Modelling anisotropic wave propagation in oceanic inhomogeneous structures using the parallel multidomain pseudo-spectral method

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Accepted 1997 December 9. Received 1997 December 9; in original form 1997 May 22

SUMMARY
We have developed a multidomain pseudo-spectral method for 3-D anisotropic seismic waveform modelling to run in a high-performance parallel computer. The numerical scheme solves acoustic and elastic wave equations formulated by velocity and stress for fluid layers and solid spaces, respectively. Spatial variations of velocity and stress fields propagating in general anisotropic and heterogeneous media are calculated by high-accuracy Fourier and Chebyshev differential operators. The fourth-order Runge–Kutta method is employed for time-marching of the wavefields. The domain decomposition technique divides the full space into several subdomains bounded by discontinuous features with steep velocity gradients. The propagating wavefronts are separately calculated in each subdomain, then wavefield matching procedures subject to the continuity condition for the velocity and traction are imposed at the interface of subdomains. Non-periodic boundary conditions at the free surface and the non-reflected edge at the bottom of the model space are adequately represented by expansion in Chebyshev polynomials. Parallelizing the serial algorithm effectively reduces the computation time. Data locally distributed in many processors for the parallel program provides the large memory storage needed for a 3-D model. The waveforms calculated by this numerical scheme show accuracy comparable with a known analytical solution. The numerical experiments indicate the effectiveness of the multidomain approach in modelling seismic energy partitioning into reflected, refracted and transmitted waves when incident on continuous planar or curved or discontinuous structures with velocity gradients. They can also be split when they enter anisotropic media and then travel with different azimuths.

Key words: anisotropic wave propagation, Chebyshev–Fourier method, full waveform modelling, multidomain, parallel computation.

1 INTRODUCTION
Seismological evidence indicates that the interior of the Earth is inhomogeneous and anisotropic on scales ranging from a few to thousands of kilometres (e.g. Nishimura & Forsyth 1989; Crampin & Lovell 1991; Montagner & Tanimoto 1991). Heterogeneity is mainly caused by seismic wave velocity varying with the composition and physical properties of the Earth. Anisotropy is usually associated with the alignment of voids or fluid-filled cracks (e.g. Crampin & Booth 1985; Blackman & Kendall 1997), and/or the lattice preferred orientations of minerals such as olivine and pyroxene in response to shear deformation (e.g. Nicolas & Christensen 1987; Blackman et al. 1996). Seismic waves radiated from their source can generate transmitted, reflected, converted and diffracted waves when incident on continuous planar or curved or discontinuous structures with velocity gradients. They can also be split when they enter anisotropic media and then travel with different
speeds. The polarization and velocity of the split waves depend on the propagation direction, the compressional or shearing type of wave motion and the anisotropic properties of the media.

Because seismic wave propagation in both heterogeneous and anisotropic structures is complicated, synthetic seismograms are needed to understand systematically the variability of full waveforms propagating in a set of hypothetical velocity models. This is essential for the further development of the inverse problem in the determination of robust geological structures. Many approaches have been developed to calculate synthetic seismograms and anisotropic seismic wave propagation, such as asymptotic ray theory (e.g. Chapman & Drummond 1982; Kendall & Thomson 1993) and the reflectivity method (e.g. Booth & Crampin 1983). However, based on the high-frequency assumption, ray-tracing methods are valid only for smooth structures with weak anisotropy and fail to calculate accurately inhomogeneous waves in media with large velocity jumps such as the water/crust discontinuity. The reflectivity method works only for laterally homogeneous, layered anisotropic structures.

Discrete solution methods such as finite differences (e.g. Boore 1972), finite elements (e.g. Lysmer & Drake 1971) and pseudo-spectral methods (e.g. Fornberg 1975) are in principle suitable for more general anisotropic and inhomogeneous structures with 3-D variations, and are capable of solving the most general wave-motion-governing equation with no need for simplification. They track the wavefields in time, and hence any change of wavefronts in a complicated anisotropic and heterogeneous medium can be clearly visualized. Moreover, broad-band full waveforms that include inhomogeneous head or surface waves and the effects of ray collapse and amplitude singularity at caustics can be adequately simulated if a proper numerical method is used. These advantages of numerical modelling provide a great aid in the interpretation of the observed arrival phases. However, the potentially intensive computational work has hindered the broad application of numerical solutions in modelling 3-D waveforms in large-scale problems such as teleseismic studies. With currently available computational power, these solutions are becoming increasingly realistic.

The goal of this paper is to present an accurate and efficient numerical method to simulate seismic wave propagation in 3-D, generalized inhomogeneous and anisotropic media, particularly in oceanic structures that have been studied using ocean-bottom seismometers (OBSs). The technique we use is the multidomain pseudo-spectral method. In this method, the field variables are approximated by the global expansion of a set of basis functions such as Fourier series. The spatial derivatives at each grid point are calculated from all nodal values along the differentiation direction and the expansion coefficients of trigonometric interpolation rather than only using a few neighbouring nodes and constant coefficients in finite difference schemes. This global approximation of derivatives minimizes numerical dispersion in the discrete solutions and does not produce artificial anisotropy, which is favourable for our interest in seismic anisotropy. Because most methods for synthetic seismogram calculation utilize a single-domain approach with global elastic properties and a uniform grid discretization, they often have difficulties in modelling structures with large velocity contrasts or changes of physical properties across discontinuities such as the water/
crust interface or core–mantle boundary (CMB). The domain decomposition technique developed for the construction of exact wavefield phenomena in such physical spaces divides the global modelling space into several subdomains separated by interfaces at velocity discontinuities or at the boundaries where material rheologies change (e.g. Carcione 1991). Wave propagation is solved independently based on the correct continuum physics describing wave motion and mechanical behaviour in each subdomain. This method allows us to vary the grid spacing based on the different wave speeds so that an assigned source pulse can be appropriately sampled at a minimum cost everywhere along the wave path. In this paper, we extend the previous work in 2-D wave propagation (Carcione 1991; Tessmer et al. 1992) to 3-D seismic modelling in general anisotropic elastic media adjoining acoustic spaces.

