Efficient Methods in Global Seismic Wave Propagation

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presented by

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Abstract

Despite the ongoing exponential growth of computational power available on supercomputers and significant advances in numerical seismology in the recent decades, the global 3D seismic forward problem remains a computational challenge. Particularly for high frequency body waves, 3D simulations are prohibitively expensive in many applications. For that reason, approximations with respect to the model or the physics of seismic wave-propagation are commonly used. This thesis deals with a numerical method to simulate seismic wave-propagation within the entire Earth that, by assuming axial symmetry of the structural model, reduces the computational burden by orders of magnitude. The two main components of the efforts presented in this thesis are: 1) theoretical developments of the methods that are partly also applicable to the full 3D problem, 2) their numerical implementation resulting in the release of two community codes. This work enables users to study a broad range of effects in global seismic wave-propagation using the full solution of the wave equation where only approximate solutions were previously available.

The theoretical part of this thesis starts with the decomposition of the elastic wave equation into a series of uncoupled equations for its multipole components. While previous mathematical developments of this decomposition where limited to spherically symmetric models in spherical domains, we generalize the proof to general axisymmetric domains and models comprising full triclinic anisotropy and attenuation. By abstracting the problem to symmetry properties of the equation, the contribution of this thesis is directly applicable to other physical problems. The second important theoretical topic is the incorporation of viscoelastic dissipation into time-domain seismic wave-propagation methods with a focus on parameter regime representative for the global case. Since the axisymmetric approach enables the simulation of wave-propagation beyond 1000 wavelengths, special care has to be taken with respect to common physical approximations. This work argues for a criterion to choose material parameters such that the resulting error in the seismograms is minimized. An efficient means of finding these parameters in the case of weak to moderate attenuation in large scale applications is outlined. Furthermore, the 'coarse grained' memory variable approach is adapted for the spectral element method leading to a speed up of a factor five in the anelastic part of the code and
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a memory reduction by a factor two. Finally, the equations of motions in the weak form are derived including both anisotropy and attenuation and discretized using the spectral element method.

The code development includes two applications, AxiSEM and Instaseis. AxiSEM is the aforementioned axisymmetric spectral element method of which a basic implementation for the isotropic elastic case was in place at the very beginning of this project and which provided the starting point of this thesis. Besides the implementation of additional physics, this project included continuous efforts towards making the toolbox robust and user-friendly, by means of a reliable version control, nightly builds and benchmarks against reference solutions. Furthermore, it now employs a non-blocking communication scheme where communication is hidden by computation and which facilitates scaling on up to 10000 cores on modern supercomputers. These achievements enable routine solution of the elastic wave equation in previously unattainable parameter regimes and also resulted in an open source release of the code, which is now being used by several research groups. Using the capability of modern parallel file systems via the NetCDF library, AxiSEM can not only provide seismograms, but also Green’s function databases throughout the whole globe. Instaseis uses these databases to extract seismograms on the fly at high order spatial accuracy. Providing a convenient Python interface, a client/server infrastructure to allow sharing databases over the internet and a performance on the order of a few milliseconds per seismogram, Instaseis can replace approximate solutions still used in many applications by highly accurate waveforms.
Zusammenfassung

Trotz des exponentiellen Wachstums der Rechenleistung die an Rechenzentren verfügbar ist und signifikanter Fortschritte in der numerischen Seismologie in den letzten zehn Jahren bleibt das globale seismische Vorwärtsproblem eine numerische Herausforderung. Vor allem die Simulation von hochfrequenten Raumwellen in 3D Modellen ist für viele Anwendungen zu rechenintensiv und aus diesem Grund muss häufig auf Näherungen bezüglich der Wellenphysik oder des Models zurückgegriffen werden. Diese Dissertation befasst sich mit einer numerischen Methode zur Lösung der seismischen Wellengleichung auf globaler Skala, die die Rechenlast um mehrere Größenordnungen reduziert indem achsensymmetrische Strukturmodelle angenommen werden. Die beiden Schwerpunkte dieser Arbeit sind: 1) die theoretische Weiterentwicklung der Methoden, die zum Teil auch auf das volle 3D Problem anwendbar sind und 2) deren numerische Implementierung, die bis jetzt in der Veröffentlichung zweier Softwarepakete resultierte. Diese ermöglichen es den Nutzern eine breite Palette von Effekten der globalen seismischen Wellenausbreitung zu untersuchen, wobei früher häufig notwendige Näherungen entfallen und für die nun die volle Lösung verfügbar ist.

Der theoretische Teil beginnt mit der Entwicklung der elastischen Wellengleichung in eine Reihe von entkoppelten Gleichungen für die Multipole. Während frühere Beweise auf sphärisch symmetrische Modelle limitiert waren, wird die mathematische Herleitung dieser Entwicklung auf generelle achsensymmetrische Modelle inklusive trikliner Anisotropie und viskoelastischer Dämpfung verallgemeinert. Indem das Problem auf Symmetrie-Eigenschaften der Wellengleichung abstrahiert wird, ist das Ergebnis direkt auf andere physikalische Probleme anwendbar. Das zweite wichtige theoretische Thema ist die Berücksichtigung von intrinsischer Dämpfung bei der numerischen Wellenausbreitung im Zeitbereich, wobei der Fokus hier auf dem Parameterbereich der globalen Seismologie liegt. Da der achsensymmetrische Ansatz die Simulation von Wellenausbreitung über mehr als 1000 Wellenlängen erlaubt, ist es besonders wichtig, häufig benutzte physikalische Approximationen neu zu evaluieren. Für die Auswahl der Materialparameter wird ein Kriterium, das die resultierenden Fehler in den Seismogrammen minimiert, sowie eine effiziente Methode um diese Parameter im Fall von schwacher bis mittlerer Dämpfung in großen Simulationen
Zusammenfassung

zu berechnen vorgeschlagen. Außerdem wird der 'coarse grained memory variable' Ansatz für die Spektrale Elemente Methode angepasst, was zu einer Beschleunigung im anelastischen Teil der Simulation um einen Faktor fünf und einer Reduktion des Speicherbedarfs um einen Faktor zwei führt. Zuletzt werden die Bewegungsgleichungen in der schwachen Form inklusive Anisotropie und Dämpfung hergeleitet und mit der Spektralen Elemente Methode diskretisiert.

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Chapter 1

General Introduction

Motivation

Every day, several earthquakes with Magnitudes $M > 5$, which are strong enough to cause local and regional damage and to detect them globally with modern seismological instruments, occur around the globe (Fig. 1.1). Since earthquakes are amongst the deadliest and economically most devastating natural catastrophes, there has been a long-standing interest in understanding the nature of their occurrence. Given the fact that seismometers are not evenly distributed but sparse in large parts of the Earth (e.g. in the oceans, parts of Africa and the polar regions), understanding the signals recorded at large distances has great societal relevance through a variety of applications. Among these are Tsunami warning systems and rapid loss estimates (e.g. PAGER, Earle et al. 2009) to be able to respond quickly to devastating earthquakes, but also monitoring in the context of the Comprehensive Nuclear-Test-Ban Treaty (CTBT).

Seismic waves carry information about the source (earthquakes, nuclear explosions, meteorite impacts, storms), but as they propagate through Earth they are also sensitive to its structure. Large parts of the current knowledge of Earth’s deep interior were gained from the interpretation of seismic recordings: some historically prominent examples are the suggested observation of the liquid outer core by Oldham (1906) and the discovery of the inner core by Lehmann (1936). Later, routine localization of teleseismic earthquakes allowed Wilson (1965) to locate mid-ocean ridges and support the idea of plate tectonics.

In the last decades global seismology has made major progress for a several reasons (Dziewonski and Romanowicz 2007): (1) the development of broad-band seismometers and digitizers with high dynamic range and the establishment of global seismic networks and easy accessibility of the digital data through the internet, (2) the development of digital signal processing to analyze the data and (3) theoretical progress in wave-propagation and tomography together with a rise in computational power. In this context, the work presented in this thesis falls mainly into category (3) and
Figure 1.1: Numbers of worldwide earthquakes per year and energy equivalents. Events with magnitude larger than about five can be observed globally with seismometers. Image source: IRIS (2011)
1.1. The Global Seismic Wavefield

Even when assuming spherically symmetric Earth models and approximating the earthquake with a point source, the global seismic wavefield is surprisingly complex. This can be seen both in a snapshot of the wavefield in Fig. 1.2 and a 'global stack', that is the seismograms as recorded at Earth’s surface averaged over azimuth as a function of epicentral distance, see Fig 1.3 (a high frequency version focused on the body waves can be found in Fig. 5.1). As proven theoretically by Poisson (1831) and first observed by Oldham (1900), there are two types of body waves propagating inside the elastic parts of Earth: the faster rotation free compressional $P$-waves and the slower but larger amplitude dilation free $S$-waves (Stokes 1849). Multiple reflection and refraction at the internal discontinuities as well as the surface generate a multitude of so called 'phases' (see Fig. 1.4). Jeffreys and Bullen (1940) first published a table of expected arrival times for various source depths and a large number of seismic phases based on the model by Jeffreys (1926). It is remarkable that this work was done with a mechanical calculator only.

Additionally to the body-waves, there are two types of waves that travel along the surface of elastic media: Rayleigh (1885) showed the existence of the first type of these surface waves in a homogeneous half-space as a superposition of two motions in the plane vertical to the surface and parallel to the travelling direction. These waves have since been called Rayleigh waves. However, seismologists in the early 20th century also observed motion perpendicular to the travelling direction arriving within the surface wave train. This phenomenon was first addressed by Love (1911) who showed that if the $S$-wave velocity in the half-space increases with depth, there exists a second type of surface waves. These are polarized transversely and have since been called Love waves. Finally, Stoneley (1924) realized that elastic waves can also travel along interfaces within the medium, such as the boundary between the solid mantle and the liquid outer core of the Earth by an effect called diffraction.

All of these can be clearly seen in Fig. 1.3 and the different phases can be identified by their arrival times, the shape of the travel time curves and their polarization (the color). For example, reflections off the discontinuities, such as the one emerging from the core-mantle boundary (CMB), adopt the form of hyperbolae (e.g. $PcP$, $ScP$, $ScS$). Phases arriving as a $P$-waves are depicted in the range of blue to green,
Figure 1.2.: Snapshot of global seismic waves originating from a strike slip earthquake in the Apennines about 13 minutes after the event in the anisotropic PREM model (Dziewoński and Anderson 1981) with continental crust simulated with AxiSEM. The inner sphere is just below the core-mantle boundary. Color scale: logarithm of absolute value of particle velocity in the vertical component.
those arriving as S-waves are shown in red to yellow, where red is purely transverse polarisation (SH). Yellow is the additive mixture of green and red, revealing the simultaneous arrival of transversely and vertically polarized S-wave (SH and SV). Surface waves are the broad linear features traversing all epicentral distances where Rayleigh waves are blue to green (movement in the source receiver plane) and Love waves red (transverse polarization). In both types of surface waves, dispersion (i.e. dependency of the phase velocity on the frequency) leads to a broadening of the wave train with distance.

Teleseismic waves cover a bandwidth ranging from the longest natural oscillation (≈ 54 min) up to about 2 Hz, hence the frequencies span about four orders of magnitude. While the limit at the longest periods is a consequence of Earth’s finite size, the high-frequency limit is due to attenuation: Higher frequencies are emitted by earthquakes, but too weak to be observed at large distances. After a large earthquake has happened, the Earth remains vibrating on certain frequencies for weeks, akin to the ringing of a bell.

While spherically symmetric Earth models such as PREM (Dziewoński and Anderson 1981) in conjunction with simple source models are able to explain a large portion of the observed seismic records (compare Fig. 1.5), the remaining few percent of unexplained difference in the seismograms with respect to these simple models conceal the most valuable information about dynamic processes inside Earth and the finite extent of the source.

1.2. The Seismic ‘Forward’ Problem

The seismic ‘forward’ problem refers to predicting Earth’s displacement due to an assumed source and 3D structure. At least on the global scale, it remains a computationally extremely challenging endeavour. Although substantial progress has been made in the last 15 years (Igel et al. 2000; Komatitsch and Tromp 2002; Tromp 2007; Tromp et al. 2010), the simulation of the highest frequencies observed in the seismic records is still prohibitively expensive and therefore not performed on a routine basis. Noteworthy, however, the efforts made to overcome these challenges have been recognized in neighbouring fields of computational science and, for example, several seismic wave propagation solvers have made it to the Gordon bell finalists (Heinecke et al. 2014; Ichimura et al. 2014; Carrington et al. 2008) and winners (Komatitsch et al. 2003). So one face the obvious question: why is the global seismic forward problem so hard? Tromp (2007) reviews the entire range of challenges and attempts for solutions focussing on the global scale, here I summarize the most relevant points:
1.2. The Seismic ‘Forward’ Problem

**Figure 1.3.** Global stack (i.e. averaged over azimuth) of 200 min seismograms accurate to a shortest period of 5 s for an earthquake in 27 km depth. Phase arrivals are clearly visible and a selection of them annotated with their names. The displacement is color-coded as indicated in the top left and using additive mixture of colors. An automatic gain control is used to balance large amplitude variations between the various phases.

**Figure 1.4.** Examples of seismic rays and their nomenclature, most of which are clearly visible in Fig. 1.3. Ray paths computed with the Taup toolkit (Crotwell et al. 1999) in the iasp91 model (Kennett and Engdahl 1991).
1. General Introduction

Figure 1.5: Snapshort of the seismic wavefield in a heterogeneous mantle simulated with *AxiSEM*: differences to the radially symmetric case are subtle and for the body waves mostly amount to slight time shifting of the main arrivals. The mantle model is a random medium with exponential distribution and maximum relative perturbations of 10% in $S$-wave velocity, density and $P$-wave velocity perturbations scaled to $S$-wave velocity perturbations with scaling factors of 0.4 and 0.55 respectively.

**Spherical Geometry / Meshing** In any numerical scheme, the domain has to be discretized into a grid or a mesh. In the spherical geometry, regular discretization as popular in local or regional problems leads to concentration of grid points around the poles and in the center of the planet. Unstructured meshing is hence necessary, which compared to structured meshing substantially increases the complexity of numerical implementations.

**Free Surface, Discontinuities, Solid Fluid System** Global models include disconti-
nuities of the seismic velocities as well as the free surface and fluid parts (outer core and oceans). Surface and diffracted waves are very sensitive to accurate implementation of the boundary conditions and location of the discontinuities. Many elastic numerical schemes cannot be directly applied to fluids, making a separate implementation of the fluid system and coupling of the two systems necessary.

**Scale Differences** While Earth has a diameter of 12,742 km (average of the Geoid), crustal layers and oceans that have a significant effect on surface waves are on the order of a few km only. The structural scales that need to be resolved by the grid hence span three to four orders of magnitude. An alternative is to define a long spatial wavelength equivalent, that supposedly has similar properties as seen by the waves. This can be done by matching surface wave dispersion curves (Fichtner and Igel 2008), homogenization (Capdeville and Marigo 2007; Guillot et al. 2010) and replacing oceans by a loading equivalent (Komatitsch and Tromp 2002).

**Attenuation / Dispersion, Rotation and Gravity** Additional physics beyond the purely elastic response of the medium is significant especially at the edges of the seismic frequency range. At long periods (above about 100 s), the effect of Coriolis forces induced by Earth’s rotation and changes in the gravitational field induced by the seismic waves affect the wave propagation. On the other hand, at short periods, attenuation strongly reduces amplitudes and leads to dispersion.

**Anisotropy** Wave speeds in Earth generally bear directional dependency, i.e. the physical properties are anisotropic. Possible reasons are the orientation of crystals or small scale heterogeneities in the in mantle flows (Long and Becker 2010) as well as thin layers of different material (Backus 1962). For radially symmetric models, radial anisotropy is often assumed to explain differences in Love and Rayleigh wave dispersion. Accounting for anisotropy substantially increases the complexity of the equations as well as memory and CPU requirements of the simulation.

**High Order Accuracy** High frequency body waves travel more than a thousand wavelength across the planet before being recorded. Simulating these at adequate accuracy requires high order space and time integration schemes to keep dispersion errors small.

**Size** Probably the biggest challenge, however, still is the sheer size of the problem, which makes efficient parallelization a necessity to scale on massively parallel
systems. While at the largest supercomputers available, solving the global forward problem at the high frequencies is becoming possible (Carrington et al. 2008), this remains prohibitively expensive for most scientists. This is especially the case for the 'inverse' problem (i.e. inferring Earth’s structure from the seismic recordings), where the forward problem has to be solved numerous times.

1.2.1. Relation of 'Forward' and 'Inverse' Problem

Both the complexity of the wavefield and the challenges in computing synthetic seismograms over the whole frequency range historically led seismologists to carefully select specific features of the seismic waves that are sensitive to the physical effects to be studied and where appropriate theory and tools existed for interpretation. Common approaches are the limitation to long period spectra, where normal-mode coupling-theory allows to include all relevant physics (Woodhouse and Dahlen 1978; Woodhouse and Deuss 2007) or the limitation to arrival times of seismic phases, which could already early be predicted using ray-theory (Jeffreys and Bullen 1940; Crotwell et al. 1999). Approaches like the reflectivity method (Fuchs and Müller 1971), frequency-wavenumber integration (Kikuchi and Kanamori 1982) or WKBJ (Chapman 1978) allow to accurately predict the shape of single phases. Hence, most forward solvers in seismology were intimately connected to such specific measurements and the related 'inverse' problem, i.e. inferring information about the structure and the source from the data.

However, seismologists always urged to extract as much information from the data as possible and pushed towards the development of methods to provide 'full' 3D synthetic waveforms (see Tromp 2007, for an overview). Together with the adjoint method (Tarantola 1988; Tromp et al. 2005; Fichtner et al. 2006a, 2006b), this allows in principle to use arbitrary portions of the seismograms with any measurement, e.g. time-frequency misfits (Fichtner et al. 2008), multi-taper travelt ime (Tape et al. 2010) or cross-correlation travelt ime in multiple passbands (Dahlen et al. 2000; Sigloch and Nolet 2006). While several regional models have been published based on adjoint methods (e.g. Fichtner et al. 2009; Zhu et al. 2012), this is not the case for the global scale where the computational demands are huge even at long periods. However, the resolution that can be achieved in tomography depends on the frequency content of the signals used, a feasible compromise for broadband body wave tomography is the finite-frequency approach (Dahlen et al. 2000; Montelli et al. 2004b, 2004a), which allows to invert waveforms of well separated phases.
1.2. The Seismic ‘Forward’ Problem

In the axisymmetric approach, the 3D problem is decomposed into a series of radiation patterns and a 2D mesh. This way, the wavefield remains 3D, while the structure is assumed symmetric to an axis through the source and the center of Earth (red). Hence this method is also called 2.5D.

1.2.2. The Axisymmetric Approach

This thesis deals with a method to solve the global seismic forward problem where the Earth models are assumed to be symmetric with respect to an axis through the center of the Earth and the source. This method is based on a decomposition
1. General Introduction

Figure 1.7.: Artistic representation of axisymmetric structure in a global model and its interaction with the wavefield: any non-spherically symmetric structure is effectively mapped into ringlike structures symmetric with respect to an axis through the source and the center of Earth.

of the wave equation into a series of uncoupled 2D equations (see Fig. 1.6) for which the dependence of the wavefield on the azimuth can be solved analytically. Four independent equations up to quadrupole order appear as solutions for moment-tensor sources located on the symmetry axis while single forces can be accommodated by two separate solutions up to dipole order. This decomposition gives rise to an efficient solution of the 3D wave equation in a 2D axisymmetric medium.

Relying on axisymmetry has three major computational advantages:

1. It enables the storage of the wavefields that provide the basis for computing Fréchet sensitivity kernels (Dahlen et al. 2000; Nissen-Meyer et al. 2007), which
1.2. The Seismic ‘Forward’ Problem

is not feasible with full 3D methods due to disk space requirements. The same wavefields are used to build Green’s function databases for \textit{Instaseis} as detailed in chapter 5.

2. It allows the inclusion of 2.5D lateral heterogeneities that are effectively modeled as ringlike structures around the symmetry axis (compare Fig.1.7) giving rise to various applications in a high-frequency approximation that are not tractable with 1D or full 3D methods. Several examples can be found in chapter 4.

3. It is computationally several orders of magnitude less expensive than full 3D methods and hence allows the routine simulation of the highest frequencies observed on the global scale in for actual scientific applications often requiring a large number of simulations.

Axisymmetric approaches have been used earlier based on finite difference (Alteman and Karal 1968; Igel and Weber 1995, 1996; Chaljub and Tarantola 1997; Thomas et al. 2000; Takenaka et al. 2003; Toyokuni et al. 2005) or pseudospectral methods (Furumura et al. 1998), but most of these studies assume azimuthally symmetric sources (monopoles) and hence cannot model arbitrary earthquake sources, but rather resemble explosive sources or a certain geometry for strike slip events (Jahnke et al. 2008). More recently, Toyokuni and Takenaka (2006, 2012) generalized their method to include moment tensor sources, attenuation and the Earth’s center. However, these methods are all based on isotropic media. Also, when using the finite-difference method, one has to deal with large dispersion errors for waves which are sensitive to discontinuities. This particularly affects surface waves and diffracted waves. The pseudospectral method uses global smooth basis functions, so it can only be used with smooth media and cannot be efficiently parallelized to scale on modern high-performance systems.

The Spectral Element Method

These limitations can be overcome using the spectral element method (SEM, Faccioli et al. 1997; Seriani 1998; Komatitsch and Vilotte 1998; Komatitsch and Tromp 1999). The SEM for general axisymmetric systems has been derived by Bernardi et al. (1999) and applied to the Navier-Stokes equation by Fournier et al. (2004). Nissen-Meyer et al. (2007, 2008) applied it to the isotropic elastic wave-equation and their theoretical work and implementation (\textit{AxiSEM}) forms the basis of this thesis.
1. General Introduction

Figure 1.8.: In the Spectral Element Method (SEM), the wavefield is expanded in Lagrangian polynomials defined on the Gauss-Lobatto-Legendre (GLL) points of each element in the mesh. Left: Lagrangian polynomials $l_n(\xi)$ of fourth order in one dimension. Right: GLL points inside an element (gray) and its neighbours. Coordinates $\xi$ and $\eta$ are the reference coordinates of the gray element, points on the edges (black squares) are shared between neighbours.

Figure 1.9.: Snapshot of a global wavefield with a shortest period of 50 s: the spatial representation in the SEM is smooth across element boundaries and the boundary conditions at the free surface and internal discontinuities are implicitly accommodated. The element size is adapted to the local shortest wavelength and accommodates the layers of the model exactly.
1.2. The Seismic ‘Forward’ Problem

The SEM is based on the weak form of the equations of motion and thus naturally includes the boundary conditions at the free surface and internal discontinuities at the order of accuracy of the spatial discretization. Also, including sources of higher order multipoles as in full moment tensors can be accommodated in a straightforward manner. In the SEM, the field variables are expanded in terms of Lagrangian polynomials defined on the Gauss-Lobatto-Legendre (GLL) points on each element of a quadrilateral mesh, see Fig.1.8. This way it combines high order accuracy and the ability to mesh arbitrary geometries, in our case the semicircular domain, Fig. 1.6. The displacement is assumed continuous at the element boundaries, leading to a smooth representation of the wavefield across element boundaries (Fig.1.9). The combination of Lagrangian polynomials with the GLL integration rules leads to a diagonal mass-matrix, which allows to use simple explicit time schemes. For this reason, the SEM lends itself well for parallelization on modern supercomputers.

1.2.3. Thesis Outline

In chapter 2 we generalize the axisymmetric approach to seismic wave propagation to fully anisotropic media. First, we prove the validity of the decomposition of the wavefield into a multipole series in the presence of general anisotropy. Then we use this decomposition to derive the reduced 2D equations of motions and discretize them using the SEM. Finally, we benchmark the numerical implementation for global wave propagation at 1 Hz and consider inner core anisotropy as an application for global high-frequency wave propagation in anisotropic media.

In chapter 3, we include attenuation and propose a method to minimize the error in the wavefield for a fixed complexity of the anelastic medium. Furthermore, we derive an analytical time-stepping scheme for the memory variables that encode the strain history of the medium. Then we develop the coarse grained memory variable approach for the SEM and benchmark it using the 2.5D code AxiSEM for global body waves. Showing very good agreement with a reference solution, it also leads to a speed-up of a factor of 5 in the anelastic part of the code (factor 2 in total) in this 2.5D approach.

Chapter 4 is the release paper for AxiSEM and highlights its main features and a diverse range of applications ranging from normal modes to small-scale lowermost mantle structures, tomographic models, comparison to observed data, and discusses further possible applications of this methodology.

Chapter 5 is the release paper for Instaseis and presents a new method to store global Green’s functions in a database which allows for near-instantaneous extraction of arbitrary seismograms. Using AxiSEM, the generation of these databases, based
1. General Introduction

on reciprocity of the Green’s functions, is very efficient. In this chapter, we present
the basic rationale and details of the method as well as benchmarks and illustrate a
variety of applications.

In Appendix A, we present a new method to compute Fréchet kernels for $Q$ and
its possible power law dependence on the frequency using adjoint techniques. Being
based directly on the memory variables, these kernels can be computed with no
additional cost compared to computing Fréchet kernels for elastic properties only.
To illustrate our developments, we present examples from regional- and global-scale
time-domain wave propagation.

A General Note to the Reader

The following chapters are all based on previous publications in peer-reviewed jour-
nals, which is why they are self-contained and may to a certain extent be redundant
(also with respect to this introduction). The title, journal and coauthors list as
well as notes on changes of the versions included in this thesis with respect to the
papers can be found in footnotes on the first page of each chapter. Major changes
are additionally marked by footnotes on the respective pages.

References


838.

propagation using SPECFEM3D_GLOBE”. In *Proc. ACM / IEEE Supercomput.

Chaljub, E., and A. Tarantola. 1997. “Sensitivity of SS precursors to topography on


1. General Introduction


IRIS. 2011. How Often Do Earthquakes Occur?


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Abstract

We present a numerical method to compute 3D elastic waves in fully anisotropic axisymmetric media. This method is based on a decomposition of the wave equation into a series of uncoupled 2D equations for which the dependence of the wavefield on the azimuth can be solved analytically. Four independent equations up to quadrupole order appear as solutions for moment-tensor sources located on the symmetry axis while single forces can be accommodated by two separate solutions up to dipole order. This decomposition gives rise to an efficient solution of the 3D wave equation in a 2D axisymmetric medium. First, we prove the validity of the decomposition of the wavefield in the presence of general anisotropy. Then we use it to derive the reduced 2D equations of motions and discretize them using the spectral element method (SEM). Finally, we benchmark the numerical implementation for global wave propagation at 1 Hz and consider inner core anisotropy as an application for high-frequency wave propagation in anisotropic media at frequencies up to 2 Hz.
2. Seismic Wave Propagation in Fully Anisotropic Axisymmetric Media

2.1. Introduction

Seismic anisotropy describes directional dependence of seismic wavespeeds and occurs in the Earth for various reasons: most importantly, mantle flow tends to align intrinsically anisotropic crystals causing lattice-preferred orientation which is expected to account for the bulk of the upper mantle anisotropy (Long and Becker 2010). Secondly, anisotropy can be caused by preferential alignment of small scale heterogeneities, called shape-preferred orientation: 3D structure of purely isotropic material on a sub-wavelength scale can cause apparent anisotropy, which was realized for layered media by Backus (1962) and is used for computational benefits using homogenization techniques to upscale Earth models (e.g. Guillot et al. 2010).

Anisotropy is globally observed in the upper mantle, where different velocities for horizontally and vertically polarized shear waves are needed to explain observed Love and Rayleigh wave speeds. The upper mantle of the 1D Earth model PREM (Dziewoński and Anderson 1981) has radial anisotropy while ak135 (Kennett et al. 1995) is isotropic. Wang et al. (2013) analyze whether the anisotropy in 1D models is due to intrinsic anisotropy or can be explained by fine layering. The study by Auer et al. (2014) is the most recent example of a tomographic model for shear wave anisotropy on a whole mantle scale and compares various anisotropic models (Kustowski et al. 2008; Panning et al. 2010) to identify regions in which the anisotropic models have reached a certain maturity. Also, structures above the core mantle boundary (CMB) such as ultra low velocity zones (ULVZ) and large low shear velocity provinces (LLSVP) are expected to be anisotropic (e.g. Panning and Romanowicz 2004; Long 2009; Nowacki et al. 2011; Walker et al. 2011; Cottaar and Romanowicz 2013). In the inner core, hexagonal anisotropy with a fast axis in north-south direction is observed both with normal modes (Deuss et al. 2010) and inner core body waves (Irving and Deuss 2011).

