-D FFTs. For this reason it has long been experimented the use of high-performance transforms such as fast Hartley transform (*e.g.*, see Saatcilar and Ergintav, 1991) and the FFT for real-sequenced numbers (Furumura *et al.*, 1993). However, such a FFT for a 1-D data can not efficiently be implemented on the current super computers because the 1-D FFT with relative short data (*e.g.*, N=128, 256) contains very small vector operations and the overhead of the vector calculation is considerably large. Recently, parallel pseudospectral computing as an alternative attractive approach is receiving attentions for a practical application of large scale pseudospectral modeling. For example, Renaut and Woo (1992) examined an efficiency for a parallel-FFT and applied for the calculation of 1-D scalar wavefield using

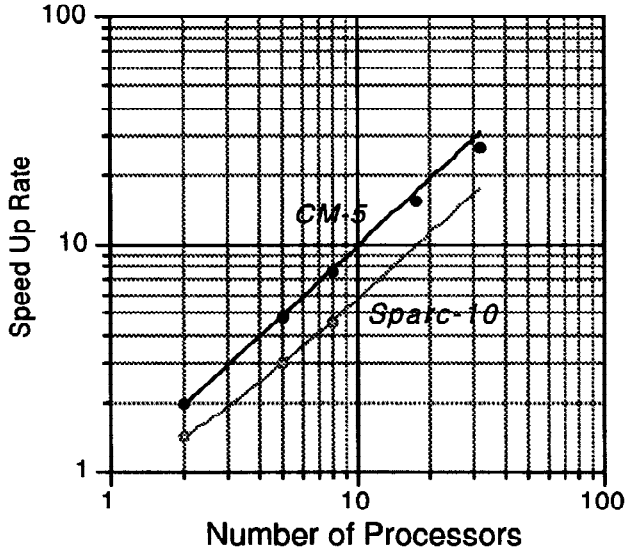

Fig. 3. Theoretical (line) and experimental (mark) efficiency for speed up rate of parallel computing with a number of processors using the CM-5 and SPARC-10 workstation clusters.

a 32-node Intel iPSC1 hyper-cube parallel computer. Sato *et al.* (1985) applied 128-node NCUBE/1 hyper-cube parallel machine for calculating a 2-D acoustic wavefield. Liao and McMechan (1993) calculated 2-D viscoacoustic wavefield by use of a a Intel iPSC860 distributed-memory multi-processor system. A parallel 3-D pseudospectral code for elastic wavefield was first developed by Furumura *et al.* (1995). In the following section we briefly review the parallel 3-D pseudospectral modeling based on the decomposition of the wave field and then a simple example of the surface wave propagation in the basin is simulated to show the feasibility of the method.

Domain decomposed parallel pseudospectral computation

The parallelization of a problem is achieved by dividing the 3-D domain into NP subdomains each with the same number of grids and assigning onto NP processors (Fig. 2). Such a parallelism is a special kind of parallel computing style, where the same operation is repeated on each processor for the subdomain with inter communication between processors, and the data is stored into its local memory.

In each subdomain spatial differentiation of horizontal (x, z) direction is calculated individually by each processor and only the vertical (z) differentiation requires communications between the subdomains. Exchange of data between processors are achieved by use of a "message passing" programming for which we utilized the "P4" parallel programming library (Butler and Lusk, 1994). The p4 is a standard library of macros and subroutines for parallel programming supporting a variety style of parallel machines such as shared-memory multi-CPU machine, distributed-memory multi-CPU computers and workstation-clusters connected with computer network, thereby the code is easily implemented on several kind of parallel computers without modification of the program.