The following section describes the principle of the multidomain, pseudo-spectral method (Chebyshev–Fourier) and its formulation, along with the numerical treatment of boundary and continuity conditions at the interfaces between elastic/elastic or fluid/elastic subdomains. An optimization scheme for the parallelization of the serial program is introduced to render a 3-D, large-scale simulation practical in a connected network of workstations. In Section 3, we test the numerical accuracy of the method. Section 4 presents the simulations of seismic wave propagation in isotropic and anisotropic models, and begins to explore the characteristic features of waveforms that identify the nature of the anisotropy. Finally, we construct two-domain models in which the isotropic or anisotropic space is in contact with a water layer to simulate wave propagation in oceanic structures. This capability is particularly important for studying data recorded at OBSs, because the contamination of primary phases by large-amplitude water reverberations can cause difficulty in analysing the OBS data (Blackman, Orcutt & Forsyth 1995).

2 FORMULATION OF THE PARALLEL MULTIDOMAIN PSEUDO-SPECTRAL METHOD

The pseudo-spectral method was initially proposed to solve the hyperbolic equations (e.g. Kreiss & Oliger 1972; Orszag 1972) and has been applied to a variety of problems in the field of fluid dynamics since then (e.g. Canuto et al. 1988). It was first introduced by Gazdag (1981) to model acoustic wave propagation and by Kosloff & Baysal (1982) to model elastic waves in 2-D isotropic media. In principle, this method employs a set of basis functions such as Fourier series to expand field variables and the discrete Fourier transform to calculate the derivatives in physical equations.

Theoretically, the length spanning two nodes is the smallest wavelength that can be resolved by the pseudo-spectral method in a homogeneous model. In heterogeneous and/or anisotropic media, five–10 grid points sampling the minimum wavelength are required to construct accurate wavefields. In 2-D models, the Fourier method with a fourth-order, time-stepping scheme needs a factor of 3–4 less CPU time and memory storage to perform calculations equivalent in accuracy to the fourth-order finite difference method (Daudt et al. 1989). The saving in memory is more pronounced for 3-D problems, since the global approximation in the pseudo-spectral method allows coarser grids to simulate higher-frequency seismic waves in large, inhomogeneous, even anisotropic structures. Here we
present a multidomain, Chebyshev–Fourier method accompanying a parallel algorithm to simulate 3-D wave propagation accurately and efficiently in both inhomogeneous and anisotropic media, particularly in oceanic structures with rapidly varying velocity.

2.1 Basic equations

The two primary equations needed to describe elastic wave propagation in an inhomogeneous, anisotropic medium undergoing infinitesimal deformation are the equation of momentum conservation and the generalized constitutive law. These two equations expressed in terms of the velocity-stress variables are written as (e.g. Orrey 1995):

\[
\rho \ddot{v}_i = \sigma_{ij,j} + f_i, \quad \sigma_{ij} = c_{ijkl} e_{kl},
\]

(1)

where \( \ddot{v}_i = (v_{i,j} + v_{ij})/2 \), \( v_i \) is the velocity component in the \( i \)-th axis, \( \sigma_{ij} \) the stress tensor equivalent to the \( i \)-th component of the traction acting across the plane normal to the \( j \)-th axis, \( f_i \) the \( i \)-th component of the body force, \( c_{ijkl} \) the strain tensor, \( \rho \) the density and \( c_{ijkl} \) the fourth-order stiffness tensor with elastic coefficients for linear elastic solids. Using the symmetric properties of stress and strain tensors, eqs (1) and (2) are combined into a set of nine coupled linear first-order partial differential equations:

\[
\frac{\partial}{\partial t} [U] = \mathbf{A} \frac{\partial}{\partial x} [U] + \mathbf{B} \frac{\partial}{\partial x_2} [U] + \mathbf{D} \frac{\partial}{\partial x_3} [U] + [\mathbf{b}],
\]

(3)

where \([U] = [v_1, v_2, v_3, \sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{13}, \sigma_{23}]^T\), \([\mathbf{b}] = \left[ f_1/\rho, f_2/\rho, f_3/\rho, 0, 0, 0, 0, 0, 0 \right]^T\) and \( \mathbf{A}, \mathbf{B}, \mathbf{D} \) are \( 9 \times 9 \) matrices consisting of elastic constants, \( c_{ijkl} \), and density, \( \rho \) (see Appendix A). Subscript 3 represents the vertical dimension in the \( z \)-direction and subscripts 1 and 2 are the horizontal dimensions in the \( x \)- and \( y \)-directions, respectively. The temporal and spatial variations of the velocity and stress fields can be solved from eq. (3) once the boundary and initial conditions are specified. The boundary condition with zero traction is imposed at the surface of the Earth. The initial condition introduced in the body force term describes the mechanism and time history of seismic sources; that is, the source time function.

The advantage of using the velocity-stress formulation instead of displacement is that the former scheme has no derivative of displacement involved in the calculation of stress at the free surface, giving a more accurate representation of the traction-free boundary condition. The second-order partial differential equation (PDE) of elastic wave motion formulated in displacement is reduced to a first-order PDE in the velocity-stress expression. The velocity-stress scheme is, therefore, less sensitive to material variations since the elastic coefficients appear undifferentiated in the wave equation (Kosloff, Reshef & Lowenthal 1984).

2.2 Domain decomposition in 3-D anisotropic media

In the multidomain calculation, the model space is divided into \( N \) subdomains based on wave velocity and physical properties. Eq (3) is solved independently in each individual subdomain to yield a set of velocity and stress variables. These variables at the collocation points of the domain interface need modification to satisfy the continuity conditions. Tessmer et al. (1992) introduced the application of the continuity condition at the subdomain interfaces in a 2-D isotropic medium. Tessmer (1998) derived the explicit forms of the characteristic variables in general anisotropic elastic media for the boundary treatment on the free surface. Following their work we extend the utilization of characteristic variables in computing the matching solutions of wavefields across the discontinuous interfaces in 3-D anisotropic media, namely for the stresses and velocity at the boundaries between solid-solid or fluid-solid domains. We assume the \( i \)-th elastic subdomain overlies the \((i + 1)\)-th elastic subdomain and the interface between these two domains is a horizontal plane. The velocity and traction wavefields have to be continuous when crossing a common interface. Therefore, the outgoing characteristic variables from the \( i \)-th subdomain towards the \((i + 1)\)-th subdomain need to be matched with the incoming characteristic variables from the \((i + 1)\)-th subdomain. The nodal values of the velocity and normal traction at the interface are respectively equalized by solving a \( 6 \times 6 \) system of linear equations in a matrix form:

\[
\mathbf{E}[\mathbf{W}]^{(o)} = [\mathbf{X}]^{(o)},
\]