To capture these diverse appearances of seismic anisotropy across the scales, full waveform modelling is needed, preferably up to high resolution (1−2 Hz) as observed in waveforms for lowermost mantle and inner-core anisotropy. While anisotropy is included in many numerical wave-propagation solvers (e.g. Igel et al. 1995; Komatitsch et al. 2000; de la Puente et al. 2007; Moczo et al. 2007), full 3D wave propagation is not feasible for the observed body wave frequencies on the global scale due to its tremendous cost in solving for up to $10^{12}$ degrees of freedom at these resolutions. In a series of papers, Nissen-Meyer et al. (2007a, 2007b, 2008) developed a novel approach to global seismic wave propagation that is based on a decomposition of the 3D wave equation into a series of uncoupled 2D equations that is valid for axisymmetric models. The axisymmetric approach has three major advantages over
full 3D methods: 1) it enables the storage of the wavefields that provide the basis for computing Fréchet sensitivity kernels (Dahlen et al. 2000), which is not feasible with full 3D methods due to disk space requirements; 2) it allows the inclusion 2.5D lateral heterogeneities that are effectively modeled as ringlike structures around the symmetry axis giving rise to various applications in a high-frequency approximation that are not tractable with 1D methods; 3) it is computationally several orders of magnitude less expensive than full 3D methods and hence allows the simulation of higher frequencies. Axisymmetric approaches have been presented earlier using finite difference (Alterman and Karal 1968; Igel and Weber 1995, 1996; Chaljub and Tarantola 1997; Thomas et al. 2000; Takenaka et al. 2003; Toyokuni et al. 2005) or pseudospectral methods (Furumura et al. 1998), but most of these studies assume azimuthally symmetric sources (monopoles) and hence cannot model arbitrary earthquake sources, but rather resemble explosive sources or a certain geometry for strike slip events (Jahnke et al. 2008). More recently, Toyokuni and Takenaka (2006, 2012) generalized their method to include moment tensor sources, attenuation and the earth center. Furthermore, these methods are all based on isotropic media and especially the finite difference methods have to deal with large dispersion errors for interface sensitive waves like surface waves and diffracted waves. Here we generalize the spectral element method by Nissen-Meyer et al. (2007a) to fully anisotropic axisymmetric media to overcome these issues. This in combination with 2) and 3) above enables the simulation of high-frequency body waves in anisotropic structures such as the D" and the inner core in a 2.5D approximation.

The numerical implementation (AxiSEM) was recently published under GNU general public license (www.axisem.info) and a whole variety of applications is presented by Nissen-Meyer et al. (2014). Stähler et al. (2012) use this method to compute finite frequency sensitivity kernels for triplicated P-waves, which is inaccurate with other methods such as the one by Dahlen et al. (2000) due to the strong influence of the upper mantle discontinuities in comparison to their sensitivity to mantle heterogeneity. Colombi et al. (2012, 2014) compute boundary topography kernels, analyze the sensitivity of different phases in comparison to there sensitivity to mantel heterogeneity and invert for CMB topography. Boué et al. (2013) use AxiSEM to compute synthetic reference seismograms to interpret noise correlations.

This paper is structured as follows: in the first section, we discuss analytically that the decomposition of the elastic wave equation into a multipole series remains valid in the presence of general anisotropy by means of two arguments based on normal mode coupling and commuting operators. In the second section we apply this decomposition to derive the 2D weak form of the reduced wave equations and discretize them spatially based on a spectral element method (SEM). In the third
section, we benchmark the new implementation at high (1 Hz) and low frequency
(normal modes observed at frequencies of a few mHz) against reference solutions
and find excellent agreement. In the last section, we apply our method to inner-core
anisotropy at 2 Hz as an example of the anisotropic parameter regime covered by
AxiSEM. Comprehensive appendices list the full discretized stiffness terms for the
multipole expansion explicitly.

2.2. Multipole Expansion

For clarity and generality, we outline two different approaches which show that
the decomposition into a multipole series remains valid and still results in a series
of uncoupled equations in the presence of general anisotropy: The first one takes
a normal mode perspective and generalizes the argument by Nissen-Meyer et al.
(2007a) that is valid for spherically symmetric non-rotating elastic isotropic (SNREI)
Earth models by expressing the wavefield in the normal mode basis and analyzing
the mode coupling selection rules. The second approach is more abstract and general
as it is based on two essential properties of the physical system under consideration:
invariance under rotation and linearity, thereby dropping the necessity for a spherical
domain and including a variety of other equations.

2.2.1. Statement of the Problem

In the cylindrical coordinate system \((s, \varphi, z)\), any square integrable function \(u\)
defined on a domain \(\Omega\) symmetric with respect to the polar axis \(\hat{e}_z\) (Fig. 2.1) can be
decomposed by applying a Fourier transform in the angular coordinate \(\varphi\) as

\[
\begin{align*}
    u(s, z, \varphi) &= \sum_{m=-\infty}^{\infty} \left[ u^m_s(s, z) \hat{e}_s(\varphi) + u^m_{\varphi}(s, z) \hat{e}_{\varphi}(\varphi) + u^m_z(s, z) \hat{e}_z \right] e^{im\varphi}. \\
      &=: u_m(s, \varphi, z) e^{im\varphi}. (2.1)
\end{align*}
\]

Equivalent expressions with \(\sin \varphi\) and \(\cos \varphi\) as used by Nissen-Meyer et al. (2007a)
can be found by summing over pairs of \(\pm m\) and using the fact that \(u\) is real. The
question is whether the wave equation

\[
\dot{\hat{K}}u + \rho \partial_t^2 u = f (2.2)
\]
in the expansion eq. (2.1) can be split into a series of independent equations, i.e. if
there exist operators \(\hat{K}_m\) such that the set of equations
2.2. Multipole Expansion

Figure 2.1.: The cylindrical coordinate system \((s, \varphi, z)\) and the reduced semicircular 2D domain \(\Omega_D\) for global wave propagation in axisymmetric media.

\[
\hat{K}_m \mathbf{u}_m + \rho \hat{\nabla}_\tau^2 \mathbf{u}_m = \mathbf{f}_m \tag{2.3}
\]

is equivalent to the wave equation eq. (2.2), where \(\mathbf{f}_m\) denotes an expansion corresponding to eq. (2.1). While this is a well known fact for spherically symmetric Earth models (which are a special case of axial symmetry and only include transversely isotropic media, see e.g. Dahlen and Tromp 1998), we prove here that this expansion is valid for a fully anisotropy medium, as long as it is azimuthally invariant:

\[
c_{ijkl}(s, \varphi, z) = c_{ijkl}(s, z), \quad (i, j, k, l = s, \varphi, z). \tag{2.4}
\]

In the normal mode context, this type of symmetry is often referred to as zonal symmetry (Dahlen and Tromp 1998). Fig. 2.2 shows an example for a structure from this symmetry class.
2. Seismic Wave Propagation in Fully Anisotropic Axisymmetric Media

Figure 2.2.: Artistic visualization of an axisymmetric anisotropic structure: while the doughnut represents isotropic structure as in Fig. 1.7, the sprinkles visualize the additional directional dependence of the physical properties (e.g. the fast axis of a hexagonally symmetric medium).

2.2.2. Proof 1: Normal Mode Coupling due to Zonally Symmetric Anisotropy

Nissen-Meyer et al. (2007a) show that the decomposition eq. (2.3) is valid for SNREI Earth models and derive the series of equations explicitly for moment tensor and single force point sources on the polar axis, where $m$ takes values between $-2$ and 2. Their argument was based on identification of the angular dependences in eq. (2.1) with analytic solutions of the wave equation using a normal mode expansion.

The strategy in this proof is to show that the angular dependence of the wavefield is not altered by the zonally symmetric anisotropy and hence the argument by Nissen-Meyer et al. (2007a) remains valid. After introducing the normal-mode solution, what remains to be shown is that only singlets with the same azimuthal dependence are coupled, as this leaves the total dependence on azimuth unchanged. This is equivalent to the selection rule $m = m'$, where $m$ is the azimuthal order.
2.2. Multipole Expansion

A Solution to the Wave Equation

Consider the elastic wave equation eq. (2.2) where

\[ \hat{K}u = -\nabla \cdot (c : \nabla u). \] (2.5)

As \( \hat{K} \) is self-adjoint, it is diagonalizable in the space of square integrable functions \( L_2 \) on the domain \( \Omega \) and the basis of eigenfunctions is orthogonalizable and countable (for more details refer to Woodhouse and Deuss 2007). Now assume any countable basis \( s^{(k)} \) of the \( L_2 \) that is orthonormal in the sense

\[ \int_{\Omega} \rho s^{(k)*} \cdot s^{(k')} \, d^3x = \delta_{kk'}. \] (2.6)

In this basis, eq. (2.2) can be written as an infinite dimensional matrix equation (Woodhouse 1983)

\[ Ku + \partial_t^2 u = F, \] (2.7)

with the coupling matrix \( K \) having elements

\[ K_{kk'} = \int_{\Omega} s^{(k)*} \cdot \hat{K} s^{(k')} \, d^3x \] (2.8)

and the source vector \( F \) and \( u \) being the vector of coefficients for the displacement \( u \) in this basis. For an instantaneous point source, the coefficients of the source vector \( F \) are

\[ F_k = \left( \sum_i F_i s_i^{(k)}(r_s) + \sum_{ij} M_{ij} \partial_j s_i^{(k)}(r_s) \right) h(t), \] (2.9)

where \( F_i \) are the components of a force vector, \( M_{ij} \) a moment tensor and \( h(t) \) the Heaviside function. To avoid confusion, summation over repeated indices is always written explicitly throughout the paper. The solution to Eq. (2.7) can then be written as (Woodhouse 1983)

\[ u(t) = K^{-1} \left[ 1 - \cos \left( \sqrt{\hat{K}}t \right) \right] F. \] (2.10)
This time evolution is trivial, if \( s^{(km)} \) are eigenvectors of \( \hat{K} \), i.e.
\[
\hat{K} s^{(km)} = \rho \omega_k^2 s^{(km)},
\]
(2.11)
because then the coupling matrix \( K \) is diagonal. The additional index \( m \) accounts for possible degeneracy of the eigenfrequencies \( \omega_k \). In the case where \( \hat{K} \) is the elastic operator corresponding to the SNREI Earth, the set of degenerate eigenfunctions \( s^{(km)} \) corresponding to an eigenfrequency \( \omega_k \) is called normal mode or the multiplet \( k \). \( k \) then incorporates the angular order \( l \), the overtone number \( n \) and the mode type (spheroidal or toroidal) and \( m \) is called the azimuthal order.

The problem of finding solutions to the wave equations is then reduced to finding eigenfrequencies and eigenvectors of the operator \( \hat{K} \), followed by application to a specific source and summation of the eigenfunctions according to eq. (2.10).

**Mode Coupling Selection Rule** \( m = m' \)

While in the SNREI Earth the spherical parts of the eigenfunctions are found to be spherical harmonics, it is impractical to compute them explicitly in an Earth with lateral perturbations. A numerically exact solution can still be found by expressing \( \hat{K} \) in the normal mode basis and diagonalizing \( K \) numerically (Deuss and Woodhouse 2001). Once this is done, the eigenfunctions can be expressed in a normal mode sum as well. The time evolution is then nontrivial, because it is affected by coupling between modes.

To evaluate the elements of the coupling matrix, it is useful to express the strain \( E \) and the perturbed elastic stiffness tensor \( c_{ijkl}(r, \theta, \phi) \) in terms of generalized spherical harmonics \( Y_{lm}^N \) (Phinney and Burridge 1973; Dahlen and Tromp 1998, (C.164)):
\[
E^{(km)}(r) = \frac{1}{2} \left( \nabla s^{(km)}(r) + (\nabla s^{(km)}(r))^T \right)
= \sum_{\alpha\beta} F_{\alpha \beta}^{(l)}(r) Y_{lm}^N(\theta, \phi) \hat{e}_\alpha \hat{e}_\beta
\]
(2.12)
with \( \alpha, \beta = -1, 0, 1 \) and \( N = \alpha + \beta \) and \( l \) is determined by \( k \) (see above). \( \hat{e}_{\alpha,\beta} \) are the canonical basis functions (Dahlen and Tromp 1998, (C.50))
\[
\hat{e}_{-1} = \frac{1}{\sqrt{2}} (\hat{\theta} - i \hat{\phi}) , \quad \hat{e}_0 = \hat{r} , \quad \hat{e}_{+1} = -\frac{1}{\sqrt{2}} (\hat{\theta} + i \hat{\phi}) .
\]
(2.13)
2.2. Multipole Expansion

Similarly, we can write for the elastic tensor (Dahlen and Tromp 1998, (D.100)):

\[ c(r) = \sum_{l \alpha \beta \gamma \delta} \sum_{\gamma' \delta'} c_{l \alpha \beta \gamma \delta}^{\gamma' \delta'} Y_{l \alpha \beta \gamma \delta}(r, \gamma', \delta') \hat{e}_\alpha \hat{e}_\beta \hat{e}_\gamma \hat{e}_\delta \]  

(2.14)

with \( \alpha, \beta, \gamma, \delta = -1, 0, 1 \) and \( N = \alpha + \beta + \gamma + \delta \). Zonal symmetry is then defined by \( c_{l \alpha \beta \gamma \delta}^{\gamma' \delta'}(r) = 0 \) if \( m \neq 0 \), i.e. the elastic tensor is independent of azimuth \( \varphi \). The coupling matrix elements can then be written as (Woodhouse and Dahlen 1978; Dahlen and Tromp 1998, (D.115)):

\[ \langle km | \hat{K} | k'm' \rangle = \int_\Omega s^{(km)*} \cdot \hat{K} s^{(k'm')} d^3x \]

\[ = \int_\Omega E^{(km)*} : c : E^{(k'm')} d^3x \]

\[ = \sum_{\alpha \beta \gamma \delta} \sum_{\gamma' \delta'} \sum_{st} \int_0^r E_{km}^{\alpha \beta \gamma \delta} c_{st}^{\alpha \beta \gamma \delta} E_{k'm'}^{\gamma' \delta'} g_{\gamma' \delta'} r^2 dr \]

\[ \times \int Y_{lm}^{N*} Y_{s0}^{N+N'} Y_{t'm'}^{N'} d\Omega \]  

(2.15)

where \( N = \alpha + \beta, N' = \gamma' + \delta' \) and \( g \) the metric tensor with \( g_{00} = 1, g_{-11} = g_{1-1} = -1 \) and \( g_{\alpha \beta} = 0 \) if \( \alpha + \beta \neq 0 \) and \( d\Omega \) the solid angle. Using the zonal symmetry (\( t = 0 \)) and the definition of the generalized spherical harmonics (Phinney and Burridge 1973, Eq. (1.5)) the angular integral in eq. (2.15) can be expressed as

\[ \int Y_{lm}^{N*} Y_{s0}^{N+N'} Y_{t'm'}^{N'} d\Omega \]

\[ = \int_0^\pi P_l^{N*} (\cos \theta) P_s^{(N+N')} (\cos \theta) P_{t'm'}^{N'} (\cos \theta) \sin \theta d\theta \times \int_0^{2\pi} e^{i(m'-m)\varphi} d\varphi \]

\[ = 0 \quad (m \neq m'). \]  

(2.16)

As no assumption about the elastic tensor \( c_{ijkl} \) was made apart from zonal symmetry, the selection rule \( m = m' \) is a direct consequence of this symmetry independent of anisotropy. The advantage of this first proof is its rather intuitive perspective of mode coupling, but it has the disadvantage of relying on the decomposition into spherical harmonics and is hence limited to spherical domains.


2.2.3. Proof 2: Commuting Operators

The second proof is more abstract but also more general as it is valid for all linear equations defined in the space of square integrable functions $L^2$ on domains $\Omega$, if both the domain and the equation are invariant under rotations around a symmetry axis. For the seismic wave equation, this includes local domains as needed e.g. for seismic exploration (suggested for explosive sources and isotropic media by Takenaka et al. 2003) and especially, as self-adjointness is not required, it readily includes linear viscoelasticity as well. Furthermore, this approach is applicable to a variety of other equations, e.g. the anisotropic acoustic wave equation that is frequently used in exploration geophysics (Alkhalifah 2000) or the Poisson and incompressible Stokes equations, see Bernardi et al. (1999) for a rigorous mathematical treatment. The method by Fournier et al. (2004) for the nonlinear Navier-Stokes equation is different in that it only treats axisymmetric solutions, while the solutions discussed here can take arbitrary form and the equation needs to have the symmetry.

Let $\Omega \subset \mathbb{R}^3$ and $\hat{T}_\psi$ a rotation of the coordinate system by the angle $\psi$ and $\Omega$ is invariant under the rotation. The action of $\hat{T}_\psi$ on a function $u: \Omega \rightarrow \mathbb{R}^3$ then is

$$\hat{T}_\psi u(x) = R_\psi u(R_\psi^T x) \quad (2.17)$$

where $R_\psi$ is the rotation matrix corresponding to the rotation around the symmetry axis of $\Omega$. As stated above, any function $u: \Omega \rightarrow \mathbb{R}^3$ that is square integrable can be expanded as in eq. (2.1). The basis vectors of the cylindrical coordinate system are symmetric with respect to the axis, i.e. $\hat{T}_\psi \hat{e}_{\{s,\varphi,z\}} = \hat{e}_{\{s,\varphi,z\}}$. The action of the rotation operator in this decomposition therefore simplifies to

$$\hat{T}_\psi \left( u_m(s, \varphi, z)e^{im\varphi} \right) = e^{-im\psi} u_m(s, \varphi, z)e^{im\varphi}. \quad (2.18)$$

Now consider the equation

$$\hat{H}u = f, \quad (2.19)$$

where the operator $\hat{H}$ is linear, the equation has a unique non-trivial solution $u$ and $\hat{H}$ commutes with $\hat{T}_\psi$, i.e.

$$\hat{H}\hat{T}_\psi u = \hat{T}_\psi \hat{H}u, \quad \text{for all } u \in L_2. \quad (2.20)$$
In other words, whether the function is first rotated and $\hat{H}$ is applied subsequently or $\hat{H}$ is applied first and the resulting function then rotated does not affect the final result. In the case of the elastic wave equation, $\hat{H}$ is the elastodynamic operator $\hat{K} + \rho \partial_t^2$ which fulfills these criteria if the medium is symmetric with respect to the z-axis, see Eq. (2.4).

Similar to $u$, the source $f$ has a decomposition as in Eq. (2.1) with $f = \sum_{m'} f_{m'} e^{im'\varphi}$ and the behaviour under rotation as in Eq. (2.18). Because of the linearity of $\hat{H}$, we can first consider solutions for $\hat{H} u = f_{m'} e^{im'\varphi}$ and sum over $m'$ later. If we apply the rotation $\hat{T}_\psi$ to the linear wave equation and use the commuting property, we have

$$\hat{H} \hat{T}_\psi u = e^{-im'\psi} f_{m'} e^{im'\varphi}.$$  

(2.21)

Using the uniqueness of the solution and linearity of $\hat{H}$ this implies

$$\hat{T}_\psi u = e^{-im'\psi} u = e^{-im'\psi} \sum_{m=-\infty}^{\infty} u_m e^{im\varphi}.$$  

(2.22)

On the other hand, using Eq. (2.18):

$$\hat{T}_\psi u = \sum_{m=-\infty}^{\infty} e^{-im\psi} u_m e^{im\varphi}.$$  

(2.23)

Because of the orthogonality of $e^{-im\psi}$, both relations hold for all $\psi$ if and only if

$$u_m = 0, \quad \text{(for all } m \neq m').$$  

(2.24)

In conclusion, eq. (2.19) can be separated into a series of independent equations

$$\hat{H} u_m e^{im\varphi} = f_m e^{im\varphi}, \quad (m \in \mathbb{N}).$$  

(2.25)

An equivalent set of reduced equations with functions $\tilde{u}_m(s,z)$ and $\tilde{f}_m(s,z)$ defined on $\Omega_D$ with $\Omega = \Omega_D \otimes [0,2\pi]$ can be defined such that
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\[ \hat{H}_m \hat{u}_m(s, z) = \hat{f}_m(s, z), \quad (m \in \mathbb{N}). \]  

These are derived explicitly for \( m = 0, \pm 1, \pm 2 \) (as these are the only contributions for a moment tensor or single force point source on the symmetry axis) for the wave equation in the isotropic elastic and fluid cases in section 4.5 to 4.6 and appendix A in Nissen-Meyer et al. (2007a) and will be presented in the next section for the anisotropic elastic case.

2.3. The Axisymmetric System

2.3.1. Equations of Motion

In this section, we derive the equations of motions of the reduced 2D equations in the weak form explicitly. This step essentially consists of projecting the wave equation onto test functions having the azimuthal dependence of monopole, dipole and quadrupole sources as defined in eq. (2.1). Taking the dot product of Eq. (2.2) with a test function \( w \), integrating over the domain \( \Omega \) and using partial integration and the free surface boundary condition yields

\[
\int_{\Omega} \left( \rho w \cdot \dddot{u} + \nabla w : (c : \nabla u) \right) d^3x = \int_{\Omega} w \cdot f d^3x. \tag{2.27}
\]

If this equation holds for all \( w \), this so called weak form is equivalent to the original wave equation. When inserting the specific dependence of the wavefield \( u \) and the test function \( w \) on the azimuth \( \varphi \), the integral in \( \varphi \) can be solved analytically leaving only the integral over the two-dimensional semicircular domain \( \Omega_D \), see Fig. 2.1. The domain \( \Omega \) of interest here is the solid part of the Earth, for the full solid-fluid system see Nissen-Meyer et al. (2008). Both source and mass term are independent of the elastic tensor \( c \), so we only consider the stiffness terms to generalize Eqs. (5-7) in Nissen-Meyer et al. (2007b) to anisotropic Earth models.

Stiffness Terms

For the monopole \( (m = 0) \), integrating the stiffness terms over \( \varphi \) results in (omitting the integral over \( \Omega_D \) on both sides)
2.3. The Axisymmetric System

\[ \frac{1}{2\pi} \int_0^{2\pi} \nabla w : (c : \nabla u) \, d\varphi \]  
\[ = \partial_s w_s \left( C_{11} \partial_s u_s + C_{13} \partial_z u_z + C_{15} (\partial_s u_z + \partial_z u_s) + C_{12} \frac{u_s}{s} \right) \]
\[ + \partial_z w_s \left( C_{15} \partial_s u_s + C_{35} \partial_z u_z + C_{55} (\partial_s u_z + \partial_z u_s) + C_{25} \frac{u_s}{s} \right) \]
\[ + \frac{w_s}{s} \left( C_{12} \partial_s u_s + C_{23} \partial_z u_z + C_{25} (\partial_s u_z + \partial_z u_s) + C_{22} \frac{u_s}{s} \right) \]
\[ + \partial_s w_z \left( C_{15} \partial_s u_s + C_{35} \partial_z u_z + C_{55} (\partial_s u_z + \partial_z u_s) + C_{25} \frac{u_s}{s} \right) \]
\[ + \partial_z w_z \left( C_{13} \partial_s u_s + C_{33} \partial_z u_z + C_{35} (\partial_s u_z + \partial_z u_s) + C_{23} \frac{u_s}{s} \right), \]

where \( C_{ij} \) is the elastic tensor \( c_{ijkl} \) in Voigt notation with the index mapping

\[ \{ss\} \rightarrow 1, \quad \{\varphi\varphi\} \rightarrow 2, \quad \{zz\} \rightarrow 3, \]
\[ \{\varphi z\} \rightarrow 4, \quad \{zs\} \rightarrow 5, \quad \{s\varphi\} \rightarrow 6. \]  
(2.29)

Equivalent expressions for dipole and quadrupole sources can be found in the appendix 2.7.1. At this point we have carried out the integration in azimuth in Eq. (2.27) and end up with an equation of motion in the weak form with a domain of definition that spans the semi-circular domain \( \Omega_D \), see Fig. 2.1.

**Effective Elasticity Tensor**

Inspection of eqs. (2.28, 2.48 and 2.49) reveals that 8 out of the 21 independent coefficients in the elasticity tensor drop out in the integration of the stiffness terms over \( \varphi \) for all source types, namely \( C_{14}, C_{24}, C_{34}, C_{16}, C_{26}, C_{36}, C_{45}, C_{56} \). These are exactly the coefficients that are antisymmetric with respect to the s-z plane, i.e. change sign under coordinate transform \( \varphi \rightarrow -\varphi \). By setting these coefficients to zero, an effective elasticity tensor can be defined that is symmetric with respect to the s-z plane, i.e. invariant under coordinate transform \( \varphi \rightarrow -\varphi \). See Fig. 2.2 and 2.3 for a visualization of this mapping.

In practice, this means that recorded seismic waveforms of a specific source-receiver combination are fundamentally insensitive to these antisymmetric coefficients so long as the 2.5D approximation is valid, i.e. for structural variations on
2. Seismic Wave Propagation in Fully Anisotropic Axisymmetric Media

![Image](image.png)

**Figure 2.3.:** Artistic visualization of the effective elasticity tensor: the wavefield only 'sees' the structure that is symmetric under coordinate transform $\varphi \rightarrow -\varphi$, the structure from Fig. 2.2 can hence be mapped onto one of the symmetry classes visualized here without any effect on the wavefield.

... a larger scale than the Fresnel zone. To image full anisotropy using high-frequency body waves, multiple crossings of a certain region are therefore necessary not only for spatial resolution as in isotropic imaging, but also to resolve the full elastic tensor.

2.3.2. Discretization

The next step is to generalize the spatial discretization of the stiffness terms from the isotropic case presented in Nissen-Meyer et al. (2007b) to the anisotropic case. The approach is the same as in the isotropic case and we refer the reader to section 3 in Nissen-Meyer et al. (2007b) for details and restrict ourselves to a short summary of the method and important aspects of the notation in the interest of brevity.

The collapsed 2D domain $\Omega_D$ is divided into non-axial elements $\Omega_e$ and axial elements $\Omega_{\bar{e}}$. The mapping between reference coordinates $\xi, \eta \in [-1, 1]$ in each element and the physical coordinates $s, z$ is provided by the Jacobian determinant.
2.3. The Axisymmetric System

\[ \mathcal{J}(\xi, \eta) = \det \begin{pmatrix} s_\xi & s_\eta \\ z_\xi & z_\eta \end{pmatrix}, \]  
(2.30)

where the subscript denotes partial derivation, \( s_\xi = \partial_\xi s \) etc. Both the test function \( w \) and the displacement \( u \) are expanded in Lagrangian polynomials \( l_i \) of order \( N \) (defined on the integration points, see below) within each element

\[ u^\alpha(\xi, \eta, t) = \sum_{ij} u^\alpha_{ij}(t) l_i(\xi) l_j(\eta) \]  
(2.31)

for each component \( \alpha \in (s, \varphi, z) \) and equivalently for \( w \). For the axial elements \( \xi = 0 \) is the axis. The integral over the domain \( \Omega_D \) is then split into a sum of integrals over elements and approximated using the Gauss Lobatto integration rule

\[ \int_{\Omega_e} u(s, z) s \, ds \, dz \approx \sum_{pq} \sigma_p \sigma_q s(\xi_p, \eta_q) u_{pq} \mathcal{J}(\xi_p, \eta_q) \]  
(2.32)

with Gauss Lobatto Legendre (GLL) integration weights \( \sigma_p \) and integration points \( \xi_p \) and \( \eta_q \). For the axial elements, Gauss Lobatto Jacobi (GLJ) quadrature is used for the \( \xi \) direction with

\[ \int_{\Omega_\xi} u(s, z) s \, ds \, dz \approx \sum_{pq} \tilde{\sigma}_p (1 + \tilde{\xi}_p)^{-1} \sigma_q s(\tilde{\xi}_p, \eta_q) u_{pq} \mathcal{J}(\tilde{\xi}_p, \eta_q) \]  
(2.33)

and GLJ integration weights \( \tilde{\sigma}_p \), integration points \( \tilde{\xi}_p \) and the Lagrangian interpolation polynomial on these points \( \tilde{l}(\xi) \). This allows to use l’Hospital’s rule to calculate derivatives at the axis where needed.

Applying this discretization to Eq. (2.27), choosing the set of test functions to be 1 in one component at a specific integration point and 0 at the others and summing over all elements we obtain the global set of ordinary differential equations in time

\[ M \ddot{u}(t) + K u(t) = f(t), \]  
(2.34)

with the global mass matrix \( M \) and stiffness matrix \( K \). While the assembled mass matrix is diagonal in the GLL/GLJ basis (hence trivial to invert), it is unnecessary
to compute $K$ explicitly and we only evaluate its action on the displacement ($Ku$). This term only appears on the right hand side of the second order system

$$\ddot{u}(t) = M^{-1}[f(t) - Ku(t)]$$

which is solved by explicit numerical time integration schemes. The stiffness terms $Ku$ are solved in each element first and the global stiffness is assembled subsequently (Nissen-Meyer et al. 2007b, section 4).