Efficiency of the parallel 3-D pseudospectral code is experimented using a Thinking Machine CM-5 parallel computer, a workstation-cluster of Sun Microsystems SPARC Station-10 system connecting with the Ethernet network and the DEC-alpha multi-CPU workstation, which is agreed well with the theoretical efficiency of previous knowledge defined by the ratio of communication speed between processors to the CPU speed. Figure 3 illustrating the benchmark results of the speed-up rate of the parallel pseudospectral code implemented on many parallel platform, which shows the maximum speed-up rate of 24 for 32-node CM-5, 4.5 for eight-processors SPARC-10-cluster and 1.4 for two-CPU

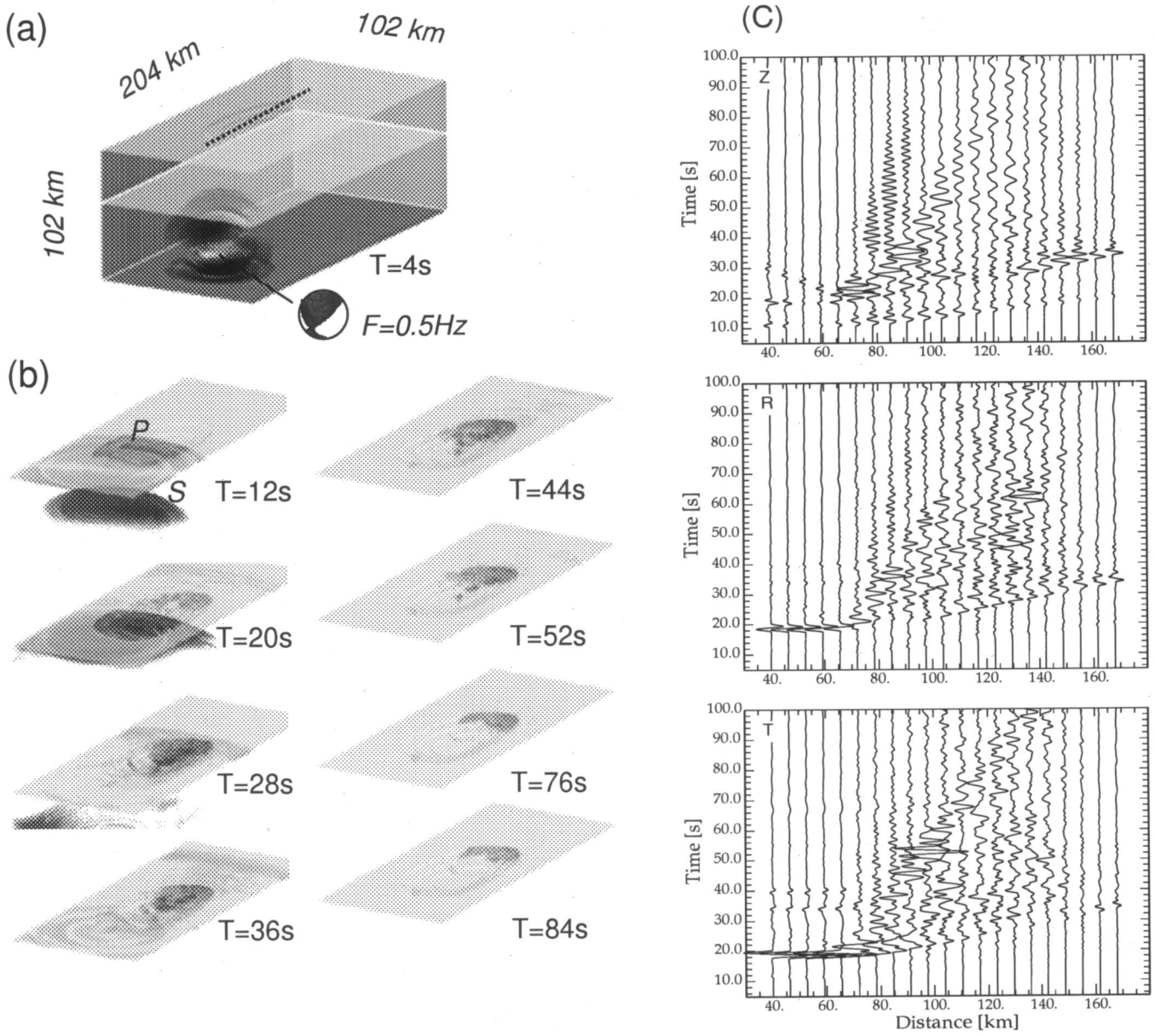

Fig. 4. Numerical modeling of 3-D wavefield in the basin model. (a) Configurations of 3-D model with an double-couple point source and seismic line array stations arranged on the surface (dashed line), (b) Snapshots of the 3-D wavefield near the free-surface, (c) Synthetic three-component seismograms of vertical, radial and transverse components.