(4)

where

\[
\mathbf{E} = \begin{bmatrix}
-\beta_{1111} & -\beta_{1133} & -\beta_{1166} & \beta_{1470} & \beta_{1840} \\
-\beta_{1313} & -\beta_{1343} & -\beta_{1366} & \beta_{1470} & \beta_{1840} \\
-\beta_{1616} & -\beta_{1646} & -\beta_{1666} & \beta_{1870} & \beta_{1840} \\
\beta_{4111} & \beta_{4133} & \beta_{4166} & \beta_{4470} & \beta_{4840} \\
\beta_{4313} & \beta_{4343} & \beta_{4366} & \beta_{4470} & \beta_{4840} \\
\beta_{4616} & \beta_{4646} & \beta_{4666} & \beta_{4870} & \beta_{4840} \\
\end{bmatrix},
\]

\[
[\mathbf{W}]^{(o)} = \begin{bmatrix}
\mathbf{e}_1^{(o)}, \mathbf{e}_2^{(o)}, \mathbf{e}_3^{(o)}, \mathbf{\sigma}_{33}^{(o)}, \mathbf{\sigma}_{23}^{(o)}, \mathbf{\sigma}_{13}^{(o)} \\
\end{bmatrix}^T
\]

and

\[
[\mathbf{X}]^{(o)} = \begin{bmatrix}
\mathbf{e}_1^{(o)}, \mathbf{e}_2^{(o)}, \mathbf{e}_3^{(o)}, \mathbf{\sigma}_{33}^{(o)}, \mathbf{\sigma}_{23}^{(o)}, \mathbf{\sigma}_{13}^{(o)} \\
\end{bmatrix}^T
\]

The \( \beta_{mn(i)+1} \) and \( \beta_{mn(i)+1} \) are the \( m \)-th row and \( n \)-th column elements of the inverse eigenvector matrix of \( \mathbf{D} \) in eq. (3) for the \((i + 1)\)-th and \((i)\)-th subdomains, respectively. The superscript \((n)\) represents the equalized solutions of the continuous traction and velocity at the overlapped interface between adjacent subdomains. The superscript \((o)\) indicates the nodal values of the characteristic variables \( \mathbf{Y} \) with the eigenvalues \(-\lambda_{11(i)+1} \leq \lambda_{66(i)+1} \leq \lambda_{66(i)+1} \) in the \((i + 1)\)-th subdomain and with \( \lambda_{11(i)+1} \leq \lambda_{66(i)+1} \leq \lambda_{66(i)+1} \) in the \((i)\)-th subdomain before the application of the continuity condition. The derivation of characteristic variables is provided in Appendix A. To avoid numerical instability when forcing the variables to satisfy the boundary or continuity conditions, the other three stress components not required to be continuous have to be updated on both sides of the subdomains based on the characteristics with zero eigenvalues (Gottlieb, Gunzberger & Turkel 1982):

\[
[\mathbf{Y}]^{(o)} = [\mathbf{Y}]^{(n)} + \mathbf{S}[\mathbf{Z}],
\]

(5)

where

\[
\mathbf{S} = \begin{bmatrix}
\beta_{16}/\beta_{14} & \beta_{17}/\beta_{14} & \beta_{18}/\beta_{14} \\
\beta_{26}/\beta_{25} & \beta_{27}/\beta_{25} & \beta_{28}/\beta_{25} \\
\beta_{36}/\beta_{35} & \beta_{37}/\beta_{35} & \beta_{38}/\beta_{35} \\
\end{bmatrix},
\]

\[
[\mathbf{Z}] = \begin{bmatrix}
\sigma_{33}^{(o)} - \sigma_{33}^{(n)}, \sigma_{23}^{(o)} - \sigma_{23}^{(n)}, \sigma_{13}^{(o)} - \sigma_{13}^{(n)} \\
\end{bmatrix}^T
\]

and

\[
[\mathbf{Y}] = [\sigma_{11}, \sigma_{22}, \sigma_{12}]^T.
\]
If the $i$th subdomain is the fluid and the $(i+1)$th subdomain is the elastic solid, the shear stresses $\sigma_{y3}$ and $\sigma_{z3}$ are zero at the common interface because the fluid cannot undergo shear deformation and the traction needs to be continuous. The continuity of the vertical velocity $v_y$ and normal stress $\sigma_{y3}$ along the interface requires that the downgoing characteristic variable with the eigenvalue $-\lambda_y$ (equivalent to the negative acoustic wave speed) from the fluid subdomain is matched to the upgoing characteristic variables with the eigenvalues $\lambda_y(i+1)$, $\lambda_{y3}(i+1)$, $\lambda_{y3}(i+1)$, from the elastic subdomain. This leads to a set of $4 \times 4$ linear equations to solve for the updated wavefield variables: the continuous vertical velocity and pressure in the fluid or the normal stress $\sigma_{y3}$ in the elastic domain, and unnecessarily continuous horizontal velocities only for the elastic domain,

$$F[R]^{(o)} = [Q]^{(o)},$$  

(6)

where

$$F = \begin{bmatrix} \beta_{4(i+1)} & \beta_{42(i+1)} & \beta_{43(i+1)} & \beta_{46(i+1)} \\ \beta_{3(i+1)} & \beta_{32(i+1)} & \beta_{33(i+1)} & \beta_{36(i+1)} \\ \beta_{2(i+1)} & \beta_{22(i+1)} & \beta_{23(i+1)} & \beta_{26(i+1)} \\ \beta_{1(i+1)} & \beta_{2(i+1)} & \beta_{3(i+1)} & \beta_{4(i+1)} \end{bmatrix},$$

and 

$$[R]^{(o)} = \begin{bmatrix} F[\lambda_{y(i+1)}] & F[\lambda_{y3(i+1)}] & F[\lambda_{y3(i+1)}] & F[\lambda_{y3(i+1)}] \end{bmatrix}^T$$

and 

$$[Q]^{(o)} = \begin{bmatrix} \epsilon_{11}^{(o)} & \epsilon_{22}^{(o)} & \epsilon_{33}^{(o)} & \epsilon_{12}^{(o)} & \epsilon_{13}^{(o)} & \epsilon_{23}^{(o)} \end{bmatrix}^T.$$  