The only difference compared to the isotropic case is in the elemental stiffness terms, which we derive here for the anisotropic case. We split the original elemental stiffness integral into contributions from each component $\beta$ of the vectorial test function $w$, denoted by the subscript $\beta$. Furthermore, we split the contributions from terms in Eq. (2.28) with two ('leading order') or less ('lower order') partial derivatives, denoted by superscripts $\partial_\beta \partial$ and $\partial$. The full elemental stiffness for the monopole is hence split as

$$Ku = \sum_{\beta \in \{s,z\}} \left( (Ku)^{\partial_\beta} + (Ku)^{\partial} \right).$$

Furthermore, we revert to a tensorial notation instead of elemental sums and define the matrix-matrix products

$$X = A \otimes B : \quad X_{ij} = \sum_k A_{ik} B_{kj}$$

and vector-matrix and vector-vector products

$$X^0 = A^0 \otimes B^0 : \quad X_{0j} = \sum_k A_{0k} B_{kj}$$

$$X^0 = A^0 \circ B^0 : \quad X_{0j} = A_{0j} B_{0j}$$

$$X = A^0 \circ B^0 : \quad X_{ij} = A_{i0} B_{0j}$$

The leading order terms have contributions from the components $\alpha$ of the displacement $u$, where the $\varphi$ component vanishes for the monopole source, thus
Table 2.1.: Definitions for precomputable matrices (that is, prior to the costly time extrapolation) of the stiffness terms, ± takes its value depending on the combination of \( x_\zeta \) as in the lower right table. Subscript reference coordinates denotes partial derivation, \( x_\zeta = \partial_\zeta x \). For consistency with the summation notation in Nissen-Meyer et al. (2007a), we use indices \( i, j \) and \( I, J \), which all take the values in \([0, N]\).

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Non-axial elements</th>
<th>Axial elements ((i &gt; 0))</th>
<th>((i = 0))</th>
<th>Axial vectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>((A)^{(ij)})</td>
<td>(\varepsilon^{ij}\sigma_i\sigma_j(s^{ij})^{-1}J^{ij})</td>
<td>(\varepsilon^{ij}\tilde{\sigma}_i(1 + \tilde{\xi}_i)^{-1}\sigma_j(s^{ij})^{-1}J^{ij})</td>
<td>0</td>
<td>((A)^{(0)}) = (\varepsilon^{0j}\tilde{\sigma}_0\sigma_jJ^{0j}(s^{0j})^{-1})</td>
</tr>
<tr>
<td>((B_{\xi\zeta})^{(ij)})</td>
<td>(\pm\varepsilon^{ij}\sigma_i\sigma_jx_\zeta^{ij})</td>
<td>(\pm\varepsilon^{ij}\tilde{\sigma}_i(1 + \tilde{\xi}<em>i)^{-1}\sigma_jx</em>\zeta^{ij})</td>
<td>0</td>
<td>((B_{\xi\zeta}^{(0)})^j = \pm\varepsilon^{0j}\tilde{\sigma}<em>0\sigma_jx</em>\zeta^{0j})</td>
</tr>
<tr>
<td>((C)^{(ij)})</td>
<td>(\sigma_i\sigma_js^{ij}(J^{ij})^{-1})</td>
<td>(\tilde{\sigma}_i\sigma_js^{ij}(1 + \tilde{\xi}_i)^{-1}(J^{ij})^{-1})</td>
<td>0</td>
<td>((C)^{(0)} = \tilde{\sigma}_0\sigma_js^{0j}(J^{0j})^{-1})</td>
</tr>
<tr>
<td>((D_{\xi}^{(ij)})^{Ii})</td>
<td>(\partial_\xi I_i(\xi_i))</td>
<td>(\partial_\xi I_i(\tilde{\xi}_i))</td>
<td>(\partial_\xi I_i(\xi_0))</td>
<td>((D_{\xi}^{(0)}) = (\partial_\xi I_i(\xi_0))</td>
</tr>
<tr>
<td>((D_{\zeta}^{(ij)})^{Jj})</td>
<td>(\partial_\zeta J_j(\eta_j) = \partial_\zeta J_j(\xi_j))</td>
<td>(\partial_\zeta L_j(\xi_j))</td>
<td>(\partial_\zeta L_j(\eta_j))</td>
<td></td>
</tr>
</tbody>
</table>

\[
\pm(x_\zeta) \quad \zeta = \xi \quad \zeta = \eta
\]

\[
\pm(x_\zeta) = \pm\left\{ \begin{array}{ll}
1 & \text{if } x_\zeta = \xi \\
-1 & \text{if } x_\zeta = \eta
\end{array} \right.
\]

\[
\frac{d^2}{d\zeta^2} = \sum_{\alpha \in \{s, z\}} (Ku)^{\beta\alpha}_{\beta\alpha} 
\]

(2.39)

with

\[
(Ku)^{\beta\alpha}_{\beta\alpha} = D_\xi \otimes \left[ C \odot E^{(1)}_{\beta\alpha} \odot (u_\alpha \otimes D_\eta) + C \odot E^{(2)}_{\beta\alpha} \odot (D^T_\xi \otimes u_\alpha) \right]
\]

\[
+ \left[ C \odot E^{(3)}_{\beta\alpha} \odot (D^T_\xi \otimes u_\alpha) + C \odot E^{(4)}_{\beta\alpha} \odot (u_\alpha \otimes D_\eta) \right] \otimes D^T_\eta.
\]

(2.40)

with \( C \) and \( D \) from table 2.1 and \( E^{(k)}_{\beta\alpha} \) defined as:
with $\varepsilon G_{k}^{xy}$ from table 2.1. Defining

\[
B_{s,s}^{(k)} = c_{11}G_{k}^{ss} + c_{14}G_{k}^{sz} + c_{15}G_{k}^{zs} + c_{55}G_{k}^{zz} \\
B_{s,z}^{(k)} = c_{15}G_{k}^{ss} + c_{13}G_{k}^{sz} + c_{55}G_{k}^{zs} + c_{35}G_{k}^{zz} \\
B_{z,s}^{(k)} = c_{15}G_{k}^{ss} + c_{13}G_{k}^{sz} + c_{55}G_{k}^{zs} + c_{35}G_{k}^{zz} \\
B_{z,z}^{(k)} = c_{55}G_{k}^{ss} + c_{35}G_{k}^{zs} + c_{35}G_{k}^{zs} + c_{33}G_{k}^{zz} \tag{2.41}
\]

with $\varepsilon A_{k}$ and $\varepsilon B_{x,\xi}$ from table 2.1 the lower-order terms read:

\[
(Ku)^{\partial}_{s} = D_{\xi} \otimes (M_{1} \otimes u_{s}) + (M_{2} \otimes u_{s}) \otimes D_{\eta}^{T} + M_{1} \otimes (D_{\xi}^{T} \otimes u_{s}) \\
+ M_{3} \otimes (D_{\xi}^{T} \otimes u_{z}) + M_{2} \otimes (u_{s} \otimes D_{\eta}) + M_{4} \otimes (u_{z} \otimes D_{\eta}) + M_{w1} \otimes u_{s} \\
+ \delta_{ee}\left\{ D_{\xi}^{0} \left[ M_{w3}^{0} \otimes (u_{z} \otimes D_{\eta}) + M_{w1}^{0} \otimes (D_{\xi}^{0})^{T} \otimes u_{s} \right] \\
+ M_{w2}^{0} \otimes \left[ (D_{\xi}^{0})^{T} \otimes u_{z} \right] \right\} \tag{2.43}
\]

\[
(Ku)^{\partial}_{z} = D_{\xi} \otimes (M_{3} \otimes u_{s}) + (M_{4} \otimes u_{s}) \otimes D_{\eta}^{T} \\
+ \delta_{ee}\left\{ D_{\xi}^{0} \left[ M_{w2}^{0} \otimes \left( (D_{\xi}^{0})^{T} \otimes u_{s} \right) \right] \\
+ M_{w3}^{0} \otimes \left( (D_{\xi}^{0})^{T} \otimes u_{s} \right) \otimes D_{\eta}^{T} \right\}. \tag{2.44}
\]

Here $\delta_{ee}$ is 1 in axial elements and 0 otherwise and is used to denote the additional terms that occur from the special treatment of derivatives at the axis.

Important, the computational cost is not increased measurably within the time-evolution compared to the isotropic version: in the monopole case the only additional term is 1D axial term with $M_{w2}^{0}$. $B_{\beta,\alpha}$ receives additional contributions, but these
are precomputed before the time loop (Table 2.1). This is similar for dipole and quadrupole sources (see appendix), so we dropped the isotropic implementation and use the new anisotropic version as well for entirely isotropic models.

2.4. Benchmarks

Solving the full 3D wave equation for arbitrary earthquake sources in axisymmetric models, \textit{AxiSEM} seems to be unique among the available codes. For benchmarking we thus have to revert to spherically symmetric models, but as the code is written in cylindrical coordinates, even transversely isotropic media lead to a stiffness tensor that is fully populated (those elements that are nonzero in the effective stiffness tensor, see above) and the full stiffness matrix is tested. As a reference, we use \textit{Yspec} by Al-Attar and Woodhouse (2008), which is a generalization of the direct radial integration method (Friederich and Dalkolmo 1995) including selfgravitation (switched off for the benchmark).

2.4.1. High Frequency Seismograms

While Nissen-Meyer et al. (2008) could only perform benchmarks down to 20 s period due to limitations in the reference normal mode solution, this limit is overcome using \textit{Yspec}. Also, \textit{AxiSEM} since then has experienced some substantial development (Nissen-Meyer et al. 2014), specifically the improved parallelization allows us to perform production runs up to the highest frequencies observed for global body waves.

Fig. 2.4 shows a record section of seismograms computed for the anisotropic PREM model (Dziewoński and Anderson 1981) with continental crust computed with \textit{Yspec} and \textit{AxiSEM}. The source is a strike slip event with a moment magnitude $M_w = 5.0$ in 117 km depth under Oaxaca, Mexico. The traces recorded at some selected GSN stations are filtered between 5 and 1 s. Due to the high-frequency content, it is necessary to zoom in to see any differences at all: the agreement between the two methods is remarkable even though the highest frequencies have traveled more than 1000 wavelengths (given the low pass filter at 1 s, the time axis is equivalent to the number of traveled wavelengths).

We use the phase and envelope misfit ($PM$ and $EM$ as defined by Kristekova et al. 2009) for quantitative comparison within the zoom windows and find phase misfits well below 1% for all windows and envelope misfits below 1.1% for all windows but the extremely small amplitude phase $ScS$ at JTS, where it reaches a maximum of 2.3%. Errors in amplitude and phase are therefore negligibly small compared to other
2. Seismic Wave Propagation in Fully Anisotropic Axisymmetric Media

Figure 2.4.: Comparison of vertical displacement seismograms (band pass filtered from 5 s to 1 s period) for a strike slip event with a moment magnitude $M_w = 5.0$ in 117 km depth under Oaxaca, Mexico, computed with AxiSEM and Yspec in the anisotropic PREM model without ocean. The traces are recorded at the GSN stations indicated in the map. The zoom windows shown in Fig. 2.5 are indicated with red rectangles.

errors when comparing these synthetics to data like e.g. noise or the assumption of a 1D model.

The total cost of this run with AxiSEM was about 70K CPU hours using a 4th order symplectic time scheme (Nissen-Meyer et al. 2008) on a Cray XE6. The mesh was built for periods down to 0.8 s and the time step chosen 30% below the CFL criterion, as this run was meant to prove convergence to the same result as Yspec. In applications where less accuracy is necessary one could either use the same traces at higher frequencies or reduce this cost substantially by choosing a larger time step and a coarser mesh.

2.4.2. Low Frequency Spectra

Normal mode eigenfrequency- and phasespectra are extremely sensitive to Earth’s structure, so they also provide a good benchmark at the low frequency end of the spectrum. For the comparison, 48 hours of synthetic seismogram were tapered with
Figure 2.5.: -continued from Fig. 2.4- The time scale is relative to the ray-theoretical arrival. *EM* and *PM* denote the envelope and phase misfit in the time window plotted (Kristekova et al. 2009).
2. Seismic Wave Propagation in Fully Anisotropic Axisymmetric Media

Figure 2.6.: Comparison of amplitude- and phase-spectra of 48h time series generated with AxiSEM and Yspec, lower two are zooms into the region marked with the red rectangle. Most differences that appear to be large in the phase spectrum (e.g. just below 5.3 mHz) are actually small and are visible only because of phase wrapping at $\pi, -\pi$.

A cosine function and transformed to the frequency domain. Fig. 2.6 shows both amplitude and phase spectra with a zoom on the frequencies just above 5 mHz. The agreement in the amplitude spectrum is striking and there is essentially no visible difference. The phase spectra agree slightly less well compared to the amplitudes due to accumulated dispersion errors in the time stepping of AxiSEM (1.7 Million time steps with a 2nd order Newmark time scheme, equivalent to 2000 propagated wavelengths at $\approx$ 10 mHz), but the most visible differences (e.g. around 5.4 mHz) arise from phase wrapping at $\pi, -\pi$.

In summary, our validation against an entirely different approach (frequency vs. time domain, 1D vs. 2.5D modelling) at the high- and low end of the relevant frequency spectrum of global seismology is very good. To the best of our knowledge no such benchmarks between two entirely different codes for both 1Hz wave propagation or for mode spectra have been published.
2.5. Applications

Hemispherical structure in the inner core of the Earth is well documented (e.g. Waszek and Deuss 2011; Deuss et al. 2010; Irving et al. 2009, 2008; Creager 1992; Morelli et al. 1986), where the Eastern hemisphere is nearly isotropic and faster on average and the Western hemisphere is anisotropic and slower than average. The observed anisotropy is of hexagonal symmetry with a fast axis approximately parallel to the rotation axis of the Earth and a slow plane parallel to the equator. Anisotropy is an important diagnostic property of the inner core since it allows to impose constraints on super-rotation (Waszek et al. 2011) and the history of inner core formation.

Inner core body waves are typically observed at frequencies around 0.5 to 2.0 Hz, which is unfeasible for 3D-discretized global seismic wave simulations. On the other hand, due to the high frequencies, the Fresnel zones are very narrow and for the early arriving inner core phases off-path scattering can be neglected. The 2.5D approximation is hence likely valid, if the medium parameters vary slowly perpendicular to the source receiver plane. Using high-frequency synthetics computed with AxiSEM one can study the problem in terms of waveform effects, potentially allowing for additional insights compared to solely analysing ray-theoretical traveltimes. Furthermore, there is an epicentral distance region around 146° where PKPab, PKPbc and PKiKP phases arrive at the receiver at the same time, see Fig. 2.7. This distance region corresponds to a depth region of turning rays, where traveltime cannot be extracted with classical ray-theoretical methods. Having full waveforms computed with AxiSEM at hand, extracting additional information about this depth region could help further constrain inner core structure.

Fig. 2.7 shows a record section zoomed in to the inner core phases for an explosive source beneath the North pole, bandpass filtered from 1 Hz to 2 Hz. The background model is isotropic PREM for the black traces and includes hexagonal anisotropy in the inner core with the fast axis in North-South direction for the red traces. This represents a model according to results for uniform anisotropy by Irving and Deuss (2011). This model is represented exactly in the 2.5D modeling of AxiSEM, the validity of the 2.5D approximation for more general models will be subject to future parameter studies. As a reference, major ray-theoretical arrivals in PREM are indicated with blue lines, PKIKP and pPKIKP for the anisotropic core with green lines.

Ray-theoretical traveltimes for PKIKP and pPKIKP in the anisotropic model can be computed using the small anisotropy approximation for the perturbation of the P-wave velocity as a function of the ray angle ζ between the fast axis and the
Figure 2.7: Vertical-displacement record section zoomed in to the inner-core phases for an explosive source bandpass filtered from 1 Hz to 2 Hz. Normalization is global. Black traces for an isotropic PREM model, red traces for a PREM with anisotropic inner core (hexagonal symmetry, fast axis in North-South direction). Major ray theoretical arrivals in PREM are indicated with blue lines, PKIKP and pPKIKP for the anisotropic core with green lines computed according to Eq. (2.45).
2.6. Conclusion & Outlook

direction of wave propagation (Morelli et al. 1986):

\[
\frac{\delta v_p(\zeta)}{v_p} = a + b \cos^2 \zeta + c \cos^4 \zeta,
\]
(2.45)

where \( v_p \) is the \( P \)-wave velocity in the isotropic background model. To define the whole elastic tensor, we use the relation of these to the Love coefficients which can be found in first order as

\[
A = \rho v_p^2 (1 + a)^2,
\]
\[
L = N = \rho v_s^2, \quad F = \rho v_p^2 (1 + a)(1 + a + b),
\]
\[
C = \rho v_p^2 (1 + a)(1 + 2a + 2b + 2c).
\]
(2.46)

The good agreement between this simple ray theoretical perturbation method and the move-out of the body wave packets in Fig. 2.7 suggests that this is a feasible method to obtain full synthetic waveforms to study inner core anisotropic structures up to 2 Hz as shown here.

2.6. Conclusion & Outlook

This paper shows how the 2.5D method by Nissen-Meyer et al. (2007a) is extended to include fully anisotropic structure. Two analytical arguments are provided to show that the terms in the expansion of the wave equation into a multipole series are still uncoupled: the first one was based on evaluation the normal mode coupling matrix which has an intuitive interpretation in the global seismology context. The second one generalizes the idea to all linear equations that are invariant under rotation around an axis.

The resulting reduced equations are discretized using the spectral element method and the numerical implementation is benchmarked against a reference solution, showing excellent agreement both for high-frequency body waves and the low frequency normal mode spectra. Inner core anisotropy is suggested as one interesting application taking advantage of the specific parameter regime covered by this new version of AxiSEM.

Future work includes benchmarks for 2.5D anisotropy and the application to more complex inner core anisotropy models as well as anisotropic D\(^n\) structures.
2. Seismic Wave Propagation in Fully Anisotropic Axisymmetric Media

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References


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2.7. Appendix

2.7.1. Dipole and Quadrupole Stiffness Terms

This section contains the results for the weak form of the stiffness term for dipole and quadrupole sources, equivalent to the results presented in section 2.3.1 for the monopole source and Nissen-Meyer et al. (2007a, section 4.6-7) for the isotropic case.

Dipole ($m = 1$)

For the dipole source, we define

$$ u_\pm = \frac{1}{2}(u_s \pm u_\varphi) \quad \Rightarrow \quad u_s = u_+ + u_-, \quad u_\varphi = u_+ - u_- \quad (2.47) $$

as this facilitates easier implementation of the axial boundary conditions (compare Nissen-Meyer et al. 2007a, section 4.8). The stiffness terms integrated over $\varphi$ then read

$$ \frac{1}{\pi} \int_0^{2\pi} \nabla w : (c : \nabla u) \, d\varphi \quad (2.48) $$

$$ = \partial_s w_+ \left( (C_{11} + C_{66}) \partial_s u_+ + (C_{11} - C_{66}) \partial_s u_- + C_{15} \partial_z u_z + (C_{15} + C_{46}) \partial_z u_+ + (C_{15} - C_{46}) \partial_z u_- + C_{13} \partial_z u_z + \frac{1}{s} (2(C_{12} + C_{66}) u_- + C_{46} u_z) \right) $$

$$ + \partial_z w_+ \left( (C_{15} + C_{46}) \partial_z u_+ + (C_{15} - C_{46}) \partial_z u_- + C_{55} \partial_s u_z + (C_{55} + C_{44}) \partial_z u_+ + (C_{55} - C_{44}) \partial_z u_- + C_{35} \partial_z u_z + \frac{1}{s} (2(C_{46} + C_{25}) u_- + C_{44} u_z) \right) $$

$$ + \partial_s w_- \left( (C_{11} - C_{66}) \partial_s u_+ + (C_{11} + C_{66}) \partial_s u_- + C_{15} \partial_z u_z + (C_{15} - C_{46}) \partial_z u_+ + (C_{15} + C_{46}) \partial_z u_- + C_{13} \partial_z u_z + \frac{1}{s} (2(C_{12} - C_{66}) u_- - C_{46} u_z) \right) $$

$$ + \partial_z w_- \left( (C_{15} - C_{46}) \partial_z u_+ + (C_{15} + C_{46}) \partial_z u_- + C_{55} \partial_s u_z + (C_{55} - C_{44}) \partial_z u_+ + (C_{55} + C_{44}) \partial_z u_- + C_{35} \partial_z u_z + \frac{1}{s} (2(-C_{46} + C_{25}) u_- - C_{44} u_z) \right) \)
2. Seismic Wave Propagation in Fully Anisotropic Axisymmetric Media

\[ + \frac{w_z}{s} \left( (C_{12} + C_{66}) \partial_s u_+ + (C_{12} - C_{66}) \partial_s u_- + C_{25} \partial_s u_z + (C_{25} + C_{46}) \partial_z u_+ \\
+ (C_{25} - C_{46}) \partial_z u_- + C_{23} \partial_z u_z + \frac{1}{s} (2(C_{22} + C_{66})u_- + C_{46}u_z) \right) \\
+ \partial_z w_z \left( C_{15} \partial_s u_+ + C_{15} \partial_s u_- + C_{55} \partial_s u_z + C_{55} \partial_z u_+ + C_{55} \partial_z u_- + C_{35} \partial_z u_z \\
+ \frac{2}{s} C_{25} u_- \right) \\
+ \partial_z w_z \left( C_{13} \partial_s u_+ + C_{13} \partial_s u_- + C_{35} \partial_z u_z + C_{35} \partial_z u_+ + C_{35} \partial_z u_- + C_{33} \partial_z u_z \\
+ \frac{2}{s} C_{23} u_- \right) \\
+ \frac{w_z}{s} \left( C_{46} \partial_s u_+ - C_{46} \partial_s u_- + C_{44} \partial_z u_+ - C_{44} \partial_z u_- + \frac{2}{s} C_{46} u_- \right) \].

Quadrupole \((m = 2)\)

In the quadrupole case we remain with the same basis as for the monopole \((u_s, u_\phi, u_z)\) and find the stiffness terms integrated over \(\varphi\) as

\[
\frac{1}{2\pi} \int_0^{2\pi} \nabla w : (c : \nabla u) \, d\varphi \tag{2.49}
\]

\[= \partial_s w_s \left( C_{11} \partial_s u_s + C_{15} \partial_z u_s + C_{15} \partial_s u_z + C_{13} \partial_z u_z + \frac{1}{s} (C_{12} u_s - 2C_{12} u_\phi) \right) \\
+ \partial_z w_s \left( C_{15} \partial_s u_s + C_{55} \partial_z u_s + C_{55} \partial_s u_z + C_{35} \partial_z u_z + \frac{1}{s} (C_{25} u_s - 2C_{25} u_\phi) \right) \\
+ \frac{1}{s} w_s \left( C_{12} \partial_s u_s + 2C_{66} \partial_s u_\phi + C_{25} \partial_s u_z + C_{25} \partial_z u_s + 2C_{46} \partial_z u_\phi + C_{23} \partial_z u_z \\
+ \frac{1}{s} ((C_{22} + 4C_{66}) u_s - 2(C_{22} + C_{66}) u_\phi + 4C_{46} u_z) \right) \\
+ \partial_s w_\phi \left( C_{66} \partial_s u_\phi + C_{46} \partial_z u_\phi + \frac{1}{s} (2C_{66} u_s - C_{66} u_\phi + 2C_{46} u_z) \right) \\
+ \partial_z w_\phi \left( C_{46} \partial_s u_\phi + C_{44} \partial_z u_\phi + \frac{1}{s} (2C_{46} u_s - C_{46} u_\phi + 2C_{44} u_z) \right) \\
+ \frac{1}{s} w_\phi \left( -2C_{12} \partial_s u_s - 2C_{25} \partial_s u_z - C_{66} \partial_s u_\phi - 2C_{23} \partial_z u_z - 2C_{25} \partial_z u_s - C_{46} \partial_z u_\phi \\
+ \frac{1}{s} (-2C_{22} u_s + 4C_{22} u_\phi + C_{66} u_\phi - 2C_{66} u_s - 2C_{46} u_z) \right) \]
\[ + \partial_s w_z \left( C_{15} \partial_s u_s + C_{55} \partial_z u_s + C_{55} \partial_s u_z + C_{35} \partial_z u_z + \frac{1}{s} (C_{25} u_s - 2C_{25} u_\phi) \right) \]
\[ + \partial_z w_z \left( C_{13} \partial_s u_s + C_{35} \partial_z u_s + C_{35} \partial_s u_z + C_{33} \partial_z u_z + \frac{1}{s} (C_{23} u_s - 2C_{23} u_\phi) \right) \]
\[ + \frac{2}{s} w_z \left( C_{46} \partial_s u_\phi + C_{44} \partial_z u_\phi + \frac{1}{s} (2C_{46} u_s - C_{46} u_\phi + 2C_{44} u_z) \right). \]

### 2.7.2. Dipole and Quadrupole Discretization of the Stiffness Terms

These stiffness terms are then discretized in the SEM using the notation defined in section 2.3.2.