DEC-alpha.

3-D modeling of the elastic wavefield

In order to demonstrate the feasibility of the parallel pseudospectral computing we have undertaken a 3-D elastic modeling for a simple basin model. The model we used here have a size of 102 km (N-S) and 205 km (E-W) long by 102 km deep, surrounded by suitable absorbing buffer zone (Cerjan *et al.*, 1985) to minimize the grid-edge effect. The domain is divided into $128 * 256 * 128$ points with a regular grid spacing of 0.8 km. We will simulate the surface wave propagation in the simplified basin model for the Tokachi plain, Hokkaido, Japan, which have a size of 100 km (N-S) by 50 Km (E-W) long and a maximum thickness of 2.6 km (see, Furumura and Sasatani, 1995). The basin structure is represented by three-layers of sediments with the P-wave velocities of α=2.2, 4.9 and 5.6 km s^{-1}, S-wave velocities of β=1.0, 2.8 and 3.2 km s^{-1} and densities of ρ=2.0, 2.5 and 2.6 Mg m^{-3}, which producing very strong velocity contrast to the the crust (α=6.6 km s^{-1}, β=3.8 km s^{-1}, ρ=2.9 Mg m^{-3}) and the uppermost mantle (α=8.0 km s^{-1}, β=4.0 km s^{-1}, ρ=3.3 Mg m^{-3}). The seismic point source for a share dislocation fault have a maximum frequency of around 0.5 Hz and is placed 100 km away from the center of the basin and a depth of 67 km (Fig. 4a). The calculation is performed using the DEC7200-620 workstation (SPECfp92:201) with two processors which used the memory of 488 MB and the CPU time of 180 hours for calculating the wave propagation of 100 s.

The sequence of snapshots of the wavefield at each time is displayed in Fig. 4b which bring us better insights into the understanding of the seismic behavior at each time and space. In the 12s flame we see the P wave incident into the basin which produce only weak S conversions at the side of the boundary and passing through the basin without affected by the crustal variations. In the 28 s flame we find the strong S-to-P conversions generated at the boundary which leads to a large surface wave. In the next few flames we can see a prominent surface wave propagating within the basin with very slow propagation speed (less than 1.0 km s^{-1}) as well as large scattering wave multiply reflected between the free-surface and the crust-basin interface. We can also discern a creeping wave propagating along the curved interface.

Synthetic seismograms of ground motion of vertical, radial and transverse components are illustrated in Fig. 4c, in which we can see a prominent of later phases generated at the south edge of the basin. We can also see the Rayleigh wave on vertical and radial components at a distances ranged from 70 to 90 km predominating a monochromatic frequencies of 2.2 Hz is agreed very well with the observations (Furumura and Sasatani, 1995).

DISCUSSION AND CONCLUSIONS

Numerical modeling of seismic wave propagation in 3-D heterogeneous media by the pseudospectral method with some corresponding numerical techniques has been reviewed in the present paper. An attractive advantage of the time domain solution of the numerical modeling method, which bring us direct insights into understanding the complex seismic behavior in the laterally heterogeneous medium through the use of a sequence of snapshots wavefield and synthetic seismograms of three-components data. High-accuracy and stable differentiation used in the pseudospectral modeling considerably reduce the computer memory for 3-D variables. Recent studies for high-performance computing by use of the parallel-computers may demonstrating the arrival of 3-D modeling age.

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