The $\epsilon_{11}$, $\epsilon_{22}$ and $\epsilon_{33}$ in the elastic subdomain are modified using the non-propagating characteristic variables as shown in eq. (5). If the elastic subdomain overlays the fluid layer instead, for instance at the CMB or a fluid magma reservoir, the continuous vertical velocity and normal stress $\sigma_{y3}$ along the interface are obtained by solving eq. (6). There the characteristic variables are replaced either by those corresponding to the eigenvalues $-\xi_1$, $-\xi_2$, $-\xi_3$ for the elastic subdomain or by those corresponding to the eigenvalue $v_p$ for the fluid layer.

### 2.3 The Chebyshev–Fourier method

In this study, we use the periodic Fourier basis functions to expand the horizontal variations of wavefield variables. As they are limited in the ability to implement explicitly the non-periodic boundary conditions at the traction-free surface and at the non-reflected base (e.g. Huang 1992; Lou & Rial 1995), Chebyshev polynomials are instead used in the vertical expansion and the partial derivatives are calculated through the expansion coefficients of the variables found by the cosine Fourier transform and the recursion relation (e.g. Kosloff et al. 1990). When the spatial derivative terms of eq. (3) are computed, the wave equation is treated as a first-order, time-derivative ordinary differential equation. The fourth-order Runge–Kutta method is then employed to update the wavefields at the incremental time step. The boundary conditions at the free surface and continuity conditions at the domain interfaces are applied after the completion of the time-advance step.

The use of the non-periodic Chebyshev functions for space discretization generates decreasing grid spacings toward the boundaries (Kosloff et al. 1990; Carcione 1996). This increases the resolution in modelling the appearance and interaction of different waves at the free surface or a discontinuous interface. However, the extremely small spacing next to the edges introduces a stringent stability criterion for the time-stepping interval (Kosloff & Tal-Ezer 1993). A coordinate transformation that rescales and stretches the Chebychev mesh is applied to remedy this restriction and thus reduce the growth in computation time (Kosloff et al. 1990). Nonetheless, the rescaled grid spacing near the boundary is still smaller than the uniform spacing in the equivalent Fourier expansion.

### 2.4 Parallelism of the FFT-based algorithm

Numerical modelling of seismic wave propagation in 3-D media usually suffers from a problem with memory. In the Chebyshev–Fourier method with the velocity–stress formulation, for instance, the nine wavefield parameters and their derivatives at two intermediate time levels in each time step, the density and the stiffness tensor (up to 21 independent elastic coefficients in general anisotropic media) at each grid point need to be stored. For surface waves (Rayleigh and Love waves), grid spacings smaller than those for body waves are needed to obtain spatial resolution equivalent to body waves at the same period, because surface waves propagate with slower speeds along the free surface. The finer grids near the surface generated from the non-uniform Chebychev mesh may also intensify the numerical cost by requiring smaller time increments. Consequently, 3-D calculations running only on a single processor not only become prohibitively slow but also require too much memory for large-scale anisotropic models. Parallel computation implemented in distributed memory computing machines provides an efficient alternative to tackle problems such as this.

The framework of the FFT-based algorithms such as the Chebyshev–Fourier method and multidomain architecture is suited for parallel computation since most of the arithmetic work is from FFT operations. The serial code can be parallelized easily by breaking the numerous FFTs sequentially performed on one processor into simultaneously running transforms on several processors since each FFT is independent. The major modification required for the parallel algorithm in waveform calculation is the complete exchange (or all-to-all communication) between processors. The message-passing model for the 3-D FFT-based algorithm is illustrated in Fig. 1. The 3-D model space is initially partitioned into $N$ slab-shaped subregions along the $y$-axis in Cartesian coordinates, where $N$ is the number of the nodes or processors. For this parallel-computing model, each node can calculate concurrently the first derivatives of the velocity and stress with respect to the $x$- and $z$-directions. As for the $y$-derivative of wavefield variables, all processors have to complete the all-to-all communication first; that is, each node sends different pieces of data in its local memory to all other nodes and then receives data from all other processors (Fig. 1). The amount of data storage remains fixed before and after the complete exchange. Once the $y$-derivative is calculated, the data will be reversely exchanged to recover the original form of data arrangement. The program will then execute the concurrent multiplication of coefficients and time advance.

In this study, the parallel algorithm was developed for implementation in the IBM Scalable POWERparallel 2 system, which connects RISC System/6000 processors via a communication network called High-Performance Switch (Stunkel et al. 1994). The Message Passing Interface (MPI) (Gropp, Lusk & Skjellum 1994), which provides standard libraries...
Figure 1. The message-passing model employed in parallelization of the FFT-based pseudo-spectral scheme for synthetic waveform calculations. The top diagram shows the configuration of data partition in a 3-D model space with a \((nx) \times (ny) \times (nz)\) grid mesh that is distributed in \(N\) processors before (left part) and after (right part) all-to-all communication. The bottom diagram schematically represents the map view of the collective data movement during the communication. The processors are narrow boxes confined by solid lines in the drawing. A, B, ..., C and D represent initially partitioned data with \((nx) \times (ny/N) \times (nz)\) data points stored in each processor \(p = 1, 2, ..., N-1, N\). They are each separated into \(N\) blocks of size \((nx/N) \times (ny/N) \times (nz)\) data points, with each block represented by \(A_K, B_K, ..., C_K, \) or \(D_K (K = 1, 2, ..., N-1, N)\). During the communication, each processor exchanges its \(K\)th data block with the \(K\)th processor in a diagonally symmetric fashion, so that the \(K\)th data blocks in all the processors will be restored into one single processor.