**Dipole**

For the dipole, we define \( \mathbf{E}^{(k)}_{\beta\alpha} \) for the leading order terms as

\[
\begin{align*}
\mathbf{E}^{(k)}_{++} &= (C_{11} + C_{66}) G^{ss}_k + (C_{15} + C_{46}) G^{sz}_k + (C_{15} + C_{46}) G^{zs}_k + (C_{55} + C_{44}) G^{zz}_k \\
\mathbf{E}^{(k)}_{+-} &= (C_{11} - C_{66}) G^{ss}_k + (C_{15} - C_{46}) G^{sz}_k + (C_{15} - C_{46}) G^{zs}_k + (C_{55} - C_{44}) G^{zz}_k \\
\mathbf{E}^{(k)}_{+z} &= C_{15} G^{ss}_k + C_{13} G^{sz}_k + C_{55} G^{zs}_k + C_{35} G^{zz}_k \\
\mathbf{E}^{(k)}_{-+} &= \mathbf{E}^{(k)}_{++} \\
\mathbf{E}^{(k)}_{-z} &= \mathbf{E}^{(k)}_{++} \\
\mathbf{E}^{(k)}_{zz} &= \mathbf{E}^{(k)}_{+-}
\end{align*}
\]

(2.50)

The leading order terms then are

\[
(Ku)_{\beta\phi}^{\partial\partial} = \sum_{\alpha \in \{+, -, z\}} (Ku)_{\beta\alpha}^{\partial\partial},
\]

(2.53)

with \( (Ku)_{\beta\alpha}^{\partial\partial} \) from eq. (2.40). For the lower order and axial terms we define
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\[ M_1 = (2C_{12} + 2C_{66})B_{z\eta} + (2C_{25} + 2C_{46})B_{s\eta} \]
\[ M_3 = C_{46}B_{z\eta} + C_{44}B_{s\eta} \]
\[ M_5 = (2C_{12} - 2C_{66})B_{z\eta} + (2C_{25} - 2C_{46})B_{s\eta} \]
\[ M_7 = 2C_{25}B_{z\eta} + 2C_{23}B_{s\eta} \]
\[ M_2 = (2C_{12} + 2C_{66})B_{z\xi} + (2C_{25} + 2C_{46})B_{s\xi} \]
\[ M_4 = C_{46}B_{z\xi} + C_{44}B_{s\xi} \]
\[ M_6 = (2C_{12} - 2C_{66})B_{z\xi} + (2C_{25} - 2C_{46})B_{s\xi} \]
\[ M_8 = 2C_{25}B_{z\xi} + 2C_{23}B_{s\xi}, \quad (2.54) \]

\[ M_{w1} = (4C_{22} + 4C_{66})A \quad M_{w2} = 2C_{46}A \quad M_{w3} = C_{44}A \quad (2.55) \]

and

\[ M_{w1}^0 = (2C_{12} + 2C_{66})A^0 \quad M_{w2}^0 = (2C_{12} + 2C_{66})B_{z\xi}^0 \quad M_{w3}^0 = C_{46}A^0 \quad M_{w4}^0 = C_{46}B_{z\xi}^0 \]
\[ M_{w5}^0 = (2C_{25} + 2C_{46})A^0 \quad M_{w6}^0 = (2C_{25} + 2C_{46})B_{s\xi}^0 \quad M_{w7}^0 = C_{44}A^0 \quad M_{w8}^0 = C_{44}B_{s\xi}^0 \]
\[ M_{w9}^0 = (4C_{12} + 4C_{22})A^0 \quad M_{w10}^0 = (2C_{25} + 2C_{46})A^0 \quad (2.56) \]

The lower order terms can then be written as

\[
(Ku)^\theta_+ = D_\xi \otimes \left[ M_1 \odot u_- + M_3 \odot u_z \right] + \left[ M_2 \odot u_- + M_4 \odot u_z \right] \otimes D_\eta^T \\
+ \delta_{\varepsilon\varepsilon} \left\{ D_\xi^0 \left[ M_{w1}^0 \odot \left( (D_\xi^0)^T \otimes u_- \right) + M_{w3}^0 \odot \left( (D_\xi^0)^T \otimes u_z \right) \right] \\
+ \left[ (M_{w2}^0 + M_{w6}^0) \odot \left( (D_\xi^0)^T \otimes u_- \right) \right] \\
+ \left[ (M_{w4}^0 + M_{w8}^0) \odot \left( (D_\xi^0)^T \otimes u_z \right) \right] \otimes D_\eta^T \right\} \\
(Ku)^\theta_- = M_1 \odot (D_\xi^T \otimes u_+) + M_2 \odot (u_+ \otimes D_\eta) + M_5 \odot (D_\xi^T \otimes u_-) \\
+ M_6 \odot (u_- \otimes D_\eta) + M_7 \odot (D_\xi^T \otimes u_z) + M_8 \odot (u_z \otimes D_\eta) \\
+ D_\xi \otimes \left[ M_5 \odot u_- - M_3 \odot u_z \right] + \left[ M_6 \odot u_- - M_4 \odot u_z \right] \otimes D_\eta^T \\
+ M_{w1}^0 \odot u_- + M_{w2}^0 \odot u_z \\
+ \delta_{\varepsilon\varepsilon} D_\xi^0 \left[ M_{w1}^0 \odot \left( (D_\xi^0)^T \otimes u_+ \right) + \left( M_{w2}^0 + M_{w6}^0 \right) \odot \left( u_+ \otimes D_\eta \right) \right] \\
+ M_{w9}^0 \odot \left( (D_\xi^0)^T \otimes u_- \right) + M_{w10}^0 \odot \left( (D_\xi^0)^T \otimes u_z \right) \right\} \\
(2.57)
\]
(Ku)_{z}^{β} = M_{3} \odot \left( D_{ξ}^{T} \otimes (u_{+} - u_{-}) \right) + M_{4} \odot ((u_{+} - u_{-}) \otimes D_{η})
+ D_{ξ} \otimes \left[ M_{7} \odot u_{-} \right] + \left[ M_{8} \odot u_{-} \right] \otimes D_{η}^{T} + M_{w2} \odot u_{-} + M_{w3} \odot u_{z}
+ \delta_{ξξ} D_{ξ}^{0} \left[ M_{w3}^{0} \odot \left( (D_{ξ}^{0})^{T} \otimes u_{+} \right) \right] + \left( M_{w4}^{0} + M_{w8}^{0} \right) \odot (u_{+}^{0} \otimes D_{η})
+ M_{w10}^{0} \odot \left( (D_{ξ}^{0})^{T} \otimes u_{-} \right) + M_{w7}^{0} \odot \left( (D_{ξ}^{0})^{T} \otimes u_{z} \right) \right]. \quad (2.59)

Quadrupole

For the quadrupole source, we define additionally to the definitions from the monopole, eq. (2.41)

\[
E_{ϕϕ}^{(k)} = C_{66} G_{k}^{ss} + C_{46} G_{k}^{sz} + C_{44} G_{k}^{zz},
E_{ϕs}^{(k)} = 0, \quad E_{sϕ}^{(k)} = 0, \quad E_{zϕ}^{(k)} = 0.
\quad (2.60)
\]

The leading order terms then are

\[
(Ku)_{β}^{γ} = \sum_{α \in \{s,ϕ,z\}} \cdot (Ku)_{βα}^{γ} \cdot .
\quad (2.61)
\]

Additionally to M_{1}, M_{2}, M_{3}, M_{4} as in the monopole case, eq. (2.42) we define:

\[
M_{5} = C_{66} B_{zη} + C_{46} B_{sη}, \quad M_{6} = C_{66} B_{sξ} + C_{46} B_{sξ}
M_{7} = C_{46} B_{zη} + C_{44} B_{sη}, \quad M_{8} = C_{46} B_{sξ} + C_{44} B_{sξ}
\quad (2.62)
\]

and partly redefine:

\[
M_{w1} = (C_{22} + 4C_{66}) A, \quad M_{w2} = -2(C_{22} + C_{66}) A, \quad M_{w3} = 2C_{46} A
M_{w4} = (4C_{22} + C_{66}) A, \quad M_{w5} = 4C_{44} A
M_{w1}^{0} = (2C_{12} + C_{22} + 4C_{66}) A^{0}, \quad M_{w2}^{0} = -2(C_{12} + C_{22}) A^{0}, \quad M_{w3}^{0} = (C_{25} + 4C_{46}) A^{0}
M_{w4}^{0} = (4C_{22} - C_{66}) A^{0}, \quad M_{w5}^{0} = -2C_{25} A^{0}, \quad M_{w6}^{0} = 4C_{44} A^{0}
\quad (2.63)
\]

The lower order terms can then be written as
\[(Ku)^{\phi}_s = M_1 \otimes (D^T_\xi \otimes u_s) + M_2 \otimes (u_s \otimes D_\eta) + M_3 \otimes (D^T_\xi \otimes u_z) + M_4 \otimes (u_z \otimes D_\eta) + 2 \cdot M_5 \otimes (D^T_\xi \otimes u_\varphi) + 2 \cdot M_6 \otimes (u_\varphi \otimes D_\eta) + D_\xi \otimes (M_1 \otimes (u_s - 2u_\varphi)) + (M_2 \otimes (u_s - 2u_\varphi)) \otimes D^T_\eta + M_{w1} \otimes u_s + M_{w2} \otimes u_\varphi + 2M_{w3} \otimes u_z + \delta_{e\xi} \cdot D^0_\xi \left[ M^0_{w1} \otimes (D^0_\xi)^T \otimes u_s \right] + M^0_{w2} \otimes (D^0_\xi)^T \otimes u_\varphi \right] + M^0_{w3} \otimes (D^0_\xi)^T \otimes u_z \quad (2.64)\]

\[(Ku)^{\phi}_\varphi = -2 \cdot M_1 \otimes (D^T_\xi \otimes u_s) - 2 \cdot M_2 \otimes (u_s \otimes D_\eta) - 2 \cdot M_3 \otimes (D^T_\xi \otimes u_z) - 2 \cdot M_4 \otimes (u_z \otimes D_\eta) - M_5 \otimes (D^T_\xi \otimes u_\varphi) - M_6 \otimes (u_\varphi \otimes D_\eta) + D_\xi \otimes [M_5 \otimes (2u_s - u_\varphi) + 2 \cdot M_7 \otimes u_z] + M_{w2} \otimes u_s + M_{w4} \otimes u_\varphi - M_{w3} \otimes u_z + \delta_{e\xi} \cdot D^0_\xi \left[ M^0_{w2} \otimes (D^0_\xi)^T \otimes u_s \right] + M^0_{w4} \otimes (D^0_\xi)^T \otimes u_\varphi \right] + M^0_{w5} \otimes (D^0_\xi)^T \otimes u_z \quad (2.65)\]

\[(Ku)^{\phi}_z = 2 \cdot M_7 \otimes (D^T_\xi \otimes u_\varphi) + 2 \cdot M_8 \otimes (u_\varphi \otimes D_\eta) + D_\xi \otimes (M_3 \otimes (u_s - 2u_\varphi)) + (M_4 \otimes (u_s - 2u_\varphi)) \otimes D^T_\eta + M_{w3} \otimes (2u_s - u_\varphi) + M_{w5} \otimes u_z + \delta_{e\xi} \cdot D^0_\xi \left[ M^0_{w3} \otimes (D^0_\xi)^T \otimes u_s \right] + M^0_{w5} \otimes (D^0_\xi)^T \otimes u_\varphi \right] + M^0_{w6} \otimes (D^0_\xi)^T \otimes u_z \quad (2.66)\]
Chapter 3

Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media

Abstract

The representation of visco-elastic media in the time domain becomes more challenging with greater bandwidth of the propagating waves and number of traveled wavelengths. With the continuously increasing computational power, more extreme parameter regimes become accessible, which requires the reassessment and improvement of the standard ‘memory variable’ methods to implement attenuation in time-domain seismic wave-propagation methods. In this paper, we propose a method to minimize the error in the wavefield for a fixed complexity of the anelastic medium. This method consists of defining an appropriate misfit criterion based on a first-order analysis of how errors in the medium representation propagate into errors in the wavefield and a simulated annealing optimization scheme to find the globally optimal parametrization. Furthermore, we derive an analytical time-stepping scheme for the memory variables that encode the strain history of the medium. Then we develop the coarse grained memory variable approach for the spectral element method (SEM) and benchmark it using the 2.5D code AxiSEM for global body waves up to 1 Hz. Showing very good agreement with a reference solution, it also leads to a speed-up of a factor of 5 in the anelastic part of the code (factor 2 in total) in this 2.5D approach. A factor of $\approx 15$ (3 in total) can be expected for the 3D case compared to conventional implementations.

This chapter was previously published in similar form as: van Driel, M., and T. Nissen-Meyer. 2014a. “Optimized viscoelastic wave propagation for weakly dissipative media”. Geophys. J. Int. 199 (2): 1078–1093, additions in this version include the generalization to frequency dependent $Q$ and the computation of partial derivatives of the coefficients needed to compute Fréchet derivatives as proposed in Appendix A.
3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media

3.1. Introduction

Ongoing advances in super-computer architecture and numerical methods enable the solution of the wave equation in increasingly extreme parameter regimes, i.e. higher frequency waves in larger modeling domains, having longer propagation distances in terms of the number of traveled wavelengths. Numerical errors as well as errors in physical approximations accumulate over these larger distances and require more precision both in the numerical solution and in the physical medium representation. We address the question of how accurate attenuation and the corresponding physical dispersion needs to be represented to accurately model seismic waves including attenuation with a focus on global body waves. Even though the quality factor $Q$ is itself poorly constrained by existing seismic studies, especially its 3D structure and frequency dependence (Romanowicz and Mitchell 2007, and references therein), we consider it an essential prerequisite to carefully evaluate the accuracy of the numerous numerical and physical approximations, before upscaling conventional methods of implementing attenuation to the more extreme regimes that modern computational seismology tries to access.

While moving from purely elastic to visco-elastic media is easy in the frequency domain via the correspondence principle and introduction of complex valued media properties, this is more involved in the time-domain since the multiplication in the constitutive relation of the elastic medium needs to be replaced by a convolution. The first method to transform the stress-strain relation into a differential form using Padé approximations is introduced by Day and Minster (1984). Later, Emmerich and Korn (1987) and Carcione et al. (1988) suggest to improve this by approximating the medium properties with a discrete relaxation spectrum (Liu et al. 1976) and fitting the parameters used to describe this spectrum to the observed behaviour numerically. These methods are still common today (e.g. Komatitsch and Tromp 2002a; Kristek and Moczo 2003; Graves and Day 2003; Käser et al. 2007; Fichtner et al. 2009; Savage et al. 2010), a more complete summary and historical overview is given e.g. by Carcione (2007) and Moczo et al. (2014). In this study we suggest several improvements to this scheme leading to better accuracy in the medium representation at zero extra cost.

Even if $Q$ is large (on the global scale the minimum observed value is about 50, Gung and Romanowicz (2004)) and the effect of attenuation on the seismograms small, accounting for it typically leads to an increase of the computational costs by a factor of two to four in both computation time and memory (e.g. Blanch et al. 1995; Käser et al. 2007). Day (1998) suggests a method called the coarse grained memory variable approach to redistribute the medium properties on the sub-wavelength scale.
such that it behaves the same for the wavefield, but is computationally significantly less expensive. Day’s method was originally developed for the acoustic wave equation and regular grid finite-difference schemes. It is generalized to the viscoelastic wave equation and improved by more appropriate averaging schemes by Day and Bradley (2001) and Graves and Day (2003). Kristek and Moczo (2003) further improved the scheme by introducing material-independent memory variables to avoid artificial averaging of material parameters at grid points where interpolation of the memory variables is necessary (e.g. in the context of heterogeneous finite-differences methods at material discontinuities or for thin layers). Ma and Liu (2006) apply the coarse grained method to a low-order finite-element scheme on unstructured grids. However, their approach can not directly be translated to higher-order methods such as the SEM, because in such schemes the elements are too large compared to the wavelength (less than four elements per wavelength). Here, we propose to redistribute the medium properties within the elements on the high-order basis functions, which again is a small scale compared to the wavelength.

On the global scale, high-frequency body waves are routinely observed at distances of 1000-2000 wavelengths and more, a regime that is hardly accessible with current global 3D solvers and computers (Carrington et al. 2008). While the methods we propose for parameter optimization are completely general and the coarse grained memory variable approach applicable to all high-order finite-element methods, we use the axisymmetric SEM AxiSEM introduced by Nissen-Meyer et al. (2007a, 2007b, 2008), further developed to include anisotropy by van Driel and Nissen-Meyer (2014b) and published open source by Nissen-Meyer et al. (2014) as an example implementation to test our theoretical arguments. The efficiency of this 2.5D approach allows very high-frequency simulations (currently up to 2Hz on the global scale) that are still impossible to reach using full 3D methods, so it provides a good basis to test common physical and numerical approximations.

Other axisymmetric approaches to global and local wave propagation have been presented (Alterman and Karal 1968; Igel and Weber 1995, 1996; Chaljub and Tarrantola 1997; Furumura et al. 1998; Thomas et al. 2000; Takenaka et al. 2003; Toyokuni et al. 2005; Jahnke et al. 2008), but only recently Toyokuni and Takenaka (2006, 2012) generalized their method to include moment tensor sources, attenuation and the Earth’s center. These methods are all based on isotropic media and especially the finite-difference methods among them have to deal with large dispersion errors for interface-sensitive waves such as surface waves and diffracted waves (Igel and Weber 1995; Igel et al. 1995). We generalize AxiSEM to viscoelastic anisotropic axisymmetric media to overcome these issues. This enables the simulation of high-frequency body waves with a particularly high sensitivity to attenuation, traveling
3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media

Figure 3.1.: Stress relaxation function $R$ for a viscoelastic medium in the time-domain, i.e. the stress response to a unit step in strain. $M_U$ and $M_R$ denote unrelaxed and relaxed modulus, respectively. Adapted from Emmerich and Korn (1987) and Christensen (1982).

distances over thousands of wavelengths such as core-transmitted, core-reflected and diffracted phases.

3.2. Theory

Here, we introduce the concepts and our notation for time-domain modelling of the memory variable approach to viscoelastic dissipation. We start with the simple 1D case (scalar instead of tensorial quantities) and generalize to the full 3D problem subsequently.

3.2.1. Preliminaries

The most general linear stress-strain relation is the convolution, i.e. the strain $\epsilon$ from all times can linearly influence the stress $\sigma$ at time $t$:

$$
\sigma(t) = \int_{-\infty}^{\infty} M(t - \tau) \cdot \epsilon(\tau) \, d\tau
$$

$$
= \int_{-\infty}^{\infty} R(t - \tau) \cdot \dot{\epsilon}(\tau) \, d\tau. \quad (3.1)
$$
3.2. Theory

Here, $R(t)$ is the stress relaxation function with the modulus $M(t) = \dot{R}(t)$, i.e. the stress response to a unit step in the strain. Assuming causality (strain in the future cannot affect the current stress state: $M(t) = 0, t < 0$), fading memory (more recent strain has a larger impact on the current state: $M(t)$ is monotonous and converges to 0 for $t \to \infty$) and solid behaviour in the limit of low frequencies (a constant strain causes a constant nonzero stress: $\lim_{t \to \infty} R(t) = M_R > 0$), the time-dependent modulus takes the general form shown in Fig. 3.1: zero for negative time and decaying to a constant positive value for positive times (Christensen 1982). This can be approximated with a discrete relaxation spectrum (Liu et al. 1976)

$$R(t) = \left[ M_R + \delta M \sum_{j=1}^{N} a_j e^{-\omega_j t} \right] H(t), \quad (3.2)$$

with $N > 0$ single peaks of strength $a_j > 0$, $\sum_j a_j = 1$ located at the relaxation frequencies $\omega_j > 0$.

This frequency dependence can be interpreted using mechanical models with combinations of springs and dash-pots such as the generalized Maxwell or Zener bodies. As shown by Moczo and Kristek (2005), these two interpretations lead to different parametrization of the medium, but result in the same mechanical behaviour. The relation between the parameter sets in the Maxwell ($a_j$ and $\omega_j$) and Zener body ($\tau_{\epsilon j}$ and $\tau_{\sigma j}$, the strain and stress relaxation times) representation is linear and can be found by comparing Eq. (8) in Blanch et al. (1995) and Eq. (11) in Emmerich and Korn (1987):

$$a_j \frac{\delta M}{M_R} = \frac{\tau_{\epsilon j}}{\tau_{\sigma j}} - 1, \quad \omega_j = \frac{1}{\tau_{\sigma j}}. \quad (3.3)$$

In this paper, we will use the Maxwell body notation as introduced by Emmerich and Korn (1987), but the results can be directly applied to the Zener body formulation using the above relations. Using the discrete relaxation spectrum, the resulting stress-strain relation can be written as

$$\sigma(t) = M_U \epsilon(t) - \sum_{j=1}^{N} \zeta_j(t), \quad (3.4)$$
where influence of the strain history on the current state of the material is encoded in the 'memory variables' \( \zeta^j \). The memory variables obey the \( N \) differential 'memory variable equations'

\[
\dot{\zeta}^j(t) + \omega_j \zeta^j(t) = a_j \omega_j \delta M \epsilon(t),
\]

that are driven by the strain of the medium \( \epsilon(t) \). The resulting frequency dependent modulus and quality factor \( Q \) are (Emmerich and Korn 1987):

\[
M(\omega) = M_R + \sum_j a_j \delta M \frac{i\omega}{i\omega + \omega_j},
\]

\[
Q^{-1}(\omega) = \frac{\text{Im} M}{\text{Re} M} = \frac{\delta M}{M_R} \frac{1}{1 + \frac{\delta M}{M_R} \sum_j a_j \frac{\omega}{\omega_j} \frac{1}{1 + \left(\frac{\omega}{\omega_j}\right)^2}},
\]

Arbitrary frequency dependency of \( Q \) can hence be approximated by a sum of absorption bands (see Fig. 3.2), by tuning the \( 2N \) parameters of the discrete relaxation spectrum \( a_j \) and \( \omega_j \). This is one nonlinear optimization problem for each set of \( Q \) and \( M \) in the model. It is important to note that this optimization is subject to the additional nonlinear constraint \( a_j > 0 \) (equivalent \( \tau_e > \tau_\sigma \) for the Zener model, compare Carcione (2007), Eq. (2.169) and (2.193)).

An important consequence of causality are the Kramers-Kronig relations stating that the real and imaginary part of \( M(\omega) \) are related by Hilbert transforms. The medium is therefore fully described by either the modulus or the phase velocity at a reference frequency \( \omega_r \), and the quality factor in the frequency range of interest \( Q(\omega) \), which in practice is often assumed to be constant or obey a power law.

Given the modulus or phase velocity at a reference frequency \( \omega_r \) inside the frequency range where \( Q \) is optimized, \( \delta M \), \( M_R \) and \( M_U \) can be found by evaluating Eq. 3.6 at this frequency. As \( \delta M \) is unknown before the optimization, a change of variables is necessary defining new coefficients \( y_j = \frac{\delta M}{M_R} a_j \). Then, with the \( y_j \) found by optimization, we can find

\[
\gamma := \frac{1}{\sum_j y_j} \sum_j y_j \frac{\omega_j^2}{\omega_r^2 + \omega_j^2}
\]

\[
\delta M = \text{Re} M(\omega_r) \left( \frac{1}{\sum_j y_j} + 1 - \gamma \right)
\]
3.2. Theory

![Inverse quality factor $Q^{-1}$ and real part of the modulus $M$ for a medium with 3 standard linear solids (see Eqs. (3.6) and (3.7)). Dashed red lines indicate contributions from the individual linear solids, black solid lines the sum. Arbitrary frequency dependency (here: constant $Q / \log$ in a limited frequency range) can be approximated by a sum of absorption bands. In the limit of large $Q$ these take the form of Debye functions.]

$$M_U = \text{Re} M(\omega_r) + \gamma \delta M$$
$$M_R = \text{Re} M(\omega_r) - (1 - \gamma)\delta M.$$  

(3.8)

A basic question is then what criterion to use in order to find the parametrization of the medium for a numerical solution to the wave equation. We strive to optimize this procedure by means of the maximal error tolerance in the wavefield as defined by amplitude and phase error estimates in the next section.
3.2.2. Optimal Q Parametrization

In this section, we analyze the influence of deviations in $M(\omega)$ and $Q(\omega)$ on the wavefield. As discussed above, the optimization problem of finding the best set of $2N$ parameters is inherently nonlinear (also for large $Q$ due to the free choice of relaxation frequencies) and has a nonlinear constraint. Taking this as given, choosing a nonlinear optimization approach such as simulated annealing also enables the free choice of optimization criteria. The goal of this section is to find such a criterion for finding the material parametrization for the discrete relaxation spectrum that minimizes the error in the wavefield.

We analyze the performance of different medium parametrizations using the dissipation operator (Müller 1983) in the approximation for large $Q$ as suggested by Emmerich and Korn (1987):

$$D(\omega) = \exp \left[ i\omega T_r \left( 1 - \sqrt{\frac{|M_r|}{M(\omega)}} \right) \right]. \quad (3.9)$$

Here $T_r$ and $M_r = M(\omega_r)$ denote the traveltime and the modulus at the reference frequency $\omega_r$. The anelastic response is then found by convolving the elastic response computed using the medium properties at the reference frequency with this dissipation operator. To evaluate the influence of errors in the representation of the medium, we separate amplitude and phase effects by writing this operator as

$$D(\omega) = A(\omega) e^{i\phi(\omega)}. \quad (3.10)$$

In the case of large $Q$, these can be approximated with $M = M_1 + iM_2 = M_1(1+i/Q)$ as:

$$A(\omega) \approx \exp \left( -\frac{1}{2} \frac{\omega T_r}{Q(\omega)} \sqrt{\frac{|M_r|}{M_1(\omega)}} \right) \quad (3.11)$$

for the amplitude and

$$\phi(\omega) \approx \omega T_r \left( 1 - \sqrt{\frac{|M_r|}{M_1(\omega)}} \right) \quad (3.12)$$
Figure 3.3.: Given acceptable amplitude (top) or phase (bottom) error, what are the requirements for the parametrization of the anelastic medium in terms of acceptable error in quality factor $Q$ and modulus $M$ for a range of number of traveled wavelengths $n_\lambda$. Shaded areas indicate typical global body waves, i.e. $t^* = 1 - 4 \, \text{s}$, period $1 - 10 \, \text{s}$, traveltime $1000 - 2000 \, \text{s}$. Note the different scales on the y-axis.
for the phase. The relative error in $Q$ is typically an order of magnitude larger than the relative error in $M_1$. This can be seen from Eqs. 3.6 and 3.7: while $Q^{-1}$ depends in first order on the frequency, $M$ is a constant plus a small frequency dependent term. Then, the first-order effect of amplitude and phase errors in the medium parametrization can be found as

$$\frac{\Delta A}{A} = \frac{1}{4\pi} \frac{\Delta Q}{Q} n_\lambda n_\lambda$$

(3.13)

and

$$\Delta \varphi = -\frac{1}{4\pi} \frac{\Delta M_1}{M_1} n_\lambda,$$

(3.14)

where $n_\lambda$ denotes number of wavelengths traveled and $\frac{\Delta Q}{Q}$ and $\frac{\Delta M_1}{M_1}$ are the relative errors in quality factor and real part of the modulus. As expected intuitively, the phase error is determined by the error in the real part of the modulus, which for large $Q$ dominates the phase velocity, while the error in amplitude is determined by the error in $Q$.

Fig. 3.3 shows how the acceptable errors in the real part of the modulus and $Q$ can be determined based on the phase and amplitude errors that are acceptable in a given application. E.g. for global high-frequency body waves ($t^* = T_r/Q = 4s$, $n_\lambda = 1000$) and an acceptable error of a few percent in phase and amplitude, we conclude that $Q$ should be approximated to well below 1% and the modulus below 0.03%. In contrast, the same seismic phase observed at lower frequencies, i.e. smaller $n_\lambda = 100$ as typically used in full 3D global simulations, is well represented with an errors in $Q$ and modulus that are ten times larger.

Optimization Criteria and Variables

It is common practice (Emmerich and Korn 1987; Blanch et al. 1995; Komatitsch and Tromp 2002a; Kristek and Moczo 2003; Graves and Day 2003; Käser et al. 2007; Savage et al. 2010) to find the medium parametrization $a_j, \omega_j$ by choosing the relaxation frequencies $\omega_j$ a priori, mostly logarithmically spaced in the frequency range of interest. Then, the $a_j$ can be found by sampling $Q(\omega)$ at a finite number of frequencies $\omega_k$ and solving an overdetermined inverse problem. We propose the following threefold strategy to improve the parametrization: 1) we suggest a specific choice of the norm for the afore-mentioned inverse problem, 2) we argue that it is
3.2. Theory

crucial not to choose the $\omega_j$ a priori, but to invert for them and 3) to fit the medium more accurately at the higher frequencies.

As can be seen from Eq. (3.11), variations in $Q$ affect seismogram amplitudes exponentially. The logarithmic error in the amplitude is therefore of the same size when $Q$ is multiplied or divided by a constant. Also, $Q$ is always positive, which motivates usage of the logarithmic error for $Q$ instead of the plain $l^2$-norm. While in the limit of small deviations these two norms are asymptotically identical, the log-$l^2$ norm emphasizes negative deviations from the optimal $Q$ that are larger than a few percent. Eqs. (3.13) and (3.14) also show that high-frequency waves that have traveled more wavelengths are more sensitive to errors in the parametrization with the factor $n_\lambda$. This motivates a linear weighting of the frequencies and we suggest to minimize

$$
\epsilon^2 = \int \left( \frac{\ln(Q_{\text{target}})}{\ln(Q_{\text{ls}})} \right)^2 \cdot w(\omega) \, d\ln \omega,
$$

where $Q_{\text{target}}$ and $Q_{\text{ls}}$ are the exact quality factor and its approximation by the linear solid from Eq. (3.7). The weights $w(\omega)$ are set to 1 by most authors (compare citations in the first paragraph of this section), the linear frequency weighting we suggest is $w(\omega) = \omega$. For the error in the real part of the modulus we use the standard $l^2$-norm, as the relative errors are very small anyway.

Fig. 3.4 visualizes the importance of including the relaxation frequencies in the optimization: for log-spaced fixed frequencies, the discretization of the medium does not converge towards the analytical behaviour, neither for increased $N$ nor for smaller bandwidth for which the medium is optimized. This is in contrast to the finding by Savage et al. (2010), Fig. 2, whose results we are only able to reproduce when ignoring the constraint $a_j > 0$. For applications where fitting of $Q$ better than 1% is needed (this is low $Q$ or many wavelength propagation as for global high-frequency body waves, compare Fig. 3.3), inversion for the relaxation frequencies is inevitable. This nonlinear optimization problem with $2N$ parameters can effectively be solved by a simulated annealing approach within seconds using $10^5$ to $10^7$ iterations for $N \leq 6$, this was also suggested by Liu and Archuleta (2006).

Fig. 3.5 shows three examples of seismograms calculated with different media representations that have the same numerical complexity in time-domain wave-propagation solvers due to the same number of memory variables. Both the reference solution and the approximations are calculated using the dissipation operator, the difference is only in $M(\omega)$. The first column represents the standard method of
choosing the relaxation frequencies of the absorption bands log-spaced. Inverting for the frequencies can reduce both the misfit in $Q$ and consequently phase and amplitude errors of the seismograms in all frequency bands by factors of 2-4 (second column). Additional frequency weighting reduces the phase and envelope misfit by another factor of 2 in the highest frequency band at the cost of worse fit in the lower frequency range (third column), resulting in same order of magnitude misfits in all frequency bands.

The Modulus

From the examples in Fig. 3.5, it can be observed that even when fitting $Q(\omega)$ with high accuracy for the high frequencies, the modulus has a maximum in the relative error close to the bounds of the frequency band. This can be understood from a relation between $Q$ and the modulus that is valid in the approximation of large and almost constant $Q$ (Dahlen and Tromp 1998, Eq. (6.75)):
\[
\frac{\partial \ln M_1(\omega)}{\partial \ln \omega} \approx \frac{2}{\pi Q(\omega)}. \tag{3.16}
\]

Thus, the modulus takes a maximum in its derivative at the peaks of \(Q(\omega)\). Another disadvantage of optimizing \(Q\) only is that the choice of the reference frequency where the modulus is known has an important effect: if it coincides with one of the maxima of the approximation of the modulus, the average value of \(M_1\) and hence the phase velocity are skewed. This can be avoided by relaxing the requirement that the approximate modulus matches the reference exactly at the reference frequency. Instead the ratio \(M_R/M_1(\omega_r)\) can be added as a parameter to the inverse problem. \(M(\omega)\) can be found via the Kramers-Kronig relations, either by numerical evaluation or analytical e.g. for constant \(Q\) (Kjartansson 1979)

\[
M(\omega) = M(\omega_r) \left( \frac{i\omega}{\omega_r} \right) \frac{2}{\pi} \tan^{-1} Q^{-1}. \tag{3.17}
\]

The fit of \(M_1\) can then be added to the inverse problem with a weighting relative to the fit of \(Q\). Fig. 3.6 shows an example, where the reference frequency was chosen particularly inappropriate \((f_r = 2 \text{ Hz})\), at the upper limit of the frequency range. If the modulus is determined by setting it to the reference value at the reference frequency, its average value is too low, leading to large phase errors. Adding the real part of the modulus to the optimization criterion circumvents this problem and makes the result independent of the choice of the reference frequency, while keeping essentially the same \(Q(\omega)\) (green). Additionally, the parametrization can be tuned towards lower amplitude or phase errors by the weighting between \(Q\) and \(M_1\) in the optimization criterion (red).

