Wave propagation in 3D spherical sections: effects of subduction zones
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Abstract

In order to understand details in the seismic wave field observed on regional and global scales on the Earth’s surface accurate modeling of 3D wave propagation is necessary. While numerical techniques are now routinely applied to local seismic wave propagation, only recently has the possibility of simulating wave propagation on larger scales in spherical geometry been investigated. We apply a high-order staggered-grid finite-difference scheme to the elastic wave equations in spherical coordinates \( \phi, \theta, r \). Using regular grid spacing in a single domain the physical space is limited to spherical sections which do not include the axis \( \theta = 0 \). While the staggering of the space-dependent fields improves the overall accuracy of the scheme, some of the tensor elements have to be interpolated to the required grid locations. By comparing with quasi-analytical solutions for layered Earth models we demonstrate the accuracy of the algorithm. Finally, the technique is used to study the effects of a source located in a simplified slab structure. The 3D technique will allow us to study the wave field due to laterally heterogeneous structures, such as subduction zones, plumes or oceanic ridges.

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1. Introduction

Many questions on the dynamics of the Earth’s interior depend on structural imaging using seismic tomography. While ray-theory based techniques offer the reconstruction of the long-wavelength structures explaining predominantly phase effects, it is desirable to be able to investigate frequency-dependent wave form effects of 3D structures due to scattering. This applies particularly to the most laterally heterogeneous areas of the mantle, the upper part with subduction zones, ridge structures and plumes and the lower part with the strongly heterogeneous lowermost mantle structure (D′′), the origin of which is still not well understood. With 3D reference Earth models in sight, the development of methods which allow the accurate simulation of the complete wave field on regional and global scales is an important step towards understanding the complexity of the observed seismic motion.

Numerical methods have been applied successfully to wave propagation problems on local scales (e.g. Graves, 1993, 1998; Olsen and Archuleta, 1996) using discretizations of the equations of motion in cartesian coordinates. Particularly the finite-difference method played an important role due to its simplicity and the ease with which it is implemented on parallel hardware. The early work of Virieux (1986) in 2D was soon extended to 3D (Witte and Richards, 1987; Mora, 1989), and anisotropic media (Igel et al., 1995). Other approaches include the pseudo-spectral method (e.g. Kosloff et al., 1984; Reshef et al., 1988; Tessmer and Kosloff, 1994; Tessmer, 1995; Furumura...
et al., 1998), the finite-element method (e.g. Padovani et al., 1994) and a combination of pseudo-spectral and finite-element methods, the spectral element method (e.g. Priolo and Seriani, 1991; Komatitsch et al., 2000).

A pioneering application of numerical techniques to wave propagation in spherical geometry was carried out by Alterman et al. (1970) using a centered finite-difference technique to solve the problem of P-SV wave propagation in spherical coordinates in the axisymmetric approximation. Along similar lines, but using high-order approaches and staggered-grid techniques, Igel and Weber (1995, 1996) studied global wave propagation (SH, and P-SV waves, respectively) and investigated the effects of heterogeneous mantle structures. Chaljub and Tarantola (1997) studied topographic effects of the upper mantle discontinuities using a finite-difference algorithm for SH waves (axisymmetric approach). These discrete grid models allowed the investigation of waveform effects of slab structures (Igel and Ita, 1997), and finite-frequency techniques, Igel and Weber (1995, 1996) studied global wave propagation in spherical coordinates. However, when the physical domain is restricted to a spherical section away from the poles, then standard techniques can be used. Igel (1999) presented a pseudo-spectral solution to this problem on a centered grid using the Chebyshev technique previously applied to cartesian systems (e.g. Tessmer and Kosloff, 1994). While the pseudo-spectral method has advantages concerning the accuracy of the spatial differential operators, the method is more difficult to implement on parallel hardware due to the global communication schemes required to perform Fourier transforms (or matrix-matrix multiplies). Therefore, we investigate the possibility of using a high-order staggered-grid method to numerically solve wave propagation in a spherical section. A similar approach was taken by Marcinkovich and Tanimoto (1999).

In the following we first present the governing equations and their numerical solution algorithm. We then discuss the accuracy of the algorithm and show examples of 3D wave propagation through models with a simple subduction zone structure in the upper mantle.