Figure 2. Testing the FFT-based parallel algorithm developed in this study by running 100 time iterations over a \(64 \times 64 \times 65\) 3-D model.
(a) The CPU time consumed when using 1, 2, 4, 8 and 16 processors.
(b) The parallel efficiency defined in the text for each timing-test run.
in turn can be directly applied to the six stress variables in
the velocity–stress formulation. To minimize the aliasing effect
resulting from the truncated expansion of a spatial delta function
in terms of the basis functions (Özdenvar & McMechan 1996),
the point source is spatially smoothed by a Gaussian function
and spread out from the centroid location \((x_c, y_c, z_c)\) to the
neighbouring nodes in all directions, i.e.
\[
F(x, y, z, t) = f(t) \exp\{-z^2[(x - x_c)^2 + (y - y_c)^2 + (z - z_c)^2]\},
\]
where \(z\) is the distance of the farthest neighbouring node at
which the amplitude of the source time function is reduced by
a factor \(1/e\).
To remove spurious reflections and wrap-around from the
artificial boundaries of the finite numerical space, a non-
reflective boundary condition based on the 1-D wave equation
approximation (e.g. Clayton & Enquist 1977) is applied on the
bottom of the model space. An absorbing boundary condition
which gradually damps the amplitude of wavefields towards
the boundaries is also implemented in a strip of the region
along the side and bottom grids to help eliminate unreal
reflections from oblique incident waves (Cerjan et al. 1985).

3 Accuracy tests for numerical solutions
To demonstrate the accuracy of the multidomain pseudo-
spectral method for 3-D waveform modelling, we compare
the analytical solution of the displacement excited by a
double-couple seismic source with the synthetic seismograms
 calculated by the Chebyshev–Fourier method. The homo-
genous model space is discretized into a \(128 \times 128 \times 136\)
mesh spanning a total distance of \(50.8\) km in the horizontal
directions and \(54\) km in the vertical dimension. The \(P\)-wave
velocity is \(8\) km s\(^{-1}\), the \(S\)-wave velocity is \(4.62\) km s\(^{-1}\) and
the density is \(3.3\) Mg m\(^{-3}\). The point source with a pure
dip-slip normal fault striking along the \(y\)-axis is located at
\((x, y, z) = (24, 24, 26.8)\) km. The seismograms are recorded
1.2 and \(15.1\) km below the hypocentral depth to investigate both
near-field and far-field displacements. Fig. 3 shows the com-
parison between the numerical result and the exact solution of
an infinite space problem (Aki & Richards 1980). The excellent
match of the synthetic waveforms to the analytical solution at
distances less than or equal to a wavelength of the \(P\) wave as well
as several wavelengths away indicates that the pseudo-
spectral scheme is able to model the amplitude decay of near-
field and far-field displacements and to represent precisely the
actual ground motion excited by an earthquake.
To test the accuracy of the application of the continuity
condition at the interface of a multidomain configuration, we
perform a numerical experiment in which an artificial planar
structure traverses a homogeneous space and seismic waves
propagate from the lower to the upper subdomain. The half-
space has uniform \(P\)- and \(S\)-wave velocities, the same as those
in the model of Fig. 3. The modelling space with a total extent
of \(50.8\) km in all three dimensions is discretized into a
\(128 \times 128 \times 129\) mesh for the single-domain calculation.
The configuration of the grid mesh for the two-domain experiment
is \(128 \times 128 \times 33\) in the upper subdomain and \(128 \times 128 \times 97\)
in the lower subdomain. The non-physical discontinuity that
divides the space into the two subdomains is put at a depth
of \(12\) km. The centroid of a pure dip-slip normal fault with the
strike oriented \(45^\circ\) from the \(x\) to the \(y\) axis is located in the
lower domain at \(14\) km depth. Synthetic seismograms recorded
at the free surface and at \(0.8\) km below the centroid are
calculated from both single-domain and two-domain
approaches. In the two-domain case, the wavefield is calculated
separately in each subdomain and then the continuity condition
is imposed along the fake discontinuity. The synthetic seismo-
grams from these two different calculations are almost exactly
identical (Fig. 4), indicating that the wavefield-matching routine
we apply at the overlapped grids between two domains is
correct and no artificial converted phases or reflections appear
at the non-physical interface.
The example shown in Fig. 5 illustrates that if an abrupt

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Seismic anisotropy has been documented in many tectonic regions such as the upwelling melting zone beneath mid-ocean ridges, near mantle plumes, spreading oceanic lithosphere and upper asthenosphere, mantle wedges above subduction slabs and the D\(^\circ\) region (e.g. Bowman & Ando 1987; Nishimura & Forsyth 1989; Bjarnason et al. 1996; Kendall & Silver 1996). Shear-wave splitting, polarization anomalies and azimuthal anisotropy of seismic traveltimes are commonly employed to detect the faulting and crack alignment in shallow crustal structures (e.g. Crampin & Lovell 1991) and to study the large-scale convective flow associated with plate motion and mantle dynamics (e.g. Russo & Silver 1994).

To characterize the complication of seismic wavefields in anisotropic structures, we perform wave-propagation simulations in our elastic models with a variety of crystallographic symmetries that may occur in the Earth’s mantle or crust. The first model, A, is a reference isotropic model with a \(P\)-wave velocity of 8.94 km s\(^{-1}\) and an \(S\)-wave velocity of 5.16 km s\(^{-1}\). The second model, B, is a transversely isotropic medium with a horizontal symmetry axis oriented 45\(^\circ\) from the \(x\)- and the \(y\)-axes, i.e. in the [110] direction. The \([hkl]\) indicates the outward-directed normal to the lattice plane (\(hkl\)) and the \(\hat{h}\) is the opposite to the \(+h\) direction (Weiss & Wenk 1985). The \(x\), \(y\) and \(z\)-axes in the coordinate of the model space are orientations parallel to the directions \([100]\), \([010]\) and \([001]\), respectively. This model can simplify the general stiffness tensor to five independent elastic coefficients (Babuska & Cara 1991).