### 3.2.3. Determination of the Optimal Structural Parameters in Full-Scale Applications

In full seismic applications, the material parameters \(a_j\) and \(\omega_j\) need to be determined for many values of \(Q\) and seismic velocities, typically for each spatial grid point, i.e. \(10^6 \sim 10^9\) times. The performance of an algorithm to find them is thus important and several approaches have been suggested.

For large \(Q\)-values, Eq. (3.7) can be linearized by realizing that \(\delta M/M_R\) becomes small:
Figure 3.5.: Influence of the parametrization of the medium on the accuracy of the seismograms simulated with dissipation operators for $t^* = 4$ s (typical for teleseismic $S$ waves, see e.g. Nolet 2008) while keeping the complexity of the parametrization constant (3 absorption bands). Left to right: relaxation frequencies fixed log-spaced in the frequency band of interest (2.3 decades), optimized frequencies using simulated annealing, additional linear weighting with the frequency. Top to bottom: seismograms filtered with Gabor-bandpass filters with center period $T_c$, quality factor $Q$, modulus $M$ and relative error of the modulus as approximated with standard linear solids. $EM$ and $PM$ denote the envelope and phase misfit (Kristekova et al. 2009). Shaded region indicates the frequency range used in the parameter optimization, vertical dashed lines the relaxation frequencies $\omega_j$ and solid black lines the reference medium. Optimization criterion was the log-l2 error of $Q$, see text for details. Note the large deviations of the optimal value in the modulus at the boundaries of the frequency range.

\[ Q^{-1}(\omega) \approx \frac{\delta M}{M_R} \sum_j a_j \frac{\omega/\omega_j}{1 + (\omega/\omega_j)^2}. \]  

This was proposed by Emmerich and Korn (1987) and became more popular later named the ‘$\tau$-method’ by Blanch et al. (1995). The advantage of this method is that it results in only one inverse problem while finding the parameters for different $Q$ is trivial due to the linearity of $a_j$ in $Q^{-1}$. For low values of $Q$, this approximation introduces a logarithmic error to the resulting approximation of constant $Q$, see blue curve in Fig. 3.7. The largest error shows up at the high-frequency end of the frequency range of interest, i.e. where the wavefield is most sensitive to such errors, see above. Furthermore, this problem becomes more dominant with increasing bandwidth.

Often, the relaxation frequencies $\omega_j$ are not inverted for, but fixed log-spaced, since this allows for a linear (hence faster) inversion for the parameters $a_j$ as suggested by Emmerich and Korn (1987) by rearranging terms in Eq. (3.7). Similarly, Savage et al. (2010) use log-spaced frequencies, but a simplex approach for the non-linear inversion and suggest to use a look-up table to solve fewer inverse problems. However, these methods cannot handle the constraint $a_j > 0$. Liu and Archuleta (2006) present empirical formulae to interpolate the parameters between the largest and smallest value of $Q$ in the model and use a simulated annealing approach to solve the remaining two inverse problems. As they do not present a closed form to
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Figure 3.6.: Optimized constant $Q \approx 250$ (black) versus simultaneous optimization of $Q$ and real part of the modulus $M_1$ (red + green) using the relation by Kjartansson (1979) for a medium with 3 absorption bands: additional optimization of the modulus makes the parametrization independent of the choice of the reference frequency (here: $f_r = 2$ Hz) and allows for tuning the parametrization towards lower phase errors at the boundaries of the frequency range (red) or lower amplitude errors (green). Vertical dashed lines indicate the relaxation frequencies $\omega_j$. Frequency weighting was not used for clarity.

find the coefficients in their interpolation, their formulae can only be used for their specific setup of frequency range, number of absorption bands $N$ and $Q$ range.

Here, we suggest a correction to the linearization as an easy-to-implement and computationally light method, combining the advantages of the linearization (‘$\tau$-method’) with increased accuracy for low $Q$. As this results in a single inverse problem, the relatively expensive simulated annealing method can be used allowing to invert for the relaxation frequencies as well as including the constraint $a_j > 0$. 

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This correction can be found by realizing that the discrete relaxation frequencies are widely spaced, hence

\[
\frac{\omega_k/\omega_j}{1 + (\omega_k/\omega_j)^2} \approx \frac{1}{2} \delta_{jk} \quad (3.19)
\]

and

\[
\frac{(\omega_k/\omega_j)^2}{1 + (\omega_k/\omega_j)^2} \approx \begin{cases}
0, & (\omega_k < \omega_j) \\
\frac{1}{2}, & (\omega_k = \omega_j) \\
1, & (\omega_k > \omega_j).
\end{cases} \quad (3.20)
\]

Then, we insert these approximations into the exact relation for \(Q^{-1}\) (Eq. (3.7)) evaluated at the relaxation frequencies \(\omega_j\). Comparison to the linearized version...
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Figure 3.8.: Recursive correction for the coefficients $y_j$ as in Eq. (3.21): Frequency-weighted log l2 error in Q as a function of Q for the linearization (dashed), the correction (solid) and the exact (dotted) relation.

Eq. (3.18) leads to a correction factor for each $a_j$ due to the term in the denominator neglected in the linearization. These factors can be defined recursively starting from the lowest absorption frequency $\omega_0$ with $y_j$ as defined above:

\[
\text{recursion:} \begin{cases} 
\delta_0 &= 1 + \frac{1}{2} y_0 \\
\delta_{n+1} &= \delta_n + \left( \delta_n - \frac{1}{2} \right) y_n + y_{n+1}
\end{cases}
\]

\[y_j' = \delta_j \cdot y_j.\]  (3.21)

The performance of this correction is visualized in Figs. 3.7 and 3.8. Fig. 3.7 compares $Q$ computed using corrected parameters to the linearization and the exact result for $Q = 20$. While the linearization causes an error of almost 20% in the high frequencies, the corrected version is still quite close to the optimal solution using the exact relation. Fig. 3.8 shows tests of the approximation as a function of $Q$ for a variety of different bandwidths and numbers of absorption bands in terms of the frequency weighted log-l2 error as defined above. The more accurate the approximation of constant $Q$ is desired, the higher the $Q$-value where the linearization breaks down: e.g. at 2.2 decades bandwidth and using 3 absorption bands (red), the linearization (dashed) doubles the error for $Q$-values lower than 90, while the
corrected ones hit this error bound only for $Q < 10$. On the global scale, where $Q$ typically takes values larger than 50, this scheme allows to find the parameters $a_j$ efficiently with very high accuracy. This correction scheme has negligible computational imprint such that it may be used in the time loop which means that the $2N$ coefficients $a_j$ and $w_j$ need to be stored only once and not for each grid point.

**Frequency Dependent $Q^*$**

While $Q$ is mostly assumed to be independent of frequency in seismic wave propagation, the correction scheme proposed above also works for weakly frequency dependent cases. One common model is the power law

$$Q = Q_0 \left( \frac{\omega}{\omega_0} \right)^\alpha,$$  \hspace{1cm} (3.22)

where typical values of $\alpha$ are in the range $-0.4$ to $0.4$ (Lekić et al. 2009) and $Q_0$ is the value of $Q$ at the reference frequency $\omega_0$. Fig. 3.9 shows an example for

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*These subsections are new compared to the GJI version of the manuscript*
$Q_0 = 10$, $\omega_0 = 2\pi \cdot 10^{-3} \text{s}$ and $\alpha = 0.3$. The correction performs similarly well as in the frequency independent case.

**Fréchet Derivatives**

The approach to calculate Fréchet derivatives for $Q$ as proposed in appendix A requires the computation of partial derivatives of the coefficients $y_j$ that parameterize the $Q$-model with respect to the physical quantities $Q_0$ and $\alpha$. In appendix A we computed these coefficients for finite $Q$ values using a simulated annealing approach and finding a compromise for all values of $Q$ in the model. In that case, the coefficients were linear with respect to $Q_0$ and the partial derivative hence trivial. By using the recursive correction proposed here for moderate values of $Q$, we have an analytically closed form and can hence also find the derivatives of the corrected coefficients analytically.

For Fréchet derivatives with respect to $Q_0$, only the term $\frac{\partial y_j'}{\partial Q_0}$ is needed. Because of the linearity of the $y_j$ in $Q_0$:

$$\frac{\partial y_j}{\partial Q_0} = -\frac{y_j}{Q_0},$$ (3.23)

so for the corrected $y_j' = \delta_j y_j$

$$\frac{\partial y_j'}{\partial Q_0} = -\delta_j \frac{y_j}{Q_0} + y_j \frac{\partial \delta_j}{\partial Q_0},$$ (3.24)

where the derivatives of $\delta_j$ can be found from the recursion

recursion: $\left\{ \begin{array}{l} \frac{\partial \delta_0}{\partial Q_0} = -\frac{y_0}{2Q_0} \\ \frac{\partial \delta_{n+1}}{\partial Q_0} = \frac{\partial \delta_n}{\partial Q_0} (1 + y_n) - \left( \delta_n - \frac{1}{2} \right) \frac{y_n}{Q_0} - \frac{y_{n+1}}{Q_0} \end{array} \right.$ (3.25)

For Fréchet derivatives with respect to the exponent $\alpha$, we additionally need the partial derivatives $\frac{\partial y_j'}{\partial \alpha}$. In appendix A, we found these using finite differences by optimizing the coefficients $y_j$ for slightly perturbed values of $\alpha$. Here, we can find the $\frac{\partial y_j}{\partial \alpha}$ by equating the analytical expression for $Q_{\text{target}}$ and the linear large $Q$ approximation for the linear solids. Then, we evaluate the equation at a set of frequencies $\omega_k$ within the frequency range of interest to find a linear set of $k$ equations. Using
3.2. Theory

A number of equations $k$ that is larger than the number of unknowns, the solution is overdetermined and can be found by matrix inversion:

$$\sum_j \frac{\omega_k}{\omega_j} \frac{\partial y_j}{\partial \alpha} \approx Q_0^{-1} \left( \frac{\omega_r}{\omega_k} \right)^\alpha \ln \alpha. \quad (3.26)$$

Once the $\frac{\partial y_j}{\partial \alpha}$ are known, we can find the derivative of the corrected coefficients as

$$\frac{\partial y_j'}{\partial \alpha} = -\delta y_j + y_j \frac{\partial \delta_j}{\partial \alpha}, \quad (3.27)$$

where the derivatives of $\delta_j$ again can be found from the recursion

$$\text{recursion: } \begin{cases} \frac{\partial \delta_0}{\partial \alpha} = \frac{1}{2} \frac{\partial y_0}{\partial \alpha} \\ \frac{\partial \delta_{n+1}}{\partial \alpha} = \frac{\partial \delta_n}{\partial \alpha} (1 + y_n) + \left( \delta_n - \frac{1}{2} \right) \frac{\partial y_n}{\partial \alpha} + \frac{\partial y_{n+1}}{\partial \alpha}. \end{cases} \quad (3.28)$$

The advantage of this correction scheme is that there is no need to find a compromise in the parameterization of the medium with respect to different values of $Q$ in the model. As long as the approximation used in the iterative correction is valid (see Fig. 3.8), the partial derivatives can be computed at the actual value of $Q$ as a function of space.

3.2.4. Analytic Time Stepping

Many discrete schemes have been proposed to integrate the memory variable equation eq. (3.5) over time to determine the values of the memory variables at the next time step: e.g. finite-differences (Day and Minster 1984), some unspecified second-order scheme (Emmerich and Korn 1987), second-order central difference (Kristek and Moczo 2003), ADER (Käser et al. 2007) or fourth-order Runge-Kutta (Komatitsch and Tromp 2002b; Savage et al. 2010). To our best knowledge, integrating the equation analytically has not been published in the seismological community.

The ’memory variable’ equation is an ODE of the form

$$\dot{\zeta}_j(t) + \omega_j \zeta_j(t) = s_j(t), \quad (3.29)$$
with \( s^j(t) = a_j \omega_j \delta M \epsilon(t) \). This can be solved by the standard method of multiplication with an integrating factor and the solution is:

\[
\zeta^j(t + \Delta t) = e^{-\omega_j \Delta t} \left[ \zeta^j(t) + \int_t^{t+\Delta t} s^j(t') e^{\omega_j (t-t')} dt' \right].
\] (3.30)

The integral can then be solved depending on the global time scheme and the corresponding time dependence of \( s(t) \). For example, if the elastic equations are time integrated with a second-order scheme, where \( s(t) \) is known at two times only (with linear interpolation: \( s(t') = s(t) + \frac{t'-t}{\Delta t} (s(t+\Delta t) - s(t)) \)) the resulting discrete scheme is:

\[
\zeta^j(t + \Delta t) = \zeta^j(t) e^{-\omega_j \Delta t}
+ \frac{s^j(t)}{\omega_j} \left[ \frac{1}{\omega_j \Delta t} (1 - e^{-\omega_j \Delta t}) - e^{-\omega_j \Delta t} \right]
+ \frac{s^j(t + \Delta t)}{\omega_j} \left[ 1 - \frac{1}{\omega_j \Delta t} (1 - e^{-\omega_j \Delta t}) \right].
\] (3.31)

Expanding the exponential functions in series, this agrees with the Runge-Kutta scheme by Savage et al. (2010) up to the fourth-order in \( \omega_j \Delta t \). In contrast to numerical integration schemes, the accuracy of this analytical scheme is only bounded by the accuracy of the source term (i.e. the elastic strain), which is determined by the time scheme used for the elastic equations. Thus, our formulation automatically ties the viscoelastic accuracy to that of the global time scheme.

### 3.2.5. Generalization to 3D

Generalization to three dimensions is rather straightforward and extensive literature is available, e.g. Carcione (2007) and references therein. We restrict ourselves to slightly anisotropic media, where the effect of attenuation can still be treated as isotropic and the anisotropy of attenuation is neglected as a second-order effect. In this case, the Eigenstrains and Eigenstiffnesses are easy to find as dilation and shear stresses and the stress strain relationship remains simple and computationally light, see e.g. Carcione (1994). The validity of this approximation for global radial anisotropy as in PREM is verified by the benchmark in section 3.5.
3.3. AxiSEM Discretization

Many authors neglect the effect of bulk attenuation and take advantage by splitting the memory variable into the shear and bulk contribution such that only 5 instead of 6 memory variables for each absorption band are needed. However, this is no good approximation when there is significant contribution of the bulk quality factor $Q_\kappa$ to the P-wave quality factor $Q_p$ (e.g. Stein and Wyssession 2003, 3.7.6):

$$Q_p^{-1} = LQ_\mu^{-1} + (1 - L)Q_\kappa^{-1}, \quad (3.32)$$

$$L = \frac{4}{3} \left( \frac{v_s}{v_p} \right)^2. \quad (3.33)$$

E.g. in the PREM model (Dziewoński and Anderson 1981) this is the case in the inner core, where $Q_\kappa = 1327$ has a significant effect (around 30%) on $Q_p$. Although there is no general agreement about the location of bulk attenuation in Earth, it is needed to simultaneously fit high $Q$ radial mode data and surface wave data (Romanowicz and Mitchell 2007). Hence we choose to keep the full 6 degrees of freedom and write the 3D memory variable equation as:

$$\dot{\zeta}_l^j(t) + \omega_j \zeta_l^j(t) = \begin{cases} 
\delta \kappa a_j^\epsilon \omega_j \text{tr } \epsilon + \frac{2}{3} \delta \mu a_j^\mu \omega_j (3\epsilon_l - \text{tr } \epsilon), & (l = 1, 2, 3) \\
\delta \mu a_j^\mu \omega_j \epsilon_l, & (l = 4, 5, 6) 
\end{cases} \quad (3.34)$$

with index $l$ denoting components in the Voigt notation (index mapping: $1 \rightarrow 11, 2 \rightarrow 22, 3 \rightarrow 33, 4 \rightarrow 23, 5 \rightarrow 31, 6 \rightarrow 12$). Importantly, using the scheme from above to find the medium parameters, $\omega_j$ are the same for bulk and shear $Q$, while the $a_j$ are found depending on the actual value of $Q_\kappa$ and $Q_\mu$. Identifying the right hand side with $s(t)$ from Eq. (3.29), the analytical time stepping can readily be used in 3D.

3.3. AxiSEM Discretization

In this section, we use AxiSEM (Nissen-Meyer et al. 2014) as an example and generalize the derivation of the equations of motions of the reduced 2D equations in the weak form to include attenuation. The elastic anisotropic problem is treated by van Driel and Nissen-Meyer (2014b) and the basic framework is derived in detail by Nissen-Meyer et al. (2007a, 2007b, 2008). The reduced 2D equations are found by projecting the wave equation onto test functions having the azimuthal dependence of monopole, dipole and quadrupole sources. Taking the dot product of the wave
3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media

Figure 3.10.: The cylindrical coordinate system \((s, \varphi, z)\) and the reduced semicircular 2D domain \(\Omega_D\) for global wave propagation in axisymmetric media.

The equation with a test function \(w\), integrating over the domain \(\Omega\) and using partial integration and the free surface boundary condition yields

\[
\int_{\Omega} \left( \rho w \cdot \ddot{u} + \nabla w : \sigma \right) \, d\Omega = \int_{\Omega} w \cdot f \, d\Omega, \tag{3.35}
\]

with the visco-elastic constitutional relation

\[
\sigma = \sigma^{\text{el}} + \sigma^{\text{anel}} = c_U : \epsilon - \zeta. \tag{3.36}
\]

Here \(\zeta := \sum_{j=1}^{N} \zeta^j\) denotes the total stress contribution of all memory variables. As shown by Nissen-Meyer et al. (2007a) for spherically symmetric models and generalized to anisotropic axisymmetric models by van Driel and Nissen-Meyer (2014b), the displacement in an axisymmetric model can be expanded in the series
3.3. AxiSEM Discretization

\[ u(s, z, \varphi) = \sum_{m=-\infty}^{\infty} \left[ u^m_s(s, z) \hat{e}_s(\varphi) + u^m_\varphi(s, z) \hat{e}_\varphi(\varphi) + u^m_z(s, z) \hat{e}_z \right] e^{im\varphi}, \quad (3.37) \]

where \( s, \varphi, z \) are the cylindrical coordinates as in Fig. 3.10. In the case of a moment tensor or single force point source on the symmetry axis, all contributions for \( |m| > 2 \) vanish. Equivalent expressions with \( \sin \varphi \) and \( \cos \varphi \) can be found by summing over pairs of \( \pm m \) and using the fact that \( u \) is real. For monopole, dipole and quadrupole sources this results in

\[ u^m = [u^m_s \hat{e}_s + u^m_z \hat{e}_z] \cos(m\varphi + \varphi_0) - u^m_\varphi \sin(m\varphi + \varphi_0) \hat{e}_\varphi, \quad (3.38) \]

where \( \varphi_0 \) depends on the orientation of the source. The reduced equations of motion can then be found by inserting this into eq. (3.35) and evaluating the integral in \( \varphi \) analytically.

3.3.1. Angular Dependence and Axial Boundary Conditions of the Memory Variables

As the initial condition for the memory variables is \( \zeta = 0 \) and the memory variable equation is linear, the angular dependence is determined by the source terms in Eq. (3.34). The angular dependence of the strain can be found from Eq. (3.38) and we find

\[ \zeta_l(s, \varphi, z) = \begin{cases} 
\zeta_l(s, z) \cdot \cos(m\varphi + \varphi_0) & (l = 1, 2, 3, 5) \\
\zeta_l(s, z) \cdot \sin(m\varphi + \varphi_0) & (l = 4, 6), 
\end{cases} \quad (3.39) \]

where \( m = 0, 1, 2 \) for monopole, dipole and quadrupole sources respectively. With the same argumentation, the behaviour of the memory variables at the axis can be analyzed based on the behaviour of the strain at the axis (Nissen-Meyer et al. 2007a). For the quadrupole case, \( \zeta_4 \) and \( \zeta_5 \) vanish at the axis with \( \mathcal{O}(s) \), the others and in the case of monopole and dipole source all memory variables take finite values at the axis. These boundary conditions are needed to evaluate the Gauss-Jacobi quadrature at the axis in section 3.3.3.
3.3.2. Anelastic Stiffness Terms in the Weak Form

The elastic stiffness terms $\sigma^{\text{el}}$ remain the same as in purely elastic case, see van Driel and Nissen-Meyer (2014b), where the elastic moduli are replaced with the unrelaxed moduli. Additionally, the contribution of the memory variables to the stiffness can be found for the monopole source as:

$$
\frac{1}{2\pi} \int_{0}^{2\pi} \nabla w : \zeta \, d\varphi = \partial_s w_s \zeta_1 + \partial_z w_s \zeta_5 + \frac{w_s}{s} \zeta_2 + \partial_s w_z \zeta_5 + \partial_z w_z \zeta_3, \quad (3.40)
$$

Equivalent expressions for dipole and quadrupole sources can be found in appendix 3.7.1.

3.3.3. Spectral Element Discretization

The next step is to generalize the spatial discretization of the stiffness terms from the anisotropic elastic case presented in van Driel and Nissen-Meyer (2014b) to the anelastic case. The approach is the same as in the isotropic elastic case and we refer the reader to section 3 in Nissen-Meyer et al. (2007b) for details and restrict ourselves to a short summary of the method and important aspects of the notation in the interest of brevity. A more general and rigorous approach can be found in Bernardi et al. (1999).

The collapsed 2D domain $\Omega_D$ (Fig. 3.10) is divided into non-axial elements $\Omega_e$ and axial elements $\Omega_{\bar{e}}$. The mapping between reference coordinates $\xi, \eta \in [-1, 1]$ in each element and the physical coordinates $s, z$ is provided by the Jacobian determinant

$$
\mathcal{J}(\xi, \eta) = \det \begin{pmatrix} s_\xi & s_\eta \\ z_\xi & z_\eta \end{pmatrix}, \quad (3.41)
$$

where the subscript denotes partial differentiation, $s_\xi = \partial_\xi s$, etc. Both the test function $w$ and the field variables $u$ and $\zeta$ are expanded in Lagrangian polynomials $l_i$ of order $N_{gll}$ (defined on the integration points, see below) within each element as

$$
u^\alpha(\xi, \eta, t) = \sum_{i,j=0}^{N_{gll}} u_{ij}^\alpha(t) l_i(\xi) l_j(\eta),$$

where
3.3. AxiSEM Discretization

\[ \zeta_l(\xi, \eta, t) = \sum_{i,j=0}^{N_{\text{gll}}} \zeta^j_{i,l}(t) l_i(\xi) l_j(\eta), \]  

for each component \( \alpha \in (s, \varphi, z) \) and \( l \in \{1, \ldots, 6\} \) and equivalently to \( u \) for \( w \). For the axial elements \( \xi = 0 \) is the axis. The integral over the domain \( \Omega_D \) is then split into a sum of integrals over elements and approximated using the Gauss-Lobatto integration rule

\[ \int_{\Omega_e} u(s, z) s \, ds \, dz \approx \sum_{pq} \sigma_p \sigma_q s(\xi_p, \eta_q) u_{pq} J(\xi_p, \eta_q) \]  

with Gauss-Lobatto-Legendre (GLL) integration weights \( \sigma_p \) and integration points \( \xi_p \) and \( \eta_q \). For the axial elements, Gauss-Lobatto-Jacobi (GLJ) quadrature is used for the \( \xi \)-direction with

\[ \int_{\Omega_{\bar{\xi}}} u(s, z) s \, ds \, dz \approx \sum_{pq} \bar{\sigma}_p (1 + \bar{\xi}_p)^{-1} \sigma_q s(\bar{\xi}_p, \eta_q) u_{pq} J(\bar{\xi}_p, \eta_q) \]  

and GLJ integration weights \( \bar{\sigma}_p \), integration points \( \bar{\xi}_p \) and the Lagrangian interpolation polynomial on these points \( \bar{l}(\xi) \). This allows to use l’Hospital’s rule to calculate derivatives at the axis where needed.

Applying this discretization to Eq. (3.35), choosing the set of test functions to be 1 in one component at a specific integration point and 0 at the others and summing over all elements we obtain the global set of ordinary differential equations in time

\[ M \ddot{u}(t) + Ku(t) - z(t) = f(t), \]  

with the global mass matrix \( M \), stiffness matrix \( K \) and the additional anelastic stiffness vector \( z \). While the assembled mass matrix is diagonal in the GLL/GLJ basis (hence trivial to invert), it is unnecessary to compute \( K \) explicitly and we only evaluate its action on the displacement (\( Ku \)). This term only appears on the right hand side of the second-order system

\[ \dot{u}(t) = M^{-1} [f(t) - Ku(t) + z(t)], \]  

with l’Hospital’s rule to calculate derivatives at the axis where needed.
which is solved by explicit numerical time integration schemes, additional to the memory variable equation Eq. (3.34). The stiffness terms $K\mathbf{u}$ and $\mathbf{z}$ are computed in each element first and the global stiffness is assembled subsequently (Nissen-Meyer et al. 2007b, section 4).

We split the original elemental stiffness integral into contributions from each component of the vectorial test function $\mathbf{w}$, denoted by the subscripts $s$ and $z$. Furthermore, we revert to a tensorial notation instead of elemental sums and define the matrix-matrix products

$$X = \mathbf{A} \otimes \mathbf{B} : \quad X_{ij} = \sum_k A_{ik}B_{kj}$$

(3.47)

$$X = \mathbf{A} \odot \mathbf{B} : \quad X_{ij} = A_{ij}B_{ij}$$

(3.48)

and vector-matrix and vector-vector products

$$X^0 = \mathbf{A}^0 \otimes \mathbf{B} : \quad X^0_{0j} = \sum_k A^0_{0k}B_{kj}$$

$$X^0 = \mathbf{A}^0 \odot \mathbf{B}^0 : \quad X^0_{0j} = A^0_{0j}B^0_{0j}$$

$$X = \mathbf{A}^0 \mathbf{B}^0 : \quad X_{ij} = A^0_{i0}B^0_{0j}.$$  

(3.49)

The elemental anelastic stiffness can then be written in the monopole case as

$$\mathbf{z} = \mathbf{z}_s + \mathbf{z}_z$$

(3.50)

with the definitions from Table 3.1

$$\mathbf{z}_s = D_\xi \otimes \left( V_{z\eta} \odot \zeta_1 + V_{s\eta} \odot \zeta_5 \right) + \left( V_{z\xi} \odot \zeta_1 + V_{s\xi} \odot \zeta_5 \right) \otimes D^T_\eta + Y \odot \zeta_2$$

$$+ \delta_{ee}D^0_\xi \left[ V^0_{z\eta} \odot \zeta^0_1 + V^0_{s\eta} \odot \zeta^0_5 \right],$$

(3.51)

$$\mathbf{z}_z = D_\xi \otimes \left( V_{z\eta} \odot \zeta_5 + V_{s\eta} \odot \zeta_3 \right) + \left( V_{z\xi} \odot \zeta_5 + V_{s\xi} \odot \zeta_3 \right) \otimes D^T_\eta$$

$$+ \delta_{ee} \left\{ D^0_\xi \left[ V^0_{z\eta} \odot \zeta^0_5 + V^0_{s\eta} \odot \zeta^0_3 \right] + \left[ V^0_{z\eta} \odot \zeta^0_5 + V^0_{s\eta} \odot \zeta^0_3 \right] \otimes D^T_\eta \right\}.$$  

(3.52)

Here $\delta_{ee}$ is 1 in axial elements and 0 in all others and $\zeta^0_i$ is the vector of memory variables at the axis ($i = 0$). Equivalent terms for dipole and quadrupole case can be found in appendix 3.7.2.
3.4. Coarse-Grained Memory Variables

Table 3.1.: Definitions for precomputable matrices (i.e. prior to the costly time extrapolation) of the anelastic stiffness terms, $\pm$ takes its value depending on the combination of $x_\zeta$ as in the right table. Subscript reference coordinates denotes partial derivation, e.g. $x_\zeta = \partial_\zeta x$. For consistency with the summation notation in Nissen-Meyer et al. (2007a), we use indices $i,j$ and $I,J$, which all take the values in $\{0 \ldots N_{gl}\}$.