2. Governing equations

As we intend to solve the governing time-dependent partial differential equations with a staggered-grid finite-difference method, a first-order description of the equations as previously used in cartesian coordinates (e.g. Virieux, 1986; Tessmer and Kosloff, 1994; Tessmer, 1995) seems appropriate. In spherical coordinates \([\theta, \varphi, \rho]\) the equations of motion for elastic anisotropic wave propagation read:

\[
\begin{aligned}
\rho \ddot{v}_r &= \frac{\partial}{\partial r} \left( \frac{\sigma_{rr}}{r^2} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \sigma_{r \theta} \cot \theta \right) + \frac{1}{r} \frac{\partial}{\partial \varphi} \left( \sigma_{r \varphi} \right) + f_r \\
\rho \ddot{v}_\theta &= \frac{\partial}{\partial r} \left( \frac{\sigma_{\theta \theta}}{r^2} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \sigma_{\theta \theta} \cot \theta \right) + \frac{1}{r} \frac{\partial}{\partial \varphi} \left( \sigma_{\theta \varphi} \right) + f_\theta \\
\rho \ddot{v}_\varphi &= \frac{\partial}{\partial r} \left( \frac{\sigma_{\varphi \varphi}}{r^2} \right) + \frac{1}{r} \frac{\partial}{\partial \theta} \left( \sigma_{\varphi \theta} \cot \theta \right) + \frac{1}{r} \frac{\partial}{\partial \varphi} \left( \sigma_{\varphi \varphi} \right) + f_\varphi
\end{aligned}
\]

(1)

where \(v_r, v_\theta, v_\varphi\) are the components of velocity, \(\rho\) is the mass density, \(\sigma_{ij}\) are the components of the stress tensor, and \(f_r, f_\theta, f_\varphi\) are the force components. In general anisotropic media the stress–strain relation is given as:

\[
\sigma_{ij} = c_{ijkl} \varepsilon_{kl} + M_{ij}
\]

(2)

where \(c_{ijkl}\) are the components of the fourth-order elasticity tensor, \(\varepsilon_{ij}\) the components of the deformation tensor, and \(M_{ij}\) are the components of the source moment tensor scaled by the volume of the respective grid cell. The deformation rate is related to the velocities by:

\[
\begin{aligned}
\dot{\varepsilon}_{ij} &= \frac{1}{\rho} \left( \frac{\partial}{\partial r} \sigma_{ij} + v_j \right) \\
\dot{\varepsilon}_{r \theta} &= \frac{1}{r \sin \theta} \left( \frac{\partial}{\partial \theta} \sigma_{r \theta} + \frac{r}{\sin \theta} v_\theta \right) + \frac{1}{r} \cot \theta \frac{\partial}{\partial \varphi} v_\varphi \\
\dot{\varepsilon}_{r \varphi} &= \frac{1}{r} \frac{\partial}{\partial \varphi} \left( \sigma_{r \varphi} + \frac{r}{\sin \theta} v_\theta \right) \\
\dot{\varepsilon}_{\theta \theta} &= \frac{1}{r^2} \left( \frac{\partial}{\partial \theta} \sigma_{\theta \theta} + \frac{1}{r \sin \theta} v_\theta \right) + \frac{1}{r} \frac{\partial}{\partial \varphi} \sigma_{\theta \varphi} \\
\dot{\varepsilon}_{\theta \varphi} &= \frac{1}{r} \frac{\partial}{\partial \varphi} \left( \sigma_{\theta \varphi} + \frac{1}{r \sin \theta} v_\theta \right)
\end{aligned}
\]
\[ \partial_t \varepsilon_{\theta r} = \frac{1}{2} \left( \frac{1}{r} \partial_r v_r + \partial_{\theta} v_\theta - \frac{1}{r} v_\theta \right) \]
\[ \partial_t \varepsilon_{\theta \phi} = \frac{1}{2} \left( \frac{1}{r \sin \theta} \partial_\phi v_\theta + \frac{1}{r} \vphantom{\sin} \partial_\theta v_\phi - \cot \theta \frac{1}{r} v_\phi \right) \] (3)