The third model, C, has orthorhombic symmetry with elastic properties associated with an olivine crystal, the most abundant mineral in the upper mantle. The \(a\)-axis, the fastest propagating direction for the \(P\) wave, coincides with the \(x\)-axis and the slowest \(b\)-axis is aligned along the \(\gamma\)-axis. There are nine independent elastic coefficients in this symmetry system. The last model, D, has monoclinic symmetry in which two of the three crystallographic axes are mutually perpendicular and the third is inclined. The velocity is only symmetric to the plane containing the orthogonal \([100]\) and \([001]\) axes, which are oriented in the \(x\)- and \(z\)-directions in our calculation. The number of independent elastic coefficients extends to 13. Most minerals in the crust, such as feldspar and diopside, have this symmetry.

4.1 Phase velocities of the anisotropic models

For the three anisotropic models, we solve the eigenvalues and eigenvectors of the Christoffel matrix associated with the stiffness tensor of an elastic medium, which yield three phase velocities and the corresponding polarization directions.
SV is the slowest direction for the P wave, the [001] the intermediate, and the [010] the fastest, the SH wave is the slowest on this plane and the fastest along its striking direction points to [001] or [010]. The fastest wave travels parallel to either the [010] or the [001] direction, and the corresponding polarization direction points to [001] or [010]. The fastest S wave travels on the XZ plane, heading for the direction inclined 45° or 135° from the z-axis, and is polarized on the XZ plane normal to the propagating direction. Such a model exemplifies the anisotropic structure in the upper mantle, where the majority of the constituent minerals such as orthorhombic olivine undergo dislocation-creep deformation and preferentially orient their a-axes to the flow direction.

The velocity dependence on the direction of propagation for model D is much more complicated because of the oblique crystallographic axis and fewer symmetry planes. The most striking differences between this system and the previous ones are that the phase velocity is only symmetric to the XZ plane, and that the fastest direction is oblique to the slowest direction for both P and S waves and none of them parallel to the x-, y- or z-axis. The propagation direction for the fastest and slowest P wave is on the symmetry XZ plane, inclined 30° and 145° from the z-axis, respectively. The fastest and slowest directions for the S waves are even more obscure. They are neither mutually orthogonal nor on any planes normal to the coordinate axes. This system may exist in subduction zones or locally random symmetry properties or due to averaging over beneath spreading centres, where the a-axis of olivine tends to be dipping in such a way as to accommodate the maximum finite extension from the turning flow.

4.2 Anisotropic wavefields and synthetic waveforms

The model space for the numerical simulation is discretized into a $128 \times 128 \times 101$ mesh and extends 63.5 km in the...
Figure 6. Azimuthal equal-area projections of anisotropic velocities (km s$^{-1}$) as a function of azimuth and dip angle for Model B with hexagonal symmetry (or transverse isotropy) in the upper right diagram; Model C with orthorhombic symmetry in the lower left diagram; Model D with monoclinic symmetry in the lower right diagram. In each model, velocities of quasi-$P$, quasi-$SV$ and quasi-$SH$ phases are shown in the top, middle and bottom rows of the left column, respectively. The paired velocities in each row are projections from two opposite centres: the left is from the top (0, 0, −1) and the right from the bottom (0, 0, 1). The right column shows the wave fronts emitted from the source on the $XY$ (top), $XZ$ (middle) and $YZ$ (bottom) planes.

In an isotropic homogeneous medium such as model A, the phase velocities of the three eigenmodes are independent of path, and thus the wave fronts emitted from the point source remain spherical. Shear waves are not split since the radially and transversely polarized components propagate with the same speed. For the transversely isotropic model B, the snapshot at the surface displays elliptical wave fronts with the long axis aligned along the [110] axis, the fast propagation direction at 3.6 s after initiation of the source. We show the wavefield of the vertical displacement at the free surface ($XY$ plane). The horizontal displacement in $x$- and $y$-components is respectively shown on the vertical $XZ$ and $YZ$ planes slicing through the source point.
these axes, and they are recorded on the surface with identical wave shapes and amplitudes. Therefore, for these two models the snapshots of the wavefields on the XZ and YZ planes are equivalent in shape but opposite in polarity because of the orientation of the double-couple source.

In orthorhombic model C, the P and S waves travelling along the x-axis are faster than along the slowest y-axis and the intermediate z-axis, resulting in three distinct, non-circular wave fronts on these planes. In addition to the diversity of wave-front shapes linked to azimuthal anisotropy in phase arrival times, the change of wavefield amplitudes is also different from the previous models. On the XY and XZ planes, two horizontal bitangent lines along the x-direction, which are individually tangent to the wave-front curves at two points, exist for the quasi-SH phase (see Fig. 6). These correspond to the SV waves propagating with a local maximum speed along the nodal planes of the radiation energy (45° from the x-axis), where both the P and S waves have minimum amplitudes in the vertical component. At the free surface, the P-wave amplitudes are as small as those in models A and B, but the excited S-wave amplitudes are quite large in these directions. The most interesting features in the S wavefields are triangular-shaped regions of upward (negative) displacement and cusps pointing in the +x and −x directions, associated with the interference of the quasi SV and SH waves. The wave surfaces from these two shear phases graze each other at these planes. The amplitudes of the S waves in the y-component are relatively small on the XZ plane except near the bitangent points of the faster SH wave. The velocity variations in the y- and z-directions are more subdued, leading to more circular-like wave fronts on the YZ plane. Because the velocity contrast between the SV and SH phases is small on this plane, the split shear waves are not separated enough to be detected in the wavefield snapshot.

For monoclinic model D, the snapshots of displacement are complex due to the low degree of symmetry and the intricate shear-wave splitting. The wave surfaces on the XY plane through the source point are symmetric to the x- and y-axes (Fig. 6), but only the symmetry to the x-axis is preserved at the free surface. The upcoming P waves propagate faster towards the +x- than the −x-direction, but the S waves are slower towards the +x-direction, which yields the non-symmetric distortion of the wave fronts. The geometries and amplitudes of the wavefields are entirely different in the two x-directions. Because the crystallographic axis [010] is inclined from the y-axis, the wave surfaces on the XZ plane are distorted in a tilted configuration. The downgoing P waves are faster towards the −x- than the +x-direction. The S waves behave in the opposite way. For the downgoing S waves, the SH is the leading shear phase in the +x quadrant. The wave surfaces from the SV and SH phases intersect in the −x quadrant and thus the SV phase moves ahead of the SH (Fig. 6). Except for polarity reversal, the wave fronts on the YZ plane are symmetric with respect to the XZ plane, the only symmetry plane for this system. When the S waves propagate in the YZ plane along the y-direction, the SV and SH phases are split more than in any other direction because the SH propagates with the local maximum speed while the SV propagates with the minimum. The disturbed wavefields are kinked near the places where the two shear phases arrive close together and interfere with each other.