<table>
<thead>
<tr>
<th>Matrix</th>
<th>Non-axial elements</th>
<th>Axial elements ($i &gt; 0$)</th>
<th>($i = 0$)</th>
<th>Axial vectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(V_{x_\zeta})^{ij}$</td>
<td>$\pm\sigma_i\sigma_j x_\zeta^{ij} s^{ij}$</td>
<td>$\pm\bar{\sigma}_i\sigma_j (1 + \bar{\zeta}<em>i)^{-1} x</em>\zeta^{ij} s^{ij}$</td>
<td>0</td>
<td>$(V_{x_\zeta}^0)^j = \pm\bar{\sigma}<em>0\sigma_j x</em>\zeta^{0j} s_\zeta^{0j}$</td>
</tr>
<tr>
<td>$(Y)^{ij}$</td>
<td>$\sigma_i\sigma_j J^{ij}$</td>
<td>$\bar{\sigma}_i\sigma_j (1 + \bar{\zeta}_i)^{-1} J^{ij}$</td>
<td>0</td>
<td>$(Y^0)^j = \bar{\sigma}_0\sigma_j J^{0j}$</td>
</tr>
<tr>
<td>$(D_{\xi})^{Ii}$</td>
<td>$\partial_\xi l_i(\xi_i)$</td>
<td>$\partial_\xi \bar{l}_i(\bar{\xi}_i)$</td>
<td>$\partial_\xi \overline{\bar{l}}_i(\bar{\xi}_0)$</td>
<td>$(D_{\xi}^0)^I = \partial_\xi \overline{\bar{l}}_i(\bar{\xi}_0)$</td>
</tr>
<tr>
<td>$(D_{\eta})^{Jj}$</td>
<td>$\partial_\eta l_j(\eta_j) = \partial_\eta l_J(\xi_j)$</td>
<td>$\partial_\eta l_J(\eta_j)$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

| $\pm(x_\zeta)$ | $\zeta = \xi$ | $\zeta = \eta$ |
| $x = s$ | + | - |
| $x = z$ | - | + |

3.4. Coarse-Grained Memory Variables

In the following, we assume constant medium properties within each element. This assumption is used in the derivation of most spectral-element schemes, often without stating it explicitly. Empirically it is clear however, that correct results are obtained when this assumption is violated by small deviations only. We can then write the approximation of the theoretical or optimal modulus with standard linear solids as

$$M_{opt}(\omega) \approx M_r + \delta M(\omega), \quad (3.53)$$

with the reference frequency $\omega_r$ that should be within the frequency band of interest and the modulus at this frequency $M_r$, i.e. $\delta M(\omega_r) = 0$ (see Fig. 3.11 for a schematic sketch). This choice of reference is equivalent to the 'element specific modulus' by Graves and Day (2003), i.e. the unrelaxed modulus that is used for the elastic stiffness is not the reference and will hence be not constant over the element. The idea of coarse grained attenuation then is to find a medium where $\delta M$ is a function of
3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media

Figure 3.11.: Coarse grained attenuation schematically: constant $Q$ corresponds to $M_{\text{opt}}(\omega)$. The problem is to find $\delta M(\omega)$ using standard linear solids for the anelastic GLL points. The constraint is that averaged with the elastic GLL points with modulus $M_0$, the medium should behave as $M_{\text{opt}}(\omega)$ in the frequency range of interest (shaded in gray).

space with the constraints 1) that it behaves macroscopically as the homogeneous medium and 2) reduces the numerical burden. This calls for a method to compute the macroscopic behaviour of a medium with structure on the sub wavelength scale where the deviations are relatively small in amplitude.

In a seminal paper, Backus (1962) showed how to average a layered medium to find a homogeneous long-wavelength equivalent medium. A similar argument was introduced into the context of heterogeneous finite-difference methods by Boore (1972) and further developed by e.g. Zahradnik et al. (1993) and Moczo et al. (2002). In more recent developments of homogenization theory (e.g. Capdeville et al. 2010; Guillot et al. 2010), more rigorous analytical arguments are raised and in the 1D case, it can be shown analytically that the correct way of averaging the modulus is the harmonic average (Cioranescu and Donato 1999). Graves and Day (2003) show that harmonic averaging also yields better results than arithmetic averaging in the context of the coarse grained memory variables in the case of small values of $Q < 20$ (where $\delta M$ is relatively large) and yields the same results as arithmetic averaging if $Q > 20$. Although $Q$ is larger than 50 for most global models, it is not obvious to generalize this conclusion to global body waves, because the test cases presented by Graves and Day (2003) are dealing with an order of magnitude less wavelengths
3.4. Coarse-Grained Memory Variables

propagation distance (compare section 3.2.2). Hence we try arithmetic averaging first because of its simplicity and benchmark it in the next section, finding that it does suffice for global high-frequency body waves.

In the case of arithmetic averaging, the modulus can be defined as

\[ M(r, \omega) = M_r + w(r)\delta M(\omega), \]  

with a weighting function \( w(r) \) and subject to the normalization condition

\[ V_e = \int_{V_e} dV_e = \int_{V_e} w(r) dV_e, \]

where \( V_e \) denotes the volume of the element. The integrals are now replaced by the quadrature rules of the SEM scheme. For AxiSEM, we additionally assume an axisymmetric weighting function \( w(r) = w(s, z) \) and split the volume integral into the analytical integration in \( \varphi \) and the quadrature over the element. The constraint then reads

\[ V_e = \sum_{pq} \gamma_{w}^{pq} = \sum_{pq} \gamma_{w}^{pq} w^{pq}, \]

with

\[ \gamma_{w}^{pq} = \begin{cases} \sigma_p \sigma_q J^{pq}s^{pq}, & \text{(non-axial)} \\ \bar{\sigma}_p (1 + \xi_p)^{-1} \sigma_q J^{pq}s^{pq}, & \text{(axial, } p > 0) \\ \bar{\sigma}_0 \sigma_q J^{0q}s^{0q}, & \text{(axial, } p = 0) \end{cases} \]

and \( w^{pq} = w(\xi_p, \eta_q) \). One possible solution is to assign the weight of neighbouring elastic GLL points to the selected anelastic GLL points as sketched in Fig. 3.12. The weighting function for the fourth-order spacial scheme could then for example be chosen as:

\[ w^{11} = \frac{1}{\gamma_{w}^{11}} \left[ \gamma_{w}^{00} + \gamma_{w}^{01} + \gamma_{w}^{10} + \gamma_{w}^{11} + \frac{1}{2} (\gamma_{w}^{02} + \gamma_{w}^{12} + \gamma_{w}^{20} + \gamma_{w}^{21}) + \frac{1}{4} \gamma_{w}^{22} \right] \]

\[ w^{13} = \frac{1}{\gamma_{w}^{13}} \left[ \gamma_{w}^{03} + \gamma_{w}^{04} + \gamma_{w}^{13} + \gamma_{w}^{14} + \frac{1}{2} (\gamma_{w}^{02} + \gamma_{w}^{12} + \gamma_{w}^{23} + \gamma_{w}^{24}) + \frac{1}{4} \gamma_{w}^{22} \right] \]
3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media

Figure 3.12.: Distribution of Gauss-Lobatto-Legendre (GLL) integration points in the reference element of the fourth-order scheme. For the coarse grained attenuation, anelasticity is concentrated on the four red GLL points, while the black points are treated as elastic. During meshing, element sizes are chosen to be smaller than $\frac{2}{3}\lambda_{\text{min}}$ of the smallest wavelength, so that there are at least 3 anelastic points per wavelength.

\[
\begin{align*}
  w^{31} &= \frac{1}{\gamma^{31}_w} \left[ \gamma^{30}_w + \gamma^{31}_w + \gamma^{40}_w + \gamma^{41}_w + \frac{1}{2} \left( \gamma^{20}_w + \gamma^{21}_w + \gamma^{32}_w + \gamma^{42}_w \right) + \frac{1}{4} \gamma^{22}_w \right] \\
  w^{33} &= \frac{1}{\gamma^{33}_w} \left[ \gamma^{33}_w + \gamma^{34}_w + \gamma^{43}_w + \gamma^{44}_w + \frac{1}{2} \left( \gamma^{23}_w + \gamma^{24}_w + \gamma^{32}_w + \gamma^{42}_w \right) + \frac{1}{4} \gamma^{22}_w \right] \\
  w^{ij} &= 0, \quad \text{(else).} \quad (3.58)
\end{align*}
\]

The choice of GLL points is guided by the criterion derived by Day (1998), stating that the periodicity of the medium should have smaller scale than half the shortest wavelength to be propagated, i.e. the elastic equivalent of the Bragg condition for normal incidence. In the specific case of 5 GLL points per element in each dimension that are meshed with $\frac{2}{3}\lambda_s$ as element size, this leads to the choice of two anelastic points per element in each dimension. In principle, the dissipation mechanisms for the lower absorption bands could be placed even sparser, as they only affect longer wavelengths. While this would reduce memory usage and computational complexity in time stepping of the memory variables, we chose not to do so for simplicity in
3.4. Coarse-Grained Memory Variables

implementation and the fact that the stiffness term \( \zeta \) would end up less sparse if another distribution was chosen. Also, additional source terms for the memory variables would cause extra cost, as the strain is no field variable in our scheme. This might be different depending on the numerical scheme used: if the strain is a field variable and does not require extra computation, the decision might be different.

3.4.1. Numerical Efficiency

The performance can benefit from the coarse grained implementation in multiple ways: The number of memory variables per element is less, so these use less memory. Also, the number of memory variable equations that need to be integrated in time and hence the number of points at which the source \( s(t) \) of these equations needs to be computed is less. The precomputed matrices for the anelastic stiffness need only be computed and stored for the elastic GLL points. On top of that, the sparsity of \( \zeta \) can be exploited by using sparse implementations of the matrix products \( \otimes \) and \( \odot \).

For the Hadamard product \( C = A \odot B \) eq. (3.47) it is clear that \( C \) has the joint sparsity of \( A \) and \( B \). For the matrix product \( C = A \otimes B \) eq. (3.48), the implementation depends on which of the two matrices is sparse. In the specific case of chosen GLL points shown in Fig. 3.12 and sparse \( A \) we have

\[
C_{ij} = \begin{cases} 
A^{i1} \cdot B^{1j} + A^{i3} \cdot B^{3j}, & (i \in \{1, 3\}, \text{for all } j) \\
0, & (\text{else})
\end{cases} 
\] (3.59)

and for sparse \( B \)

\[
C_{ij} = \begin{cases} 
A^{i1} \cdot B^{1j} + A^{i3} \cdot B^{3j}, & (j \in \{1, 3\}, \text{for all } i) \\
0, & (\text{else})
\end{cases} 
\] (3.60)

The observed performance gains in AxiSEM are summarized in tables 3.2 and 3.3, showing roughly a factor of two in total memory reduction and a factor of five in computational time both for anelastic stiffness and memory variable time stepping, resulting in a total simulation speedup of around two. The additional cost of the anelastic terms compared to the elastic ones hence reduces from \( 150-200\% \) to \( 35-45\% \) for the Newmark time scheme. The ideal value for the speedup in anelastic stiffness and memory variable time stepping would be \( \frac{25}{4} = 6.25 \). In a full 3D code, the dimensionality would increase this to \( \frac{125}{8} \approx 16 \). The anelastic addition to the
Table 3.2.: Memory usage relative to the elastic case in terms of a multiplicative factor (Newmark time integration)

<table>
<thead>
<tr>
<th>N</th>
<th>full memory variables</th>
<th>coarse grained</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1.7</td>
<td>1.1</td>
</tr>
<tr>
<td>4</td>
<td>1.8</td>
<td>1.1</td>
</tr>
<tr>
<td>5</td>
<td>1.9</td>
<td>1.1</td>
</tr>
<tr>
<td>6</td>
<td>2.0</td>
<td>1.1</td>
</tr>
<tr>
<td>7</td>
<td>2.2</td>
<td>1.2</td>
</tr>
<tr>
<td>8</td>
<td>2.3</td>
<td>1.2</td>
</tr>
</tbody>
</table>

Table 3.3.: Computation time relative to elastic case in terms of a multiplicative factor (Newmark time integration)

<table>
<thead>
<tr>
<th>N</th>
<th>full memory variables runtime</th>
<th>coarse-grained variables runtime</th>
<th>total speed-up</th>
<th>anelastic stiffness speed-up</th>
<th>anelastic time step speed-up</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1</td>
<td>2.55</td>
<td>1.35</td>
<td>1.9</td>
<td>5.3</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>2.75</td>
<td>1.38</td>
<td>2.0</td>
<td>5.2</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>3.0</td>
<td>1.41</td>
<td>2.1</td>
<td>5.3</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>3.16</td>
<td>1.44</td>
<td>2.2</td>
<td>5.5</td>
</tr>
</tbody>
</table>

The elastic stiffness term in current implementations accounts for about 2/3 of the total runtime, and would then be diminished to the point where the elastic stiffness terms always dominate the computational cost.

3.5. Benchmark

Solving the full 3D wave equation for arbitrary earthquake sources in axisymmetric anisotropic models, AxiSEM seems to be unique among available codes. For benchmarking we thus revert to spherically symmetric models. As a reference, we use Yspec by Al-Attar and Woodhouse (2008), which is a generalization of the direct radial integration method (Friederich and Dalkolmo 1995) including selfgravitation (switched off for the benchmark). While Nissen-Meyer et al. (2008) could only per-
form benchmarks down to 20 s period due to limitations in the reference normal mode solution, this limit is overcome using \textit{Yspec}. Also, \textit{AxiSEM} since then has experienced some substantial development (Nissen-Meyer et al. 2014), specifically the improved parallelization allows us to perform production runs up to the highest frequencies observed for global body waves.

Fig. 3.13 shows a record section of seismograms computed for the anisotropic PREM model (Dziewoński and Anderson 1981) with continental crust computed with \textit{Yspec} and \textit{AxiSEM}. The source is a normal faulting event with a moment magnitude $M_w = 5.0$ in 117 km depth under the Tonga islands. The traces recorded at some selected GSN stations are filtered between 10 and 1 s period. Due to the high frequency content, it is necessary to zoom in to see any differences at all: the agreement between the two methods is remarkable even though the highest frequencies have traveled more than 1000 wavelengths (given the low pass filter at 1 s, the time axis is equivalent to the number of traveled wavelengths).

We use the phase and envelope misfit ($PM$ and $EM$ as defined by Kristekova et al. 2009) for quantitative comparison within the zoom windows and find phase misfits below 1.6% for all windows and envelope misfits below 3.1% for all windows but the extremely small amplitude phase ScS at KNTN, where it reaches a maximum of 4.4%. These differences between \textit{AxiSEM} and \textit{Yspec} are slightly larger than in the purely elastic case (van Driel and Nissen-Meyer 2014b), which is not surprising for a number of reasons: While $Q$ is approximated using standard linear solids in \textit{AxiSEM}, \textit{Yspec} uses exactly logarithmic dispersion. The symplectic time scheme was developed for conservative systems (Nissen-Meyer et al. 2008), while here the attenuation causes a slight energy loss. Also, the coarse grained memory variable approach was implemented using arithmetic averaging instead of harmonic averaging and we neglected attenuation in the fluid outer core. However, the errors in amplitude and phase are still negligibly small compared to other errors when comparing synthetics to real data like e.g. ambient noise or the assumption of a 1D model.

The total cost of this extreme-case, demanding run over 1800 traveled wavelengths at 1% accuracy with \textit{AxiSEM} was about 88K CPU hours on 11048 cores (4 simultaneous parallel jobs according to the decomposition described by Nissen-Meyer et al. (2007a)) using a fourth-order symplectic time scheme and 5 relaxation frequencies on a Cray XE6. The mesh was built for periods down to 0.8 s and the time step chosen 30% below the CFL criterion, as this run was meant to prove convergence to the same result as \textit{Yspec}. In applications where less accuracy is necessary one could either use the same traces at higher frequencies or reduce this cost substantially by choosing a larger time step and a coarser mesh (for instance, a dominant period of 1.6 s at otherwise fixed parameters is already an order of magnitude cheaper to
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Figure 3.13.: Comparison of vertical displacement seismograms (band pass filtered from 10 s to 1 s period) for a moment magnitude $M_w = 5.0$ event in 126 km depth under the Tonga islands, computed with AxiSEM and Yspec in the anisotropic PREM model without ocean but including attenuation. The traces are recorded at the GSN stations indicated in the map. The zoom windows shown in Fig. 3.14 are indicated with red rectangles.

compute due to the scaling with the third power of the period). The additional cost for attenuation using the fourth-order symplectic time scheme and coarse grained memory variables compared to a purely elastic simulation was only 26%.

3.6. Conclusion & Outlook

In this paper we presented two improvements for more efficient implementation of attenuation in time-domain wave-propagation methods. First, we showed how to find the optimal set of medium parameters to minimize errors in the wavefield at a fixed numerical complexity. To do so, we analyzed first-order effects of errors in this parametrization onto the wavefield. Also, we derived an approximate method to find these parameters in a full-scale application, i.e. for $10^6$ or more different values of $Q$ and the modulus. Furthermore, we suggested an analytical time stepping scheme, that ties the error of the anelastic time integration to that of the global scheme.
3.6. Conclusion & Outlook

Figure 3.14: -continued from Fig. 3.13- The time scale is relative to the ray-theoretical arrival. _EM_ and _PM_ denote the envelope and phase misfit in the time window plotted (Kristekova et al. 2009). The largest envelope error is 4.4% for the small amplitude phase ScS at KNTN.
3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media

These findings are completely independent of the spatial scheme.

Second, we generalized the coarse grained memory variable approach to the spectral element scheme, noting that the same method could be used in other high-order finite-element schemes. This is a physical approximation reducing the cost of attenuation by a factor of five in the 2D case of AxiSEM. Future work includes implementation of the coarse grained scheme into high-order 3D methods including homogeneous averaging for lower $Q$ values.

Acknowledgements

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References


References


3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media


3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media


3.7. Appendix

3.7.1. Anelastic Stiffness Terms in the Weak Form

The anelastic stiffness in the weak form for the dipole source \((m = 1)\) reads

\[
\frac{1}{\pi} \int_{0}^{2\pi} \nabla w : \zeta \, d\varphi = \partial_{s}w_{+}(\zeta_{1} - \zeta_{6}) + \partial_{z}w_{+}(\zeta_{5} - \zeta_{4}) + \partial_{s}w_{-}(\zeta_{1} + \zeta_{6}) + \partial_{z}w_{-}(\zeta_{5} + \zeta_{4}) + 2\frac{w_{s}}{s}(\zeta_{2} - \zeta_{6}) + \partial_{s}w_{z}\zeta_{5} + \partial_{z}w_{z}\zeta_{3} - \frac{w_{z}}{s}\zeta_{4},
\]

and for the quadrupole source \((m = 2)\):

\[
\frac{1}{2\pi} \int_{0}^{2\pi} \nabla w : \zeta \, d\varphi = \partial_{s}w_{s}\zeta_{1} + \partial_{z}w_{s}\zeta_{5} + \frac{w_{s}}{s}(\zeta_{2} - 2\zeta_{6}) - \partial_{s}w_{\varphi}\zeta_{6} - \partial_{z}w_{\varphi}\zeta_{4} + \frac{w_{\varphi}}{s}(\zeta_{6} - 2\zeta_{2}) + \partial_{s}w_{z}\zeta_{5} + \partial_{z}w_{z}\zeta_{3} - 2\frac{w_{z}}{s}\zeta_{4}.
\]

3.7.2. Spectral Element Discretization

In the spectral element discretization, the anelastic stiffness terms for the dipole source are

\[
z = z_{+} + z_{-} + z_{z}
\]

with

\[
z_{+} = D_{\xi} \otimes \left[ V_{z_{n}} \circ (\zeta_{1} - \zeta_{6}) + V_{s_{n}} \circ (\zeta_{5} - \zeta_{4}) \right] + \delta_{\xi\xi} \left[ D_{0}^{0} \left[ V_{z_{n}}^{0} \circ (\zeta_{1}^{0} - \zeta_{6}^{0}) + V_{s_{n}}^{0} \circ (\zeta_{5}^{0} - \zeta_{4}^{0}) \right] \right]
\]

\[
+ \left[ V_{z_{n}}^{0} \circ (\zeta_{1}^{0} - \zeta_{6}^{0}) + V_{s_{n}}^{0} \circ (\zeta_{5}^{0} - \zeta_{4}^{0}) \right] \otimes D_{\eta}^{T},
\]

\[
z_{z} = D_{\xi} \otimes \left[ V_{z_{n}} \circ (\zeta_{1} - \zeta_{6}) + V_{s_{n}} \circ (\zeta_{5} - \zeta_{4}) \right]
\]

\[
+ \delta_{\xi\xi} \left[ D_{0}^{0} \left[ V_{z_{n}}^{0} \circ (\zeta_{1}^{0} - \zeta_{6}^{0}) + V_{s_{n}}^{0} \circ (\zeta_{5}^{0} - \zeta_{4}^{0}) \right] \right]
\]

\[
+ \left[ V_{z_{n}}^{0} \circ (\zeta_{1}^{0} - \zeta_{6}^{0}) + V_{s_{n}}^{0} \circ (\zeta_{5}^{0} - \zeta_{4}^{0}) \right] \otimes D_{\eta}^{T},
\]

\[
z_{-} = D_{\xi} \otimes \left[ V_{z_{n}} \circ (\zeta_{1} - \zeta_{6}) + V_{s_{n}} \circ (\zeta_{5} - \zeta_{4}) \right] + \delta_{\xi\xi} \left[ D_{0}^{0} \left[ V_{z_{n}}^{0} \circ (\zeta_{1}^{0} - \zeta_{6}^{0}) + V_{s_{n}}^{0} \circ (\zeta_{5}^{0} - \zeta_{4}^{0}) \right] \right]
\]

\[
+ \left[ V_{z_{n}}^{0} \circ (\zeta_{1}^{0} - \zeta_{6}^{0}) + V_{s_{n}}^{0} \circ (\zeta_{5}^{0} - \zeta_{4}^{0}) \right] \otimes D_{\eta}^{T},
\]
3. Optimized Visco-elastic Wave Propagation for Weakly Dissipative Media

\[
\begin{align*}
\mathbf{z}_- &= \mathbf{D}_\xi \otimes \left[ \mathbf{V}_z \otimes (\zeta_1 + \zeta_6) + \mathbf{V}_s \otimes (\zeta_5 + \zeta_4) \right] \\
&\quad + \left[ \mathbf{V}_{z\xi} \otimes (\zeta_1 + \zeta_6) + \mathbf{V}_{s\xi} \otimes (\zeta_5 + \zeta_4) \right] \otimes \mathbf{D}^T_\eta + 2\mathbf{Y} \otimes (\zeta_2 - \zeta_6) \\
&\quad + \delta_{ee} \mathbf{D}^0_\xi \left[ \mathbf{V}_{z\eta} \otimes (\zeta_1^0 + \zeta_6^0) + \mathbf{V}_{s\eta} \otimes (\zeta_5^0 + \zeta_4^0) + 2\mathbf{Y}^0 \otimes (\zeta_2^0 - \zeta_6^0) \right], \\
\mathbf{z}_z &= \mathbf{D}_\xi \otimes \left( \mathbf{V}_z \otimes \zeta_5 + \mathbf{V}_s \otimes \zeta_3 \right) + \left( \mathbf{V}_{z\xi} \otimes \zeta_5 + \mathbf{V}_{s\xi} \otimes \zeta_3 \right) \otimes \mathbf{D}^T_\eta - \mathbf{Y} \otimes \zeta_4 \\
&\quad + \delta_{ee} \mathbf{D}^0_\xi \left[ \mathbf{V}_{z\eta} \otimes \zeta_5^0 + \mathbf{V}_{s\eta} \otimes \zeta_3^0 - \mathbf{Y}^0 \otimes \zeta_4^0 \right]
\end{align*}
\]

(3.64)

and for the quadrupole source

\[
\mathbf{z} = \mathbf{z}_s + \mathbf{z}_\varphi + \mathbf{z}_z
\]

(3.65)

with

\[
\begin{align*}
\mathbf{z}_s &= \mathbf{D}_\xi \otimes \left( \mathbf{V}_z \otimes \zeta_1 + \mathbf{V}_s \otimes \zeta_5 \right) + \left( \mathbf{V}_{z\xi} \otimes \zeta_1 + \mathbf{V}_{s\xi} \otimes \zeta_5 \right) \otimes \mathbf{D}^T_\eta \\
&\quad + \mathbf{Y} \otimes (\zeta_2 - 2\zeta_6) + \delta_{ee} \mathbf{D}^0_\xi \left[ \mathbf{V}_{z\eta} \otimes \zeta_1^0 - \mathbf{Y}^0 \otimes (\zeta_2^0 - 2\zeta_6^0) \right], \\
\mathbf{z}_\varphi &= -\mathbf{D}_\xi \otimes \left( \mathbf{V}_z \otimes \zeta_6 + \mathbf{V}_s \otimes \zeta_4 \right) - \left( \mathbf{V}_{z\xi} \otimes \zeta_6 + \mathbf{V}_{s\xi} \otimes \zeta_4 \right) \otimes \mathbf{D}^T_\eta \\
&\quad + \mathbf{Y} \otimes (\zeta_6 - 2\zeta_2) + \delta_{ee} \mathbf{D}^0_\xi \left[ -\mathbf{V}_{z\eta} \otimes \zeta_6^0 + \mathbf{Y}^0 \otimes (\zeta_6^0 - 2\zeta_2^0) \right], \\
\mathbf{z}_z &= \mathbf{D}_\xi \otimes \left( \mathbf{V}_z \otimes \zeta_5 + \mathbf{V}_s \otimes \zeta_3 \right) + \left( \mathbf{V}_{z\xi} \otimes \zeta_5 + \mathbf{V}_{s\xi} \otimes \zeta_3 \right) \otimes \mathbf{D}^T_\eta \\
&\quad - 2\mathbf{Y} \otimes \zeta_4 + \delta_{ee} \mathbf{D}^0_\xi \left[ \mathbf{V}_{z\eta} \otimes \zeta_3^0 \right].
\end{align*}
\]

(3.66)
Chapter 4

AxiSEM: Broadband 3D Seismic Wavefields in Axisymmetric Media

Abstract

We present a methodology to compute 3D global seismic wavefields for realistic earthquake sources in visco-elastic anisotropic media, covering applications across the observable seismic frequency band with moderate computational resources. This is accommodated by mandating axisymmetric background models which allow for a multipole expansion such that only a 2D computational domain is needed, whereas the azimuthal third dimension is computed analytically on-the-fly. This dimensional collapse opens doors for storing space-time wavefields on disk which can be used to compute Fréchet sensitivity kernels for waveform tomography. We use the corresponding publicly available open-source spectral-element code AxiSEM (www.axisem.info), demonstrate its excellent scalability on supercomputers, a diverse range of applications ranging from normal modes to small-scale lowermost mantle structures, tomographic models, comparison to observed data, and discuss further avenues to pursue with this methodology.

4.1. Introduction

Seismology currently enjoys transformative progress upon a simultaneous surge in instrumentation, software, and hardware. The dawn of high-performance computing and sophisticated numerical techniques to address seismic wave propagation in a physically robust and realistic manner has enabled seismologists to capture relevant physics of wave propagation in the seismic far-field, and resolve structures for which direct comparisons to waveform data are feasible. This in turn opens doors to incorporating full waveforms into inversion algorithms, using, for instance, adjoint methods in conjunction with 3D wave propagation (e.g. Tromp et al. 2005).

Traditionally, global seismic tomography (consult Rawlinson et al. 2010, for a comprehensive summary) has been based upon ray theory utilizing traveltimes, rather than full waveforms. Indeed, phase delays relate to wavespeed variations in a more robust manner than amplitude information. So why would numerical methods, within the realm of tomography at least, strive to capture the entire waveform? Most modern measurements of “traveltimes” such as cross-correlation (Nolet 2008), time-frequency phase delays (Fichtner and Igel 2008a), or instantaneous phase (Bozdağ et al. 2011) are based on waveforms, and therefore necessitate full wavefield modeling. Moreover, high-frequency waveform modelling (e.g. Thorne et al. 2007) is often employed to fit smaller-scale heterogeneities. Such studies are subject to significant tradeoffs especially if secondary measurements such as traveltimes were used. Thirdly, accurate computation of the gradient of measurements with respect to model variations, often termed Fréchet derivative, requires the convolution of a forward-propagating wavefield with a backward-, or adjoint wavefield, both of which need to be sampled in 3D space and time (Nissen-Meyer et al., 2007a). For the purpose of this paper, let us postulate a desire for a method to deliver

1. 3D wavefields for realistic sources and structures,

2. across the observable frequency band,

3. at a reasonable computational cost for tomography.

We will now delve into some of these issues in more detail, and present our compromise for a solution which covers a significant, realistic and relevant fraction of these aspirations.
4.1. Introduction

4.1.1. Effective Earth Models and Data

Spherically symmetric models are widely established as a common basis for Earth properties not only in seismology, but also as a bridge to mineral physics and geodynamics. This popularity stems not only from the relative simplicity in modeling 1D structures, but largely from the fact that such laterally averaged models represent and fit a large majority of seismic (traveltime) data, as has been established since the traveltime tables by Jeffreys and Bullen (1940) and subsequent models such as PREM (Dziewonski and Anderson 1981), IASP91 (Kennett and Engdahl 1991), and ak135 (Kennett et al. 1995). Our understanding and interpretation of the Earth’s interior has come a long way from the detection of its radial structure, and has been significantly fueled by means of seismic tomography (Rawlinson et al. 2010). At the global scale, 3D tomographic models usually amount to a few percent wavespeed perturbation from spherically symmetric models (Becker and Boschi 2002), and behave close to linear in seismic traveltimes (Mercerat and Nolet 2012).