The elasticity parameters are conveniently described in the condensed notation:
\[ \sigma_p = c_{pq} \epsilon_q, \quad p, q = 1-6 \] (4)

where, in spherical coordinates, the mapping: 1 \mapsto \theta \theta, 2 \mapsto \phi \phi, 3 \mapsto r r, 4 \mapsto \phi r, 5 \mapsto \theta r, 6 \mapsto \theta \phi \] applies. The corresponding elements of the elasticity tensor are then given by:
\[
\begin{bmatrix}
\sigma_{\theta \theta} & \sigma_{\phi \phi} & \sigma_{r r} & \sigma_{\phi r} & \sigma_{\theta r} & \sigma_{\theta \phi}
\end{bmatrix}
\times
\begin{bmatrix}
\epsilon_{\theta \theta} & \epsilon_{\phi \phi} & \epsilon_{r r} & \epsilon_{\phi r} & \epsilon_{\theta r} & \epsilon_{\theta \phi}
\end{bmatrix}
\] (5)

and they reduce to:
\[ \epsilon_{\theta \theta} = \epsilon_{\phi \phi} = \epsilon_{r r} = \frac{1}{2} \right \}
\[ \epsilon_{\phi r} = \epsilon_{\theta r} = \epsilon_{\theta \phi} = 0 \] (6)

in the isotropic elastic case, where \( \lambda \) and \( \mu \) are the Lamé constants and all other elements are zero.

In the following, we will present a numerical solution to these equations for the isotropic case based on a staggered-grid finite-difference method.

3. Numerical solution

All space-dependent fields (velocities, stresses, material parameters) are defined on an equidistant grid in spherical coordinates \([\theta, \phi, r]\). As mentioned above, due to the singularities present in the equations of motion, the physical domain is limited to regions away from the axis \( \theta = 0 \), where motion is not defined.

A convenient choice is to center the spherical section around the equator. In Fig. 1 a spherical section with angular ranges \(80^\circ\) (for both \(\phi\) and \(\theta\)) is shown with a depth extent of 5000 km. Centering the domain around the equator minimizes the range of grid increments on the spherical section along the axis \( \theta = 0 \) we center the model on the equator (solid lines). Geographical models can be rotated accordingly.
Fig. 2. (a) Staggered grid used in the finite-difference calculations. The elements of a cell unit are linked by lines. Note that some of the elements need to be interpolated to calculate the acceleration (see text). (b) Locations where material parameters are defined. Note that in heterogeneous media the material parameters (e.g. $\rho$) may vary within a grid cell.
the spherical shell thus optimizing the stability for a particular model range.

The first-order formulation of the equations of motion suggests the use of a staggered-grid scheme as applied in several cartesian algorithms (e.g., Virieux, 1986; Graves, 1993; Frankel, 1993; Igel et al., 1995; Olsen et al., 1995). The staggering of the vector and tensor elements as well as the material parameters is shown in Fig. 2. Note that due to the spherical coordinate system geometrical terms appear in the equations and $r$ and $\theta$ need to be defined at all the staggered locations. The finite-difference operators are convolutional operators as used by Igel et al. (1995). In the numerical tests carried out below a four-point operator is being applied. The time extrapolation is carried out by a first-order Taylor expansion.

We define the material parameters ($\rho$ and tensor of elastic constants $c_{pq}$) at the grid locations where the diagonal elements of the stress tensor are defined. This implies that those parameters that are needed elsewhere in the grid cell have to be interpolated to these locations. This interpolation is carried out using a second order scheme. To accurately model the location of interfaces or sources at material discontinuities such interpolations are necessary (e.g., Igel et al., 2002). In comparison with cartesian schemes a further

Fig. 3. Comparison of synthetic seismograms (vertical velocity component) by the FD method (solid lines) with seismograms calculated using the reflectivity technique (dashed lines, slightly offset) for a homogeneous model ($v_p = 8.08$ km/s, $v_s = 4.47$ km/s, $\rho = 3.37$ g/cm$^3$). The source is a vertical force at 100 km depth. The dominant period is 12 s.
complication occurs: as can be seen from Eqs. (1) and (3) the staggering does not lead to a completely decoupled scheme as the calculation of velocity or stress components requires terms which are not defined or centered at the corresponding grid locations. For example, to calculate the acceleration $\frac{\partial v_\theta}{\partial t}$ (left-hand side of the top Eq. (1)) the stress components $\sigma_{\theta\theta}$, $\sigma_{\phi\phi}$, $\sigma_{\rho\theta}$ need to be interpolated to the location of $v_\theta$. These interpolations are carried out using a second-order scheme.