In Fig. 9 we show azimuth-dependent variabilities of arrivals and waveforms in synthetic seismograms for these four models. Four receivers are placed on the free surface at the same distance of 15.1 km from the centroid of the source. The locations of the stations and their ray paths are shown in Fig. 7. No azimuthal anisotropy is shown in the transversely isotropic model because the azimuths of these four particular stations are off from the symmetry axis by the same degree and the seismic waves go through the same velocity variation along the ray paths. Although there is not much difference in P waveforms between the isotropic and transversely isotropic models at these azimuths, the S waveforms show diagnostic distinctions. The single, one-cycled pulse shown in the isotropic model is split into two on the vertical and horizontal components of the transversely isotropic model. In the orthorhombic model, the P- and S-wave velocities are symmetric around the x- and y-axes, so there are no differences in waveforms or arrival times between Stations 1 and 2 or between Stations 3 and 4 (except for changes in polarity on the horizontal components). However, the azimuth of the ray path for Station 2 is near the fastest axis while Station 3 is close to the slowest axis, so there are significant differences between P and S arrival times and S waveforms for this station pair. Shear-wave splitting is clearly seen on the two horizontal components of Stations 1 and 2. The monoclinic model shows variations of P-wave arrival time and non-symmetric, complicated waveforms at all four stations because the YZ plane (100) is not the symmetry plane. The P wave travels fastest and the S wave propagates mostly slowly towards Station 1, resulting in the largest S-P differential times. The effect at Station 2 is just the opposite because the P wave travels mostly slowly while the S wave is much faster.

4.3 Wave propagation in the space containing a water layer

To illustrate that the multidomain method can effectively simulate energy partitions in models with discontinuities, we add a 2 km deep water layer on the top of an isotropic (Model A) and an anisotropic half-space with orthorhombic symmetry (Model C). A normal-faulting earthquake with 45° strike is excited at location (32, 32, 11) km. Fig. 10 schematically
Figure 9. Comparison of waveforms of the four models recorded on the free surface at the same distance, but at several different azimuths. Dashed lines represent the vertical components of displacement. Horizontal components pointing to the $x$- and $y$-directions are indicated by dotted and solid lines, respectively.

Figure 10. The geometry of the model space, seismic source and recording stations for the simulations of wave propagation in the elastic models (A and C) overlain by a water layer. Solid triangles indicate the 10 receivers located at the water-solid interface, denoted by S1, S2, ..., S9 and S10. The ray paths are shown by solid lines. The dark grey region represents the 2 km water layer. Three light grey planes are the places where the snapshots in Fig. 11 are recorded. The focal sphere shows the normal fault exerted at the hypocentre projected onto the $XY$ plane. Black quadrants indicate compressional $P$-wave motions. The side view along the strike shows the slip motion on the fault plane.

distances, is the inhomogeneous $P$ wave. The wave front that forms in the centre region of the $XY$ plane is the reverberated phase, $spwP$, which is converted from $S$ at the water/solid interface and bounces once in the water layer. The multiple water reverberations are clearly shown in the snapshots of the $XZ$ and $YZ$ planes.

In Fig. 12, we show the vertical displacement and pressure recorded at the water/solid contact with a variety of azimuths and distances. The positions of the receivers and the
Figure 12. Comparison of synthetic seismograms for the isotropic and the orthorhombic half-spaces overlain by a 2 km water layer. Pressure and vertical displacement are recorded at the medium interface as a function of distance and azimuth. The former is shown at the top of each paired trace by a solid line and the latter at the bottom by a dashed line (a) for the isotropic model; (b) for the orthorhombic model. The number in degrees shown on each paired record indicates the azimuth of the ray path.

corresponding ray paths are shown in Fig. 10. Differences in amplitude and waveform between these two models are clearly illustrated on both displacement and pressure records, particularly for the shear wave and S-to-P reverberated phases. For instance, the amplitude of the S wave at station S2 for the orthorhombic model is small and nearly invisible compared to that in the isotropic model. Shear waves are split when seismic waves do not propagate along the symmetry axes, such as those arriving at the stations S4, S5 and S6. The head-wave P phases that appear between direct P and S at horizontal distances greater than 17 km are converted from the SV component when the incident angle exceeds 60° and is beyond the critical angle for the reflected P wave. In addition, the water-reverberated phases such as pwP and spwP are well constructed. The multiple reverberations bouncing within the water column are separated by an equal time delay of about 2.6 s for the two-way traveltime in the 2 km water layer. The polarity of the pwP phase is reversed on the free surface relative to the direct P phase in pressure, but not in displacement. Therefore, the multiple pwP and swP phases change polarity in the pressure recording when bouncing once in the water layer. The much larger amplitude of pwP relative to P in pressure is due to the constructive superposition of incident and reflected energy at the water/solid interface. For displacement, however, the incident P wave from the water layer reflected at the interface reverses in polarity. Destructive interference between the incident and reflected waves at the seafloor causes a low amplitude of the multiple reverberations on the vertical component. These observations are consistent with predictions of simple ray theory and reflectivity synthetics (Blackman, Orcutt & Forsyth 1995).