Global tomographic models exhibit considerable agreement up to spherical harmonic degree 5 (Becker and Boschi 2002; Auer et al. 2014), that is, for very large-scale structures, but often diverge at smaller length scales due to shortcomings such as insufficient data coverage and modeling. In this multi-scale context, it is important to remember that any discrete Earth model used in a numerical method is inherently upscaled (either by its own nature, or by porting to the discrete mesh), and at best a blurred rendition of reality. The challenge lies in tying the background model to both the desired frequency range and type of measurement extracted from the wavefield in a feasible, realistic manner.

Clearly, utilizing a maximal amount of broadband data is as desirable as capturing complexities in structure and wave physics. Even in times of a surge in data acquisition, source-receiver geometries are still largely controlled by continents, tectonic boundaries and the Northern hemisphere. It thus seems desirable to seek a compromise for modeling between broad frequency ranges, realistic effective Earth models, while exploiting a maximal amount of usable data.

4.1.2. Numerical Wave Propagation

Unlike disciplines subject to more complex, non-linear physical systems such as fluid dynamics, the availability of mature, comprehensive seismic wave-propagation codes such as SPECFEM3D_GLOBE (e.g. Komatitsch and Tromp, 2002b) seems to have resolved most challenges in capturing the underlying physics of wave propagation. Instead, it appears to shift attention for achieving realistic wave propagation simu-
Figure 4.1.: The cost of global wavefield simulations in “real-time” (i.e. seismogram length equals wallclock simulation time) for different methods. Each data point is based on actual simulation times, and gives as a result the number of processors needed to achieve this, assuming perfect scalability. The cost of normal-mode solutions (mineos, available from geodynamics.org) and wave propagation in 3D domains (SPECFEM3D_GLOBE, geodynamics.org) scales with the seismic period to the fourth power, whereas the axisymmetric method (AxiSEM) scales to the third power. We calculate the cost estimation upon saving $10^6$ spatial points, a moderate task to compute wavefields. This is especially noteworthy for the mode solution whose cost scales directly with the number of saved spatial points.

In summary, we are concerned with:

- feasible choices for source and structure,
- usability of the method,
- availability of computational resources.

While all of these issues are common to any numerical method and not easily resolvable, the latter point is especially stringent. Worse still, for global seismology the prohibitive cost will remain a dominant limitation on the maximally resolved frequencies and exponentially increasing number of usable data with millions of recorded waveforms (IRIS annual report 2011, www.iris.edu) for years to come.
4.1. Introduction

Come. Full 3D models in spherical geometry can be incorporated by spherical finite-differences (Igel et al. 2002), or spectral-element methods (Komatitsch and Tromp, 2002a; Chaljub et al. 2007). As the computational cost scales with the frequency to the fourth power (three space, one time dimension), such comprehensive methods are still extraordinarily expensive for global-scale wave propagation at high resolution, and certainly more so if large numbers of simulations are needed as in most cases of geophysical interest. Alternative attempts such as high-order expansions of the Born series (Takeuchi et al. 2000) is similarly prohibitive for complex media and high frequencies. This is unfortunate, as especially the domain of seismic periods below 10 seconds (see Fig. 4.1) offers both a wealth of seismic data and a resolution harboring many open geophysical questions. The plot in Fig. 4.1 is an approximate, order-of-magnitude estimation of computational cost, and minor algorithmic optimization does not affect this overarching trend drastically. The slightly increased cost for AxiSEM above 10 seconds represents the fact that the thin crustal layers at these long periods start to dominate the smallest element size and thus increase the relative cost due to this geometric constraint on the global timestep. This is not seen in SPECFEM3D_GLOBE, since intra-crustal layers are not explicitly meshed. Further commentary on Fig. 4.1 is given in Section 4.2.7.

Considering desirable features for the inversion such as comprehensive model-sampling, uncertainty analysis, or probabilistic approaches, this represents not only a formidable challenge, but is essentially not computable even with most optimistic estimates of the evolution of computation on a decadal time-scale, especially in 3D. Several strategies of speeding up numerical methods exist, focused on either the physical system or the implementation. Code optimization may exploit dedicated hardware infrastructures such as GPUs (Rietmann et al. 2012), or algorithmic tasks such as tensor-vector products (Nissen-Meyer et al., 2007b), irregular meshing (Zhu et al. 2009) or local time-stepping. These approaches usually lead to a performance speedup of about 2-3 in total CPU time. Physics-based approximations often limit the frequency range either on the high end (as implicitly done due to prohibitive cost in 3D methods) or lower end (ray theory). Additionally, we commonly find cost reductions related to reduced dimensionality (e.g., 2D, Zhu et al. (2009)), rheology (e.g. acoustic wave propagation), or structural complexity by means of homogenization (Capdeville et al. 2013). Such approximations can lead to orders of magnitude faster codes, but need to be chosen carefully depending on each application.
4. AxiSEM: Broadband 3D Seismic Wavefields in Axisymmetric Media

4.1.3. 3D Waves in Axisymmetric Media

Several methods have been developed to effectively accommodate various levels of complexity in background structures. For spherically symmetric Earth models, normal-mode summation (Dahlen and Tromp 1998) elegantly tackles the grave end of the spectrum including such effects as gravity and rotation (Dahlen 1968). For higher frequencies, the direct-solution method (Kawai et al. 2006), GEMINI (Friederich and Dalkolmo 1995), or Yspec (Al-Attar and Woodhouse 2008) have proven efficient in delivering accurate seismograms. While in principle doable, all of these methods become computationally expensive if an entire wavefield is needed as for sensitivity kernels (Nissen-Meyer et al., 2007a), and do not allow for lateral heterogeneities. Axisymmetric finite difference methods (Toyokuni and Takenaka 2006; Jahnke et al. 2008) may accommodate this effectively, but suffer various shortcomings such as approximate sources, lack of fluid domains and anisotropy (Jahnke et al. 2008), and high dispersion errors for large propagation distances of interface-sensitive phases such as surface or diffracted waves. However, recent advances include a full moment tensor, attenuation, and the Earth’s center (Toyokuni and Takenaka 2012).

The purpose of this paper is to introduce the axisymmetric spectral-element implementation AxiSEM as a new and publicly available, production-ready method and code for global wave propagation, which taps into parameter regimes that have been previously unavailable at similar computational cost. We motivate the relevance of these parameter regimes by various examples and present ideas for further extensions and applications. Exploitation of moment-tensor source and single-force radiation patterns allow the computational domain to be collapsed to a 2D semi-disk, and the azimuthal third dimension is computed analytically. Radiation pattern symmetries require all sources to be located along the axis, and lateral heterogeneities are translated into a 2.5-dimensional torus-like structure. Due to the dimensional reduction, global wave propagation at typical seismic periods can be tackled serially on workstations. Novel features in this manuscript with respect to the methodology already described in Nissen-Meyer et al. (2007b, 2008) include 2D parallelization, scalability to $> 8000$ cores, benchmarks at 1Hz and for normal modes, extensions to visco-elastic anisotropic media, fluid spheres, finite sources, axisymmetric structures, tomographic models, comparison to data, generic post-processing for arbitrary source-receiver settings, sensitivity kernels, and availability as an open-source code.

This paper is organized as follows. A methodological chapter briefly summarizes the mathematical background of our approach, delegating more details to previous publications, and focusing instead on practical matters such as scalability, runtime requirements, I/O, and code availability. Chapter 4.3 describes those source types
4.2. Methodology

that may be simulated with AxiSEM, ranging from moment-tensors, single forces, to finite faults and stochastic sources. Chapter 4.4 similarly describes a range of background models to be discretized in AxiSEM, including anisotropy, intrinsic attenuation, classical 1D Earth models, solar models, small-scale 2.5D heterogeneities and tomographic cross-sections, random media and explicit mesh representations of the crust and oceans (oceans are not part of the current code as of April 2014). Chapter 4.5 shows simulation results for a selection of the previously mentioned ranges of applicability, covering the entire seismic frequency spectrum, 3D wavefield visualization, lowermost mantle structures, simulations for 2.5D slices through a tomography model, comparison with observed data from lowermost mantle and core phases, and sensitivity kernels. A concluding chapter discusses the general applicability, limitations and an outlook on future developments.

AxiSEM is a mature methodology and code, able to address a number of intriguing scientific questions. As should be commonly known per any software implementation, the level of automatism for the applications listed here is diverse, and readers should refer to the manual of the most recent release version for up-to-date features of the code.

4.2. Methodology

The mathematical foundation and validation of spherically symmetric, solid-fluid lower-frequency settings is detailed in previous publications (Nissen-Meyer et al., 2007b, 2008). In this section, we only sketch key methodological concepts, while focusing on new additions and practical matters related to usability, functionality and applicability. Our approach accurately simulates 3D wavefields in axisymmetric Earth models, and distinguishes itself by

1. decreasing the computational costs by orders of magnitude compared to 3D method by running in 2D,

2. taking no limiting assumptions about wave-propagation physics (except for very long-period effects such as rotation (see section 4.4.7)) or kinematic earthquake radiation.

It therefore falls in between traditional end members that are typically optimized for either end of the frequency spectrum (e.g. ray theory, normal-mode summation) and 3D modeling, by not compromising on essential wave-propagation physics or the coverage of the entire recorded frequency band between 0.001-1Hz. The efficiency
gain is grounded upon assuming axisymmetric background models, which reduces the numerical cost to a 2D domain whereas the third dimension is tackled analytically. We shall forego detailed treatment of classical spectral-element methods to highlight the peculiarities associated with this axisymmetric setting.

### 4.2.1. Equations of Motion

The 3D integral (weak-form) elastodynamic equations of motion in the solid Earth read

\[
\begin{align*}
\text{mass term: } & M(u) \\
\text{stiffness term: } & K(u) \\
\text{source term: } & F(u)
\end{align*}
\]

\[
\int_{\oplus} \rho \mathbf{w} \cdot \partial_t^2 \mathbf{u} \, d^3x + \int_{\oplus} \nabla \mathbf{w} : C : \nabla \mathbf{u} \, d^3x = \int_{\oplus} \mathbf{w} \cdot \mathbf{f} \, d^3x
\]  

(4.1)

where \( \mathbf{u} \) is the sought displacement vector, \( \mathbf{w} \) a suitably chosen test vector, \( \mathbf{f} \) the source term, \( \rho \) the mass density, and \( \mathbf{C} \) the anisotropic fourth-order elasticity tensor with 21 independent parameters (consult Nissen-Meyer et al. (2007b) for details). It may be time-dependent for intrinsic attenuation in which case the double contraction : implies a convolution.

### 4.2.2. Axisymmetric Dimensional Collapse

As shown in Nissen-Meyer et al. (2007a), one may analytically separate radiation patterns into individual responses to each moment-tensor element \( M_{ij} \) factorized in azimuthal functions

\[
\mathbf{u}_m(x) = \begin{pmatrix} u_s(\tilde{x}) \cos m\varphi \\ u_\varphi(\tilde{x}) \sin m\varphi \\ u_z(\tilde{x}) \cos m\varphi \end{pmatrix},
\]

(4.2)

where \( m = 0,1,2 \) are monopole, dipole, quadrupole radiation types, respectively (Fig. 4.2), and \( \tilde{x} = (s,z) = (r,\theta) \) spans a two-dimensional domain (Fig. 4.3) by cylindrical \((s,\varphi,z)\) or spherical \((r,\theta,\varphi)\) coordinates, respectively. This relation is accurate for axisymmetry in source \( \mathbf{f} = \mathbf{f}(\tilde{x}) \) and structure \( \rho = \rho(\tilde{x}), \mathbf{C} = \mathbf{C}(\tilde{x}) \).

After solving the set of 2D problems, seismograms and wavefields at any location \((s,\varphi,z)\) are obtained by multiplication with these azimuthal radiation factors in Eq. (4.2) during the post-processing stage (Section 4.2.5). Conceptually, 3D integrals in \( \oplus \) over any integrand \( \psi \) that contains azimuthal dependencies such as in Eq. (4.2) are then collapsed to 2D integrals in \( D \) as
4.2. Methodology

Figure 4.2.: Radiation patterns for monopole (top), dipole (middle), and quadrupole angular orders of the respective moment tensor elements. The azimuthal radiation patterns encapsulated by $f_l \phi$ depend on multipole order $m$ as well as component $l$, that is, no summation is implied by the above products.

$$u_l = u_l(s, z)$$

$$u_l = u_l(s, z) \odot f_l(\sin \varphi, \cos \varphi)$$

$$u_l = u_l(s, z) \odot f_l(2 \sin \varphi, \cos(2 \varphi))$$

by evaluating integration over $\varphi$ analytically. This delivers solutions for the 3D displacement vector $u$ within a 2D computational domain (Fig. 4.3). Symmetry about the axis (blue in Fig. 4.3) mandates all structural heterogeneities away from it to adopt a torus-shaped, azimuthally invariant elongation, whereas the point source remains along the axis. Such lateral in-plane heterogeneities may prove useful for parameter studies at sufficiently high frequencies (see Section 4.4.4).
Figure 4.3.: The 2D computational domain D upon which the collapsed numerical system operates with a symmetry axis (blue). The method solves the three-dimensional equations of motion, but allows for an analytical representation within the azimuthal dimension (green). Sources and structure therefore obey axisymmetry with respect to the axis. Colors denote compressional velocities of the PREM model (Dziewonski and Anderson 1981), and black lines an elemental mesh for a seismic period of 20s. Zoom panels show a higher-resolution version (5s) with upper-mantle discontinuities honored by the mesh (b), as well as the rotated-coordinate meshing below the inner-core boundary (ICB) (Nissen-Meyer et al. 2008).
4.2.3. Spatial Discretization

Finite-element based methods compute derivatives and integration upon reference coordinates. This entails a mapping \( \mathbf{x} = \mathbf{x}(\xi) \) from a generic reference coordinate frame \( \xi \) to the physical domain \( \mathbf{x} \), represented by the Jacobian

\[
J(\xi) = \left| \frac{\partial \mathbf{x}}{\partial \xi} \right|, \quad (4.4)
\]

where \( |\cdot| \) is the determinant. This mapping is purely analytical for all element types of \textit{AxiSEM}'s automated mesh generator with the exception of the cube at the center of the sphere (Nissen-Meyer et al. 2008). We then expand the wavefield within each elemental integral upon a basis of order \( N \) (typically 4, 5, 6) as

\[
\mathbf{u}(\xi) \approx \sum_{i,j=0}^{N} \mathbf{u}_{ij} l_{ij}(\xi), \quad (4.5)
\]

with two-dimensional Lagrange polynomials \( l_{ij} \) (Nissen-Meyer et al., 2007b). Partial derivatives \( \partial_{\xi} \mathbf{u}(\xi) \) are given by analytically differentiating \( l_{ij} \) along \( \xi \). These derivative operations are responsible for the bulk of the computational cost in typical spectral-element methods. Having performed these algebraic operations at the level of elements, these elemental contributions are gathered to define the discrete global stiffness \( \mathbf{Ku} \) and mass terms \( \mathbf{Mu} \). Our formulation with cylindrical coordinates leads to singularities of the type \( s^{-1} \) (Fig. 4.3) in the gradients at the symmetry axis. This is accommodated by a different basis compared to the interior domain, l'Hospital’s rule (Fournier et al. 2005), and asymptotic expressions to accommodate boundary conditions (Nissen-Meyer et al., 2007a). By choice of either kind of basis function, the mass matrix is exactly diagonal.

4.2.4. Temporal Discretization

Such a discrete system leads to a set of ordinary differential equations in time, which may be rearranged as

\[
\ddot{\mathbf{u}}(t) = \mathbf{M}^{-1} (\mathbf{f}(t) - \mathbf{Ku}(t)), \quad (4.6)
\]

This system is conveniently solved by various explicit time-evolution schemes such as second-order Newmark, or higher-order symplectic schemes (Nissen-Meyer et al. 2008) up to eighth-order accuracy. Note that for the case of solid-fluid domains, the
4. \textit{AxiSEM}: Broadband 3D Seismic Wavefields in Axisymmetric Media

Figure 4.4: A Google-Earth rendition of the source-receiver geometry used in an \textit{AxiSEM} simulation. A generic output of the post-processing embedded within \textit{AxiSEM}, this \textit{kml}-file contains earthquake parameters (red dot), and actual seismogram images as links at the station locations (yellow pins).

time-stepping becomes a combined system of these two domains, and needs to be iterated appropriately across the solid-fluid interface (Chaljub and Valette 2004).

4.2.5. Post-Processing: Summation, Rotation, Filtering

Unlike most seismic wave-propagation codes, \textit{AxiSEM} requires a crucial sequence of post-processing steps to retrieve the full solution, see Eq. (4.2). While this may seem as an undesirable additional burden, it represents a high level of flexibility, leaving a maximum amount of parameter choices to this post-processing step instead of having them fixed for the bulk simulations. For instance, one does not need to decide on the source mechanism, source-time function, filtering, instrument response, and receiver components at the time of the actual simulation but can defer this to post-
4.2. Methodology

processing. The only necessary geophysical choices at the time of the simulation are source depth, receiver distances, maximal frequency, and background model. Fig. 4.4 depicts an example of an automated output from postprocessing to be read by Google Earth, containing source (red dot) and receiver (yellow pins) locations. Each receiver pin is linked to an image of the corresponding post-processed seismograms, and source information is provided as text (see Fig. 4.4). Section 4.5.3 sketches a generalization of this post-processing that fully exploits its flexibility in the context of solving the forward problem once-and-for-all, deferring the choice of the source-receiver geometry to post-processing as well.

Recasting the 3D equations of motion into a suite of 2D problems yields a system of four independent wave equations to represent all six independent elements of the moment tensor ($M_{rr}, M_{\phi \phi}, M_{\theta \theta}, M_{r \phi}, M_{r \theta}, M_{\theta \phi}$) separately (see Fig. 4.7). This collapse from six to four independent systems honors azimuthal redundancy between the dipoles $M_{r \theta} \sim M_{r \phi}$ as well as quadrupoles $(M_{\theta \theta} - M_{\phi \phi}) \sim M_{\theta \phi}$ (Nissen-Meyer et al., 2007a). Consequently, AxSEM simulations are by construction always given for each individual element of the moment tensor. The task to sum to a full moment-tensor is described in Section 4.3.1. Additional features of post-processing are rotation from the pole-centric to an actual source-receiver geometry, bandpass filtering, convolution with a source-time function, rotation to arbitrary seismogram component systems, choice between displacement and velocity seismogram. A similar set of operations applies to 3D wavefield visualizations. Users may for this visualization case also specify rendering perspectives, wavefield components, 3D cuts, hypersurface extractions within post-processing. In effect, this allows for in-situ visualization and merges seismic trace analysis with visualization on-the-fly.

4.2.6. Parallelization

At frequencies around 1Hz, the required run-time memory (roughly 20GB) for 1 Million elements exceeds the typical memory of contemporary cluster cores. More importantly, the CPU time-to-solution becomes prohibitively lengthy if the system is simulated on a single core (although possible). We thus incorporated a generic, automated 2D domain decomposition into $2N_\theta N_r$ domains, where $N_\theta N_r$ represent positive integers for the number of latitudinal and radial slices, respectively (see Fig. 4.5 for an example). This guarantees the simultaneous realization of the three crucial factors for scalability: 1) a minimal amount of neighboring domains (maximally eight), 2) minimal interfaces size (i.e., length of messages), and 3) exact load balancing. The non-blocking, asynchronous message passing implementation is entirely hidden behind the computation of the stiffness term, which will be seen in the
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Figure 4.5.: A typical mesh decomposition for the PREM model running at dominant period of 9 seconds on 96 cores. Load balancing is exact, and the arbitrary permissible multiplication between number of horizontal and radial slices guarantees flexibility for adapting numerical settings to existent hardware infrastructures.

excellent scaling in the next section.

4.2.7. Performance & Scaling

The reduction of 3D wave propagation to a 2D computational domain is reflected by the method’s performance compared to 3D methods (Fig. 4.1). This equally holds true against methods which are extremely efficient and fast in delivering singular seismograms such as normal-mode summation or DSM, but whose computational cost depends on the amount of desired output locations. To compute sensitivity
4.2. Methodology

Figure 4.6.: Scalability of *AxiSEM* on a Cray XE6 at CSCS (Switzerland). Left: Strong scaling, i.e. fixed global problem size (8 Million 2D elements) as a function of the number of used cores communicating via the message-passing interface, for 12000 time steps. *AxiSEM* scales super-optimal, which is mostly due to the more efficient usage of run-time memory if less memory is used per core. Right: Weak scaling, i.e. fixed problem size per core (1000 elements) for 1000 time steps. The desired constant time-to-solution is exceeded by 4% for >8000 cores in which case communication is not entirely hidden behind the computation of the stiffness terms.

Kernels for the inverse problem, one needs to save the entire space-time wavefield everywhere, and hence such dependencies become inefficient especially when moving to higher resolutions. Fig. 4.1 gives a flavor of the computational task along a typical range of global-scale seismic periods, quantified in terms of required amount of CPU cores to achieve real-time simulations (seismogram time equals CPU wall-clock time), assuming perfect scalability. Fig. 4.6 shows strong as well as weak scaling results on a Cray XE6 supercomputer installed at CSCS, Switzerland. In both cases, the performance is excellent: Strong scaling (fixed global degrees of freedom) is even super-optimal due to efficient memory usage. Weak scaling shows a slightly sub-optimal behavior at 96% for >8000 cores, still a remarkable figure indicating that message passing and parallelization are essentially hidden within the code. It is noteworthy to recognize that *AxiSEM* has little run-time memory, and applications at the high-frequency end benefit from vast multi-core systems mainly to reduce wall-clock time, unlike 3D seismic methods which are often memory-bound.

As in any (2D) time-domain discrete method, it is important to recognize that half the dominant period takes about 8 times longer if seismogram length is fixed:
The mesh is about 4 times larger, and the time step about twice as small. Note that monopole source types run faster than dipoles and quadrupoles due to their sparser stiffness terms (Nissen-Meyer et al., 2007b).

As a rough estimate, each 2D element occupies 1.5 wavelengths and about 2.5 kB, and for seismic periods of 5 seconds approximately 400,000 elements are needed. The code requires about eight microseconds simulation time per time-step and element.

### 4.2.8. Excessive Input/Output

Spectral-element methods of the kind presented here have excellent scalability properties in general (Fig. 4.6). The bottleneck, especially when moving to higher resolution and larger parallelization, lies in disk access which is necessary for saving wavefields and seismograms at run-time. For storage of synthetic seismic data, especially for a database of precomputed waveforms (see sect. 4.5.3), platform-independence of the data is needed. However, the storage format of Fortran binary files is not even compiler-independent. To ensure true platform independence, AxiSEM fully supports the widely accepted NetCDF4 (http://www.unidata.ucar.edu/netcdf/) format to store seismograms and wavefields, but users may also revert to Fortran binary if desired. A NetCDF4 file is a container, in which very large variables (e.g. wavefields) as well as single scalar values (e.g. general simulation information) can be stored. The format allows transparent compression of the variables using the SZIP algorithm (Yeh et al. 2002), which saves around 50% of hard drive space for a typical seismic wavefield with respect to generic binary format. The container character of a NetCDF file means that direct access to selected data is possible, i.e. small amounts of data such as time series can be read from a (potentially very large) file, without loading the whole file into memory. The code allows to store all simulation output in one self-contained NetCDF4 file, which facilitates handling of a large number of simulation results, for example in parameter studies.

NetCDF4, which is based on the HDF5 format, allows for parallel writing into one file. Since this makes use of parallel file systems very efficiently, it might provide big performance gains on the next generation of supercomputers. On the current generation however, the installation of parallel NetCDF4 is not generally reliable yet. Therefore and to increase compatibility with older machines, AxiSEM uses a serial round Robin-scheme for writing data to disk. All processors buffer their respective wavefield output locally. After a set number of time steps, one instance spawns a new thread and transfers its wavefield buffer to it. This new thread then opens the output file and compresses and writes the buffer to disk, while the original processor continues to simulate the wavefield. This non-blocking IO scheme has been tested.
to work well up to 224 parallel instances, in that wavefield storage marginally affects CPU time and performance. \(^1\)

4.2.9. Implementation and Availability

The AxiSEM code is written in Fortran2003 combined with MPI message passing, requiring corresponding compilers. Optional additional packages are NetCDF4 (Rew and Davis 1990) for improved I/O, fftw3 (Frigo and Johnson 2005) for post-processing in the frequency domain, TauP (Crotwell et al. 1999) for traveltime picks, paraview for visualization of vtk- and xdmf-based wavefields, Matlab for visualization of source-receiver geometries and seismograms on the sphere, python wrappers for streamlined input/output and linkage to Obspy (Beyreuther et al. 2010). The Fortran2003 code is divided into a Mesher utilizing OpenMP, a Solver utilizing the message-passing interface (MPI) for communication between separate domains, and extensive post-processing for ease of visualization, filtering, source-time functions, various receiver component systems, and moment-tensor solutions. The number and meaning of input parameters for AxiSEM are kept at a generic, streamlined minimum, providing a robust basis in an effort to reduce failure. This is amended by a comprehensive number of sanity checks prior to the time loop, including critical tests upon mesh configurations, source, model, receiver settings parallelization, discrete volume and mass of the Earth, accuracy of internal surfaces, numerical quadrature, mass matrix and boundary terms.

AxiSEM is available through a release version with GPL license from www.axisem.info, and comes with no guarantee of functionality or support, but each version contains a detailed manual, examples, nightly builds and tractable subversion control system as well as an existent userbase.

4.3. Seismic Sources

In global seismology, it is customary to rely on the point-source approximation and corresponding moment tensors \(M_p\) (not to be confused with mass matrix \(M\) in the

---

\(^1\)Since publication of this paper, the situation has improved and on all supercomputers available to us, NetCDF4 compiled with OpenMPI is now preinstalled. In chapter 5 we describe the new implementation using collective IO and show that it scales well on up to several 1000 processors and reaches write speeds of a few GB per second. For jobs smaller than 100 processes however, we still recommend the scheme described here as it perfectly hides IO behind computation.
last section). The implementation of indigenous earthquake sources or single forces located at \(x_p\) is detailed in Nissen-Meyer et al. (2007b). We use temporal Dirac delta functions acting at time \(t_p\) in the simulations, such that a displacement time series is obtained by convolving a source-time function \(S_p(t)\) (incorporated into a time-dependent moment-tensor term as \(M^p(t) = M^P S^p(t)\)), with the Green’s tensor solution \(G^p\)

\[
\mathbf{u}^p(x, \omega) = M^p(\omega) : \nabla_p G^p(x, \omega),
\]

where we reverted to frequency domain \(\omega\) for concise notation, and \(\nabla_p\) denotes spatial differentiation with respect to the source coordinate (no summation implied).

Here, we focus on basic necessary post-processing operations to obtain the response to a full moment-tensor, the extension to finite kinematic faults, stochastic sources (as for example in noise seismology or helioseismology), and the problem of handling Dirac delta functions \(\delta(x)\) in a discrete world.

### 4.3.1. Moment-Tensor & Single Forces

To obtain the response to a full moment tensor (e.g., CMT catalogue, [www.globalcmt.org](http://www.globalcmt.org)), one applies posterior summation honoring the respective radiation patterns along the azimuth along with the convolution:

\[
\mathbf{u}^p(x, \omega) = \sum_{m=1}^{4} \tilde{M}^p_m(\varphi, \omega) \tilde{G}^p_m(\tilde{x}, \omega),
\]

where \(\tilde{G}^p_m\) represent 2D vectorial Green’s responses to each simulation \(m\) for point source \(p\), and \(\tilde{M}^p_m\) read

\[
\begin{align*}
\tilde{M}_1(\varphi) &= M_{rr}, \\
\tilde{M}_2(\varphi) &= (M_{\theta\theta} + M_{\varphi\varphi}) / 2, \\
\tilde{M}_3(\varphi) &= M_r \cos \varphi + M_{r\varphi} \sin \varphi, \\
\tilde{M}_4(\varphi) &= (M_{\theta\theta} - M_{\varphi\varphi}) \cos 2\varphi + M_{\varphi\theta} \sin 2\varphi.
\end{align*}
\]

Only these four independent types of radiation patterns exist (monopoles \(\tilde{M}_1, \tilde{M}_2\); dipole \(\tilde{M}_3\); and quadrupole \(\tilde{M}_4\)) in this axisymmetric framework. For a full earthquake moment tensor, four independent simulations are thus undertaken to account for the six moment-tensor elements \(M_{ij}\), whereas single forces (as needed for Lamb’s
4.3. Seismic Sources

**Figure 4.7.** Left quadrant: The four time series upon the generic moment-tensor types (see Eq. (4.9)–(4.12)). Right: Summation to the full seismogram for the 2011 M9 Tohoku (point-source) event. Plotted is the displacement in the $s$-direction (i.e., perpendicular to the symmetry axis, see Fig. 4.3), with a dominant period of 10 seconds recorded at station BILL (East Siberia) at 33° distance.