The free surface boundary condition:

$$\sigma_{rr} = \sigma_{r\phi} = \sigma_{r\theta} = 0$$ (7)

is implemented in the same way as in the case of a cartesian system by using an explicit method by Graves (1996).

Simple absorbing boundary conditions are implemented by tapering the fields as well as seismic velocities with decreasing values using Gaussian functions. There are two grid levels at which the free surface can be defined (at the level of the diagonal stress elements or the level of the radial velocity component). Note that Gottschämler and Olsen (2001) investigated these two options and concluded that the overall errors are smaller when the free surface is defined at the latter location, which is the approach we adopted. The computationally demanding algorithm is implemented using domain decomposition in the vertical direction and the message passing interface (MPI). Hereby, the 3D grid is divided into $n$ depth sections, where, $n$ is the number of computational nodes. To be able to calculate the space derivatives with respect to the vertical direction...
across the domain boundaries \( n_{op}/2 \) grid slices have to be communicated to the neighboring processor, where \( n_{op} \) is the length of the differential operator (in our case \( n_{op} = 4 \)). Typical performance data for a model of size \( 720 \times 1220 \times 406 \) and a simulation run for 4200 time steps are a memory requirement of ca. 60GBytes and a runtime of 10.5 h on 13 nodes of a Hitachi Sr8000-F1.

4. Verification, accuracy, snapshots

To assess the accuracy of the proposed algorithm we compare the numerical solutions with synthetic seismograms calculated with the reflectivity method (Fuchs and Müller, 1971; Wang, 1999) for regional wave propagation. The model parameters are \( v_p = 8.08 \) km/s, \( v_S = 4.47 \) km/s, and \( \rho = 3.37 \) g/cm\(^3\). The grid size is \( \theta, \phi, r \) and the grid distance at the Earth’s surface is approximately 4 km, leading to a cube of 800 km side length. The source is a vertical point force \( f_r \) acting at a depth of 100 km and 600 time steps were evaluated with a time increment of 0.2 s. We simulate a delta-like point source in space and time at the corresponding grid location. This leads to synthetic seismograms containing numerical artifacts that are reduced through convolution with a source time function of appropriate dominant frequency. The source-time function is the first derivative of a Gaussian.

In Fig. 3 synthetic seismograms (vertical velocity component) are shown for epicenter distances up to 400 km using both the reflectivity method and the
finite-difference algorithm. The reflectivity seismograms have been calculated with the Earth-flattening transformation. We calculate the energy misfit $\varepsilon$ of the waveforms for a particular velocity component $v$ by summing over samples $i$:

$$
\varepsilon = \frac{\sum (v_{FD}^i - v_{REF}^i)^2}{\sum v_{REF}^2}
$$

The misfit is shown in Fig. 4 as a function of dominant period and distance. As expected the error generally decreases with increasing dominant period as the wave field is sampled with a larger number of grid points per wavelength. The error also increases with propagation distance. For a dominant period of 20 s (this corresponds to approximately 22 points per dominant wavelength) the error is below 1% for distances smaller than 350 km.

Seismograms are compared for a two-layer model in Fig. 5 (vertical velocity component). The grid size is the same as for the homogeneous model. The top layer has the same properties as mentioned above. Below 240 km depth the material parameters are $v_p = 8.89$ km/s, $v_S = 4.92$ km/s, and $\rho = 3.7$ g/cm$^3$. The source is an explosion at 100 km depth and 900 time steps were evaluated with a time increment of 0.2 s. The comparison with the reflectivity seismograms shows that all signals are present in the numerical