5 CONCLUSIONS

The simulation results demonstrate that the multidomain pseudo-spectral method is able to calculate accurately synthetic seismograms and propagating wavefields in anisotropic structures with a free surface or with large velocity gradients such as that associated with the water/crust boundary. The multidomain approach, which uses an appropriate domain decomposition scheme and implements the continuity condition along discontinuous contacts provides the flexibility to change grid spacings based on the variation of wave speed and the requirement of the minimum number of grid points needed to sample a complete wavelength. Parallelization of the serial code to run in high-performance parallel computers makes the computation of 3-D simulations or large-scale problems practical, so that the discrete numerical solutions become increasingly powerful and competitive for the seismological applications of full-waveform modelling. The parallel algorithm using the message-passing model supported by the standard Message-Passing Interface library is not restricted to run only on the SP2 computer. It is portable and can be
ACKNOWLEDGMENTS

We wish to thank Jeff Orrey for providing his thesis and a 2-D isotropic code as a starting place to develop our 3-D, multidomain pseudo-spectral scheme for generalized anisotropic and heterogeneous media. We also thank Marc Parmentier and Karen Fischer for their comments at the beginning of this work. The thorough and critical reviews from Colin Thomson and two anonymous referees helped us to improve the manuscript significantly. S-HH benefitted from discussion with Paul Fischer on the parallelization of the 3-D serial code. Examples shown in the paper were run on the 24-node IBM SP2 machine sponsored by the Center for Fluid Mechanics (CFM) of the Department of Applied Mathematics at Brown University. Constantinios Evangelinos and Sam Fulcomer from CFM gave kind assistance in managing parallel jobs on the SP2 computer. This research was supported by the National Science Foundation under grants OCE-9314489 and OCE-9402375.

REFERENCES


APPENDIX A: CHARACTERISTIC VARIABLES FOR MULTIDOMAIN SPACE

The matrices $A$, $B$, $D$ containing the elastic coefficients and density of the medium have the following explicit forms:

$$A = \begin{bmatrix}
1/\rho & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1/\rho \\
0 & 0 & 0 & 0 & 1/\rho & 0 \\
C_{11} & C_{16} & C_{15} & 0 & 0 & 0 \\
C_{21} & C_{26} & C_{25} & 0 & 0 & 0 \\
C_{31} & C_{36} & C_{35} & 0 & 0 & 0 \\
C_{41} & C_{46} & C_{45} & 0 & 0 & 0 \\
C_{51} & C_{56} & C_{55} & 0 & 0 & 0 \\
C_{61} & C_{66} & C_{65} & 0 & 0 & 0 \\
\end{bmatrix}$$

$$B = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 1/\rho \\
0 & 0 & 1/\rho & 0 & 0 & 0 \\
0 & 0 & 0 & 1/\rho & 0 & 0 \\
C_{16} & C_{12} & C_{14} & 0 & 0 & 0 \\
C_{26} & C_{22} & C_{24} & 0 & 0 & 0 \\
C_{36} & C_{32} & C_{34} & 0 & 0 & 0 \\
C_{46} & C_{42} & C_{44} & 0 & 0 & 0 \\
C_{56} & C_{52} & C_{54} & 0 & 0 & 0 \\
C_{66} & C_{62} & C_{64} & 0 & 0 & 0 \\
\end{bmatrix}$$

$$D = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 1/\rho \\
0 & 0 & 0 & 0 & 1/\rho & 0 \\
0 & 0 & 0 & 1/\rho & 0 & 0 \\
C_{15} & C_{14} & C_{13} & 0 & 0 & 0 \\
C_{25} & C_{24} & C_{23} & 0 & 0 & 0 \\
C_{35} & C_{34} & C_{33} & 0 & 0 & 0 \\
C_{45} & C_{44} & C_{43} & 0 & 0 & 0 \\
C_{55} & C_{54} & C_{53} & 0 & 0 & 0 \\
C_{65} & C_{64} & C_{63} & 0 & 0 & 0 \\
\end{bmatrix}$$

where $C_{mn} = C_{nm}$ is a common $6 \times 6$ matrix expression for the fourth-order stiffness tensor $c_{ijkl}$ using symmetric properties of $c_{ijkl} = c_{klij} = c_{ikjl} = c_{ijlk}$. The formal relation between $C_{mn}$ and $c_{ijkl}$ is $C_{mn} = c_{mn}$ with $m = i = j$ if $i = j$ and $m = 9 - i - j$ if $i \neq j$, and $n = k = l$ if $k = l$ and $n = 9 - k - l$ if $l \neq l$ (Babuska & Cara 1991).

The characteristic variables for the wave equation are obtained from 1-D analysis in which only derivatives to the normal direction of the surface are considered (e.g. Tessmer et al. 1992). Therefore, eq. (3) becomes

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{D} \frac{\partial \mathbf{U}}{\partial x_3}.$$  \hspace{1cm} (A2)

Diagonalizing the matrix $D$ and multiplying its inverse eigenvector matrix $\mathbf{T}^{-1}$ on both sides of eq. (A2), we get

$$\frac{\partial \mathbf{V}}{\partial t} = \Lambda \frac{\partial \mathbf{V}}{\partial x_3}.$$  \hspace{1cm} (A3)

where $\mathbf{V} = \mathbf{T}^{-1} \mathbf{U}$ is the vector of characteristic variables, $\Lambda = \mathbf{T}^{-1} \mathbf{CT}$ is the diagonal matrix containing the eigenvalues of the matrix $D$, and $\mathbf{T}$ is the matrix composed of the column eigenvectors of the eigenvalues $(0, 0, 0, \varepsilon_1, -\varepsilon_1, -\varepsilon_2, \varepsilon_2, -\varepsilon_3, \varepsilon_3)$.

For the fluid domain, the acoustic wave equation is solved instead to obtain the velocity and pressure. The field variables $\mathbf{U}$ that appears in eq. (3) becomes $[v_1, v_2, v_3, -P]^T$. The
matrices $A$, $B$ and $D$ are simplified to

\[
A = \begin{bmatrix}
0 & 0 & 0 & 1/ho \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
K & 0 & 0 & 0
\end{bmatrix}, \quad
B = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1/ho \\
0 & 0 & 0 & 0 \\
0 & K & 0 & 0
\end{bmatrix},
\]

\[
D = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1/ho \\
0 & 0 & K & 0
\end{bmatrix}, \quad (A4)
\]

where $K$ is the bulk modulus.

Following the similar 1-D characteristic variable analysis for elastic media, the matrix $D$ in the fluid domain has two zero eigenvalues and two non-zero eigenvalues that are equal to $\pm v_p (= \sqrt{K/\rho})$, where $v_p$ is the speed of the acoustic waves. The characteristic variables are

\[
[V] = \begin{bmatrix}
v_3 - p/(\rho v_p) \\
v_3 + p/(\rho v_p) \\
v_1 \\
v_2
\end{bmatrix}. \quad (A5)
\]