![Fig. 6. The energy misfit of the traces shown in the previous figure as a function of receiver distance for seismograms with varying dominant frequency.](image)
solution. The reflections and conversions from the discontinuity at 240 km depth are indicated in Fig. 5.
Ray-theoretical arrival times were calculated using a Gaussian beam method and superimposed on the seismograms. The misfit energy as functions of distance and frequency (Fig. 6) shows that for this setup at a dominant period of 20 s the misfit is approximately 1% for all epicentral distances.
Snapshots for wave propagation simulation on a 200x grid are shown in Fig. 7 at four different times. The physical domain is 90° x 90° x 5000 km. The source is an explosion at 600 km depth and the dominant period of the wave field is approximately 40 s. The simulation was carried out for the spherically symmetric PREM model (isotropic part, no crust). The snapshots show predominantly the direct P-waves and the surface reflections and conversions (pP, pS) as well as the core–mantle boundary reflections (PcP, PcS), Fig. 7A-D.

5. Numerical example: slab effects
Subducted lithosphere constitutes the strongest laterally heterogeneous structures in the Earth’s upper mantle and it hosts the largest earthquakes on this planet. The wave field radiated by seismic sources inside subduction zones may be severely affected by their heterogeneous structure. In addition to the high-velocity anomaly associated with a cool slab, low-velocity layers due to untransformed oceanic crust at the top of the slab may exist (e.g. Hori et al., 1985), possibly containing water (Ilk and Madariaga, 1996). The effects of subduction zones on seismic waveforms and arrival times were previously investigated by Vidale (1987), Cormier (1989), Weber (1990), Vidale et al. (1991), Bostock et al. (1993), and Sekiguchi (1992). Shapiro et al. (2000) studied wave effects of accretionary prisms with evidence from long-period surface waves propagating along

![Image of snapshots showing elastic wave propagation for an explosive source at 600 km depth. The model is the isotropic part of PREM (no crust). The vertical displacement is shown at four different times: A: t = 125 s; B: t = 200 s; C: t = 260 s; D: t = 320 s. Dark and bright colors denote positive and negative vertical velocity, respectively. At the surface a gray scale is employed. Only amplitudes larger than 1% of the total wavefield are displayed. The major phases are the direct P-wave (A), pP, pS (B), PcP, PcS (D) and a P-wave (C) entering the outer core.](image-url)
As an application of our algorithm we investigate the effects of a subduction zone structure for an earthquake source inside a low-velocity layer at the top of the slab.

The background model is the isotropic part of PREM (Dziewonski and Anderson, 1981) without the crustal layers. The model with grid size $720 \times 1200 \times 406$ has a lateral extent of $22^\circ$ and $13^\circ$ in $\phi$- and $\theta$-directions, respectively. The maximum depth is 808 km. The S-velocity model is shown in Fig. 8. The slab has a maximum positive velocity perturbation of 8% and thickness of approx. 100 km. A low-velocity layer is located on top of the slab with a maximum negative perturbation of 4% and a width of 20 km.

Note that the thickness of this layer has been imposed through the still relatively coarse grid spacing. The source (black star) is located at 260 km depth and is a dip slip source with strike $\phi_s = 0^\circ$, rake $\lambda = 90^\circ$, and the fault plane (and the slab) dips at $\delta = 52^\circ$ at the source location. The slab is invariant in the $\theta$-direction. We situate a receiver profile across the slab (in the $\psi$-direction) directly above the source and a receiver semi-ring around the epicenter at a distance of $5^\circ$. The receiver strings are schematically shown in Fig. 9. In all subsequent seismogram plots the moment rate function is a Gauss function with dominant period of 6 s.

Snapshots of the simulation of wave propagation through the slab structure are shown in Fig. 10. We focus on shear wave propagation and show the curl component perpendicular to the particular model faces. The shear energy propagating in the slab direction (upwards and downwards) is characterized by an additional phase developing due to the low-velocity structure. In addition, at the top of the slab both these shear waves are reflected in the eastern direction. The vertical component of velocity along a profile across the trench. As an application of our algorithm we investigate the effects of a subduction zone structure for an earthquake source inside a low-velocity layer at the top of the slab.
Fig. 10. Snapshots of slab simulation. The component of the curl perpendicular to the relevant plane is shown. Top: wavefield after 50 s. Note the development of an additional shear wave within the slab due to the low-velocity zone. Bottom: wavefield after 120 s. In the direction of the slab two distinct shear phases develop. At the top of the slab shear waves are reflected in eastern direction. Coastlines of South America are superimposed.
the subduction zone is shown in Fig. 11. The time window displayed contains predominantly the direct S wave arrival. The waves traveling upwards through the slab are advanced several seconds (negative distances) while the waves propagating away from the slab are unaffected (positive distances). Most noticeable are additional phases recorded at distances around $-2^\circ$ in the wake of the direct arrival. Due to the slab there is a sudden decrease in amplitude at around $-3^\circ$ indicating the edge of the high-velocity structure at the surface.

The vertical component of motion recorded on a semi-ring at $5^\circ$ distance from the epicenter is shown in Fig. 12. The P-wave arrives at approx. 75 s and the S-wave at 140 s. The slab has strong effects on relative amplitudes and wave forms of both these arrivals. (1) The amplitudes of the P-wave for azimuths greater than $100^\circ$ (away from the slab) are not affected. However, for propagation in the direction of the slab the amplitudes are reduced by up to 50%. In case these signals are used to determine the source mechanism errors may occur. (2) The S-waves are severely affected in the azimuthal range 0–$80^\circ$. This corresponds to waves propagating inside the slab. The S-pulse is advanced, broadened (i.e. two distinct phases) and
Fig. 12. Synthetic seismograms (vertical component) recorded on a semi-ring at 5° epicentral distance (W–N–E). The dominant period is 6 s. Left: seismograms for background model. Right: seismograms for model with slab.

the amplitude reduced. (3) In addition, a diffracted S-wave is propagating in an easterly direction away from the slab. The transverse component of motion recorded on the semi-ring of receivers further highlights the effects of the slab (Fig. 13). Within a very small azimuthal range (at azimuths 60° and 80°) the wave form of the S-arrival splits up into two distinct arrivals and a diffracted wave propagates away from the slab. The presence of the slab leads to considerable reduction of the amplitude of the S-wave (azimuths around 20°).

6. Discussion

To account for wave field complexities that may occur for waves propagating through strongly heterogeneous regions of the mantle (subduction zones, ridges, lowermost mantle) an accurate modeling of 3D wave propagation in general heterogeneous structures in spherical geometry is required. In this study we present a staggered-grid finite-difference solution to the isotropic elastic wave equation in spherical coordinates that is applicable to intermediate epicentral...
Fig. 13. Synthetic seismograms (transverse component) recorded on a semi-ring at 5° epicentral distance (W–N–E). The dominant period is 6 s. Left: seismograms for background model. Right: seismograms for model with slab.

In this study we apply a standard finite-difference method that in the future should be extended to incorporate recent advances in the understanding of finite-difference operator accuracy (e.g., Geller and Takeuchi, 1998; Takeuchi and Geller, 2000). Here, the algorithm was compared with quasi-analytical solutions using the reflectivity method. The comparison shows that the body waves are well modeled as long as a sufficiently large number of grid points per wavelength is employed. Further research is needed to carefully investigate the accuracy for surface wave propagation as strong effects for surface wave
propagating through subduction zones, plume heads, or along or across ridge axes are to be expected.

We applied this algorithm to simulate waves radiated by a source inside a subducting slab. The slab consists of a maximally 8% positive velocity perturbation and a maximally 4% negative velocity perturbation at the top of the slab. The source is located inside this low-velocity layer. The synthetic seismograms show pronounced effects on the direct P- and S-waves propagating upwards along the slab. With small changes of propagation direction the wave forms and their spectral content changes. The slab also affects the polarities of the first motion. This implies that errors may occur when the source mechanism is estimated using laterally homogeneous models. While the magnitude of these effects may be exaggerated through the thickness of the low-velocity zone, the simulated effects may indicate at least qualitatively what effects are to be expected. Further complications may arise through strongly heterogeneous Q-structure inside the slab. The inclusion of viscoelasticity and anisotropy into the algorithm presented here is work in progress.

These results as well as previous studies show that a systematic investigation of such effects for likely subduction zone structures is necessary. Some of the wave form effects reported could be used to further constrain the structural details in the upper mantle.

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