Problem, ambient noise, impacts, or adjoint wavefields, require two simulations (monopole vertical force, dipole horizontal force) to account for the three components (Nissen-Meyer et al., 2007b).

Fig. 4.7 depicts an example for the individual displacement solutions for each $\tilde{M}_m$ (quadrant on the left), and the final sum for a response to the full 2011 M9 Tohoku earthquake, recorded at station BILL (Eastern Siberia) at 33° distance. Note that the summed trace bears little resemblance with any of the generic solutions to radiation patterns eqs (4.9)–(4.12).

### 4.3.2. Finite Faults

Kinematic rupture over a fault plane can be modelled as a discrete sequence of point sources distributed across the fault plane, each of which may have individual
moment tensors, magnitudes and source-time functions to mimic time-dependent slip. \textit{AxiSEM} is well positioned for an effective incorporation of such finite faults: Due to the rotational symmetries outlined above, the number of simulations for an arbitrary fault is simply given by its number of discrete depth points. The solution for finite-fault displacements may be written in terms of the solution to individual point-source solutions \( u^p \)

\[
    u(x, t) = \sum_p u^p(x, t).
\]  

Note that the dependence on the point-source locations \( x^p \) exists for moment-tensor \( M^p \) (by means of radiation pattern and source-time function), and Green tensor \( G^p \) in Eq. (4.7), requiring separate solutions to the wave equation for each location \( x^p \). A significant shortcut can be made in the case of spherically symmetric media by saving seismograms at “all” distances, and applying rotational properties to the Green tensor. As such, all laterally distributed points \( x^p \) are accommodated within one simulation, and only the discrete depths need to be honored by separate simulations. This is advantageous, as most finite-fault models are mainly distributed laterally, and only require a few depth samplings. This allows for considerable flexibility should one wish to change certain properties of the fault model without conducting new simulations. In light of the common problem of local minima in (non-linear) source inversions, this offers an efficient engine to perform comprehensive studies on the behavior of different fault models and methodologies (Page et al. 2011). The modeling of finite sources is thereby largely delegated to post-processing (see sect. 4.5.3), such that existent \textit{AxiSEM} databases can simply be applied to finite sources as well, and finite faults can be naturally embedded within any application of \textit{AxiSEM} with little additional computational effort.

### 4.3.3. Stochastic Sources

The rotational invariance also facilitates applications of spatially distributed stochastic sources such as ambient noise generated by ocean-continent interactions or crustal scattering (e.g. Boué et al. 2013), or random pressure fluctuations in the Sun’s interior (Gizon and Birch 2002). Similar to finite faults, one simulates point sources at the relevant number of depths (for ocean-continent ambient noise, this is one depth) and relegates the spatial distribution and stochastic time-frequency behavior to post-processing for rotations and filtering, respectively. This helps not only for generating a diffuse wavefield for structural imaging, but also for inverting for ambient-noise source locations.
4.3.4. Discrete Dirac Delta Distribution

It is desirable to simulate Green’s functions, as they offer flexibility with respect to filtering and source-time functions after the simulation. The “source-time function” for the simulation is then a Dirac delta “function”, which, from a rigorous perspective, is meaningless in any discretized system. To retain its attractive properties as the “source time function” to generate Green’s functions, one instead utilizes a triangle function that obeys integral properties of the Dirac distribution. Should one wish to extract a downsampled time series from a simulation of this kind, then the “width” of the Delta function must be adjusted to guarantee the tradeoff between 1) its Delta-function characteristics and 2) sufficient sampling below Nyquist frequency. This is automatically computed in the code, depending on the sampling and period ranges.

4.4. Structural Properties

The definition, discretization and implementation of background models is one of the most critical aspects for accurate wave propagation. Amongst the decision factors are:

• the scale-lengths of structural variations, and their feasible upscaling from a potentially smaller-scale model,

• merging diverse models of source and structure,

• sharp versus smooth variations,

• local reliability and resolution, for instance in global tomographic models.

Uncertain choices amongst these points may lead to an entirely wrong model and consequently useless wave-propagation results. Discretization and meshing in finite-element based methods usually strive to replicate all sharp boundaries of the model. Apart from algorithmic limitations in meshing arbitrary hexahedral elements, any failure to mesh a desired interface leads to false solutions.

AxiSEM offers an internal meshing algorithm which optimally honors any discontinuities in spherically symmetric Earth models, as well as arbitrary discrete spheres of any radial distribution of solid and fluid domains. Axisymmetric structures that are invariant in the azimuthal direction may then be superimposed onto the background mesh on-the-fly in the solver. These structures can be of pre-defined shape
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Figure 4.8.: A mesh for the Sun’s interior which accommodates the radial structure of the Sun for frequencies up to 5 mHz. It honors acoustic wavespeed variations of the Sun across two orders of magnitude (left), leading to seven coarsening (doubling) layers. Density (right) varies by eleven orders of magnitude, but does not affect the meshing process so long as these variations are smooth at the scale of elements. Such a mesh represents the basis for wave propagation and imaging the solar interior utilizing stochastic noise excitation within the framework of time-distance helioseismology.

types, or arbitrarily superimposed by interpolation of discrete external grids (see Section 4.4.4).

4.4.1. Spherically Symmetric Models

Spherically symmetric models such as PREM, IASP91, and ak135 are automatically incorporated in AxiSEM. The code also allows for flexible inclusion of arbitrary 1D structures in the meshing process, such that other Earth models such as those based on mineral physics can be easily accommodated. One may also apply the methodology to other planetary bodies (e.g. Moon, Mars, Europa, not shown here) including purely fluid media to facilitate acoustic wave propagation (a computational shortcut
still popular in the exploration industry), which drastically reduces computational cost.

As a curious case of extreme medium variations readily discretized by our methodology, we reach out for our central star: The sun is a giant fluid sphere subject to turbulent redistribution of masses, magnetic field variations, and acoustic body waves (Gizon and Birch 2002). The background structure of the sun covers many orders of magnitude in density due to its huge size and gravitational force, and about two orders of magnitude in acoustic wavespeed. Only the radial wavespeed gradient matters for meshing, thus it is easily possible to adapt the AxiSEM mesh to the Sun as seen in Fig. 4.8. Surface boundary conditions for acoustic waves (i.e. vanishing pressure) pose no technical difficulty, but are not yet included in the first code release and shall be added in a timely future version.

### 4.4.2. Crustal Variations

Crustal thickness variations from 6–8 km (oceans) to 60–80 km ( continental shields) owing to lithospheric composition have a significant imprint on those seismic phases that are sensitive to shallow structure, such as surface waves which traverse the crust to large distances. Additionally, covering 70% of Earth’s surface, the oceans are also a contributor to wavefield modifications, even though most seismometers are installed on land.

The computational efficiency of a 2D numerical method allows for sufficiently small elements to explicitly mesh the crust, which is also necessary for wavelengths in the range of crustal thicknesses. This is also true for the actual oceans, which may be discretized by actual fluid-domain elements, instead of resorting to a loading equivalent (Komatitsch and Tromp, 2002b) or a homogenized crust (Fichtner and Igel 2008b). Similar to axisymmetric structures, this divides the sphere into oceanic and continental pole-centric rings. Discretized oceans are not available in the first code release, but will be added in the near future.

### 4.4.3. Random media

Spherically symmetric or axisymmetric variations in properties can be as general as desired in the method, including random media variations so long as they are sufficiently smooth and mildly deviatoric. In Fig. 4.9, we show two types of such random variations, perturbing either radial structure (left), or 2.5D structure by maximally 10% velocity variations. Wave propagation through such complex structures can deliver useful insight into wave effects as a function of spatial scale dependence,
scattering and homogenization properties, or the relation between structural heterogeneities and seismic measurements (Baig et al. 2003).

4.4.4. Localized Heterogeneities

The next level of complexity in structural properties is represented by axisymmetric media, which may have arbitrary variations in the source-receiver plane, but are invariant in the perpendicular azimuthal direction. Especially in high-frequency regimes, 3D edge effects from large-scale structures may become less dominant given the decreased ratio between seismic and structural wavelengths, such that Fresnel zones reside within the azimuthal extent of an anomaly. Axisymmetry can then
Figure 4.10.: An example of various lateral heterogeneities, representing realistic deep-mantle structures projected onto the source-receiver plane with azimuthal invariance. The large volume in yellow denotes a Large Low-shear wave Velocity Province (LLSVP), flanked by two exaggerated ultra-low velocity zones (50 km height, 10% $P$-velocity decrease, 20% $S$-velocity decrease, 10% density increase), underlying a detached uprising in the mid-mantle. The implementation is done by assigning laterally heterogeneous properties to the coefficients of the basis functions, as commonly done in high-order spectral-element methods (Peter et al. 2011) so long as elements are sufficiently small to capture variations in a smooth manner.

represent a tangible basis for waveform modelling of unknown arrivals, precursors, undetected arrival delays, oblique reflectors. The only neglected part of the wavefield compared to 3D background models are 3D wave effects from off-plane structures such as 3D elastic lense focusing and off-plane back-scattering. All other scenarios in
which structures vary preferentially in the source-receiver direction are respected, as for instance wave propagation through certain configurations for subduction zones, or forward scattering of small-scale lowermost mantle structures. Fig. 4.10 shows one example of lateral heterogeneities implemented in AxiSEM, including a Large Low-Shear Wave Velocity Province (LLSVP) (Romanowicz and Gung 2002), an Ultra-Low Velocity Zone (ULVZ) (Rost 2013), and a disconnected uprising (e.g. Zhao 2001). These variations are sufficiently smooth to be picked up by the elemental basis functions within the spectral-element mesh (see left panel). The inclusion of such lateral heterogeneities can be done by functional parameterization as shown here, but also by discrete external models. Such arbitrary models are incorporated via KD-tree (Kennel 2004) search for nearest neighbors and interpolation, and therefore allows for any shape and complexity. The accuracy of wave propagation through such models is governed by the scale of heterogeneity versus finite-element size, in that strong variations at short spatial scales tend to be smoothed in the discrete model.

4.4.5. Anisotropy

In a spherically symmetric scenario, the most complex anisotropy is transverse isotropy with 5 independent parameters. In axisymmetry, we may incorporate the full elasticity tensor with triclinic symmetry and 21 independent parameters, so long as the anisotropy does not vary within the azimuthal direction of the Fresnel zone. While logically mandated, this theoretical fact is in itself intriguing: An individual source-receiver wave senses only anisotropic variations within a sufficiently narrow azimuthal range of sensitivity. If, however, a higher complexity of anisotropy is present but varies at a scale larger than the sensitivity of the traveling wave, then this level of large-scale complexity is not extractable from singular seismograms but instead represents an effective image of the actual structure. Van Driel and Nissen-Meyer (2014b) provide a detailed analysis and implementation strategy for anisotropic wave propagation in axisymmetry, including proofs related to the multipole expansion for the presence of general anisotropy in the axisymmetric environment.

4.4.6. Attenuation

Intrinsic attenuation or visco-elastic damping is a natural property of bulk real-Earth structure at relevant frequency ranges of seismic wave propagation. Although models for the quality factor Q (inverse damping) of the mantle show little agreement and the origin of damping may be inseparably coupled with elastic small-scale
scattering, seismic attenuation on waveforms is a well-detected and significant phenomenon. We implemented an improved methodology based on coarse-grain memory variables with negligible additional computational cost compared to purely elastic wave propagation. This further includes attentuative bulk and shear deformation, relaxation mechanisms, a combined linear/non-linear approach to identify optimal sets of parameters for the range of realistic Q, and analytical time stepping. Details on this new implementation, which is applicable to any higher-order finite-element method, are described in a separate paper (van Driel and Nissen-Meyer 2014a).

### 4.4.7. Lack of Ellipticity & Rotation

The Earth’s radius differs, depending on latitude, by up to 40 km between poles and equator. For reasons of axial symmetry, AxiSEM does not allow waves to propagate from a non-polar point source through a pole-centric ellipsoid. To account for ellipticity a posteriori, three options are suggested: 1) phase correction, 2) epicentral distance correction, 3) Born perturbation theory. Phase-specific ellipticity corrections may be applied by shifting waveforms according to predicted traveltime shifts. This is useful only if individual phases are assessed, such as in most cases of tomography, and phase-specific waveform modeling. Epicentral distance correction may be conducted by recalculating receiver coordinates to account for the difference between purely spherical and ellipsoidal geometries, similar to the standard method in traditional tomography (Kennett and Gudmundsson 1996). Finally, Born theory may be applied by assuming ellipticity (including internal interfaces) to act as a boundary perturbations to the spherical model domain. This way, entire seismograms are accounted for jointly. This approach has not been implemented or tested at this point. Rotation of the polar axis can in principle be incorporate in AxiSEM, but only for a polar source, which clearly is a rather unique case of rotation. At the scale of interest where rotation comes into play (above periods of 100 seconds), one could devise a torus-shaped, off-axis source in case its azimuthal radiation is of lesser significance - as may be the case for free oscillations. This would be a field of further study and implementation. In summary, such effects grow into a visible and recordable first-order concern for rather specific cases of seismic data analysis concerned with pathological body-wave paths and very long-period seismology.

### 4.5. Wave-Propagation Applications

Our methodology and the actual code AxiSEM are production-ready and may be used to tackle a diverse range of applications. Here, we sketch some of these, ranging
from basic validation against reference solutions across the frequency spectrum, indefinite solutions to wave propagation, 3D wavefield visualization, lowermost mantle heterogeneities, tomographic models, comparison to recorded data, and sensitivity kernels. All examples are deliberately disconnected as a showcase for the diverse range of applications.

### 4.5.1. High-Frequency Body Waves

Previous publications on an early version of this method and implementation showcased the accuracy by comparison against normal-mode summation (Nissen-Meyer et al. 2008). Normal-mode summation is difficult to achieve at high method frequencies due to the computational cost in generating mode catalogues, as well as numerical issues related to determining the eigenfrequencies. We use an alternative frequency-domain reference solution $Y_{\text{spec}}$ (Al-Attar and Woodhouse 2008) capable of covering the entire relevant frequency band from 0.001 Hz to 1 Hz. Fig. (4.11) shows a record section and some details for both AxiSEM and $Y_{\text{spec}}$ modeling results in an anisotropic, visco-elastic PREM model for a Tonga event at 126 km depth, simulated at a dominant frequency of 1 Hz, i.e. at the limit of teleseismic detection of body waves. The fit is excellent for all phases and distances; the two solutions are indistinguishable almost everywhere out to 1600 propagated wavelengths. Minor differences are amplitude differences, and most probably due to a cut-off in the summation done in $Y_{\text{spec}}$. To our knowledge, this is the first accurate validation of two completely independent methods for anisotropic, viscoelastic media at such high resolution.

### 4.5.2. Free Oscillations

At the grave end of the spectrum, free oscillations dominate and have revealed a great deal about Earth’s internal structure, in particular the Earth’s density structure (Dahlen and Tromp 1998). We strive to provide a numerical method applicable to wave propagation across the observable frequency band. We thus compare amplitude spectra stemming from AxiSEM in a simulation over 48 hours, 1.7 Million time steps, against $Y_{\text{spec}}$ in Fig. (4.12). The fit is again excellent, which is not trivial considering that time-domain numerical methods are exposed to steadily growing numerical dispersion errors with increasing numbers of propagated cycles. To the best of our knowledge, this is the first direct benchmark between time- and frequency-domain methods for free oscillations of the Earth, even if for a spherically symmetric, non-rotating, non-gravitating Earth model. Phase spectra, which may be more
4.5. Wave-Propagation Applications

Figure 4.11.: High-frequency validation (1 Hz dominant frequency) between AxiSEM and Yspec. Top: Record section for vertical displacements of a M4.1 event in Tonga (depth: 126 km), recorded at the stations shown on the map (bottom left) as red triangles. The background model is PREM, including anisotropy and attenuation, and the traces are filtered between seismic frequencies of 0.1-1 Hz, i.e. at the limit of recordable signals in global seismology. The traces from AxiSEM and Yspec are virtually indistinguishable. The zoom sections for individual seismograms (bottom right) on P and S waves (red boxes) represent phases that traveled 500 and 1200 wavelengths, respectively. Time in these panels is normalized to the ray-theoretical phase arrivals (Crotwell et al. 1999), and includes phase (PM) and envelope misfits (EM) measured following Kristekova et al. (2009).
Figure 4.12.: Amplitude spectra simulated by AxiSEM and Yspec for the PREM model (Dziewonski and Anderson 1981) for frequencies below 10 mHz. The time-domain solution provided by AxiSEM extended over 48-hour time series using 1.7 Million time steps. While amplitude spectra do not exhibit issues related to numerical dispersion, the fit between these two different methods is remarkable.

informative for actual studies with normal modes, are shown in (van Driel and Nissen-Meyer 2014b).

4.5.3. Instantaneous Forward Solutions

The reduced dimensionality of AxiSEM opens doors to simulating the entire response due to a given background model once-and-for-all, for all possible source-receiver choices. This seemingly daunting task is rendered tractable by the rotational properties of the displacement vector Eq. (4.2), such that seismograms only need to be stored along the distance range $0–180^\circ$ for sources at a range of depths. This is com-
putable. The remaining problem lies in deciding on a discrete sampling for source depth and receiver spacing to mimic continuous coverage. In the case of depths, this may be defined upon depth uncertainties in different earthquake catalogues, and in the case of receivers by choosing the closest or interpolating upon epicentral distance uncertainty levels.

The computation of such a once-and-for-all solution can be conducted by taking into account the reciprocity of the Green’s function, resulting in only two simulations: one with a vertical and one with a horizontal single force, upon which the strain tensor needs to be stored for all realistic earthquake depths 0–660 km at all distances. This reciprocity shortcut is fueled by the fact that AxiSEM carries the full 3D wavefield automatically, as opposed to reflectivity, DSM, Yspec or normal-modes solutions for which the number of saved seismogram locations factors into the computational cost. The problem is thereby shifted from CPU-time to hard-drive storage. The permanent storage for the entire parameter space spanning all source-earthquake configurations and several Earth models is feasible (tens of Terabytes). Queries to such databases (such as a record section of arbitrary source-receiver geometries, filters, source-time functions, and a range of spherically symmetric Earth models), can be completed within minutes by means of the same kind of post-processing as done upon the AxiSEM code. This can be tremendously beneficial in studies that need to sample a large range of parameters such as source inversion problems, especially in a probabilistic framework (Stähler and Sigloch 2014).

4.5.4. Wavefield Visualization

Most of the applications in this section, as well as in the literature, rely upon seismogram analysis. However, one of the major benefits of this method is the availability of the full global 3D space-time wavefield, for both research and teaching purposes (Thorne et al. 2013). This is possible only due to the collapse to 2D at run-time and the convenience of on-the-fly extraction of the 3D radiation upon azimuthal factors. In practice, this means that one may save the entire 2D wavefield in space and time, and then subsequently decide on any moment tensor, summation, source-receiver geometry, and rendering choices. Fig. 4.13 depicts a snapshot of a typical simulation of a strike-slip event in Italy with a dominant period of 10s and isotropic, anelastic PREM background model. Note the characteristic dispersion in the surface wave

\[2\text{In the meantime, we implemented this approach and describe it in a separate publication, see chapter 5. The code is available at } \text{www.instaseis.net} \]
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Figure 4.13.: Snapshot of a 3D wavefield emanating from a strike-slip event in Italy after 400 seconds. The background model is isotropic, anelastic PREM, and the simulation done at a dominant period of 10s. Note the effect of the radiation pattern on the wavefield in 3D. Similar snapshots are automatically generated in the post-processing of AxiSEM. A movie is available as supplementary material.

train, the large amplitudes in the PP phase, and the 3D radiation pattern. A movie of this setting is available in the supplementary material. Such visualization may offer complementary insight into complex propagation patterns beyond singular trace analysis, in particular as they can be devised as differential wavefields for diagnostic purposes in tracing the influence of changes in model parameters.
4.5. Wave-Propagation Applications

4.5.5. Wave Propagation Through In-Plane Heterogeneities

As mentioned in Section 4.4.4, we may readily insert lateral heterogeneities and compute 3D wavefields upon those torus-like structures. To neglect the imprint of the torus-shaped azimuthal invariance, seismic frequencies should be chosen such that they represent local wavelengths that are smaller than the expected azimuthal extent of a 3D heterogeneity to be modeled. In the regime of 1 Hz, this is warranted for a number of examples, and various lowermost mantle structures have been studied and constrained by waveform modelling for decades (e.g. Igel and Weber 1996; Cottaar and Romanowicz 2013). Constraining geometry and structural composition of these features is crucial for understanding the thermo-chemical, dynamical regime of the Earth’s deep interior. In many previous applications, such structures have been modelled as azimuthally invariant with source-receiver-plane heterogeneity using approximations at frequencies below 0.07 Hz to study core-mantle boundary scattering (Thomas et al. 2000), D" layer (Thorne et al. 2007), and LLSVP structure (Sun et al. 2007). Fig. 4.14 displays seismograms and wavefield snapshots for the model in Fig. 4.10. The record sections highlight phases and distances at which the existence of a ULVZ may be tested, possibly with array methods and stacking. The wavefield snapshots represent a complementary diagnostic for differential studies, from which the most significant imprints can be traced back to the surface, affecting phases such as $PcP$, $ScS$, and $SPKS$.

Modeling of such lateral heterogeneities taps into a regime of wave propagation that offers a grasp of wave effects at resolution and computational cost that is difficult to achieve with alternative methods. Users should however, as always, be cautioned to recognize the structural assumptions imposed on such in-plane features: These may either approximate actual 3D structures well (if the above-mentioned scale separation is warranted), or act as an upper bound of waveform effects (by means of azimuthal overestimation), but conversely they may also neglect elastic focusing and thus underestimate 3D effects.

4.5.6. Tomographic Models

Global models derived from tomography can also be approximated by an in-plane rendition with AxiSEM, in that they usually deviate only mildly and smoothly from spherically symmetric Earth models. Just as in the previous example, wavefield effects captured by this methodology are those that obey forward scattering, whereas true 3D-medium effects such as off-plane scattering are neglected. Of course, this azimuthal invariance does not represent our nature’s dimensionality, but mimics
4. AxiSEM: Broadband 3D Seismic Wavefields in Axisymmetric Media
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Figure 4.14.: A forensic application of *AxiSEM* on the in-plane detectability of an azimuthally invariant representation of two adjacent structures: A “ULVZ” near a “LLSVP” (see model in Fig. 4.10). Top: Seismograms for a model with a ULVZ as in Fig. 4.10 (red traces), and one exactly the same but without the ULVZ (black traces). The underlying Earth model is isotropic PREM (Dziewonski and Anderson 1981), dominant period 2s. The \(N\)-displacement record sections are at considerably large epicentral distance ranges. Bottom: Wavefield snapshot of the same simulation with ULVZ, at time 604 seconds. Blue quadrants denote those parts of the wavefield that are most affected by the presence of the ULVZ (in comparison to a similar plot for the simulation without ULVZ).

a substantial sub-set of those data that are actually used for waveform modeling or tomography rather well and at a cost many orders of magnitude below that of simulating a 3D domain. This can be seen in Fig. 4.15, a comparison between synthetic modeling through a PREM, an in-plane collapse of tomographic model S40RTS (Ritsema et al. 2011), and SPECFEM3D_GLOBE synthetics for S40RTS and CRUST2.0 (Bassin et al. 2000). As seen by the waveforms in Fig. 4.15, many phases are largely insensitive to the added complexity in these models, partly due to the smooth nature of tomographic models (as mandated by their inversion technique). Direct body waves and other early arrivals barely notice the different models, whereas later arrivals and surface waves exhibit considerable differences, most of which can be attributed to the crustal layer. The overall imprint of crustal variations overrides that of the tomographic model. The neglected effects such as 3D backscattering may indeed not contribute all that significantly to resultant seismograms, but this is subject to further parameter-space studies. In general, this provides an efficient new approach should one wish to validate different tomographic models within a synthetic exercise, or modify local properties for a given source-receiver geometry. The actual incorporation of tomographic models is trivial in *AxiSEM* for any model that is given by discrete cartesian, spherical grids, or spherical harmonics.

4.5.7. Relating to data

The ultimate raison d’être of any seismic modeling is its capability to relate to actual observed data, at least in some useful fraction of the generally impenetrable overall parameter space. Here, we showcase a comparison of waveforms at considerably high resolution (5 seconds) to observed data (Scheingraber et al. 2013). This resolution is at the cutting edge of supercomputing with 3D methods (see Fig. 4.1),
Figure 4.15.: Modelling 3D wave propagation through a 2.5D version of tomographic model S40RTS (Ritsema et al. 2011) (top right) for an event near Antarctica (top left). Bottom: Seismograms filtered at 10s from the receivers denoted on the cross section (top right) for 1D model, 2.5D tomographic model, and SPECFEM3D_GLOBE synthetics through S40RTS and CRUST2.0 (Bassin et al. 2000), aligned with the $P$-wave arrival time.
at a frequency range applicable to tomography, and also interesting for waveform modeling of relatively small-scale features in the lower mantle. The map (top right) shows the event and station locations (red triangles for $PKiKP$, blue for $Pdiff$). Filtering has been applied at 5–15 seconds (top), and 15–45 seconds. In the latter case, we included SPECFEM3D_GLOBE synthetics for the S362ANI tomographic model (Kustowski et al. 2008) and CRUST2.0 (Bassin et al. 2000) which are accurate to about 17 seconds (Tromp et al. 2010). AxiSEM synthetics are based on an inverted moment tensor and depth, whereas SPECFEM3D_GLOBE synthetics are taken from the IRIS database, i.e. calculated for GCMT. All synthetics have been convolved with an inverted source-time function. The phases have been aligned by frequency-dependent cross-correlation, forming the basis for tomographic inversions. The waveform differences between all three traces fall within a feasible range of conducting waveform tomography. The timeshifts based on the 13 $Pdiff$ and 6 $PKiKP$ measurements are:

<table>
<thead>
<tr>
<th>filter [s]</th>
<th>method</th>
<th>$\Delta t$ ($Pdiff$) [s]</th>
<th>$\Delta t$ ($PKiKP$) [s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5 – 15</td>
<td>AxiSEM</td>
<td>2.5 ($\sigma^2 = 0.99$)</td>
<td>2.3 ($\sigma^2 = 0.5$)</td>
</tr>
<tr>
<td>15 – 45</td>
<td>AxiSEM</td>
<td>4.0 ($\sigma^2 = 0.89$)</td>
<td>3.4 ($\sigma^2 = 0.3$)</td>
</tr>
<tr>
<td>15 – 45</td>
<td>SPECFEM</td>
<td>3.7 ($\sigma^2 = 0.6$)</td>
<td>6.0 ($\sigma^2 = 0.37$)</td>
</tr>
</tbody>
</table>

Such comparisons include (as per usual) inevitable differences in processing such as event origin time and location, source time function. However, it is noteworthy to recognize the waveform similarity confirming that wave propagation in spherically symmetric Earth models provides an excellent basis for broadband waveform tomography, in particular in the regime of periods below 10 seconds.

4.5.8. Wavefield sensitivity kernels

As a final example, we present the essential and possibly most intriguing application to time- and frequency dependent sensitivity kernels (Nissen-Meyer et al., 2007a). The ability to store entire space-time wavefields from AxiSEM makes it principally trivial to compute time-dependent sensitivity kernels as a comprehensive basis for mapping seismograms to Earth structure, and thus the model-to-data operator for the tomographic inverse problem (Fuji et al. 2012; Colombi et al. 2014). As such, it logically extends existent ray-based or finite-frequency tomographies (which were based on approximate physics) by incorporating complete seismograms, arbitrary time- and frequency-windows as well as arbitrary wave effects such as triplicated
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Figure 4.16.: A comparison of AxiSEM synthetics with recorded data and SPECFEM3D_GLOBE synthetics (Tromp et al. 2010) for a Mw7.5 2009 event in Southern Sumatra at 82km depth. Top right: Event-station distribution, where red triangles are for core-phase PKiKP, blue for CMB-diffracted phase Pdiff. Left: Pdiff synthetics and observed data filtered at 5–15 seconds (top), and 15–45 seconds (bottom). In the latter case, SPECFEM3D_GLOBE synthetics are included which are accurate down to 17 seconds. Bottom right: The same for PKiKP. AxiSEM synthetics are simulated through a viscoelastic, anisotropic PREM model, SPECFEM3D_GLOBE synthetics through the S362ANI tomographic model (Kustowski et al. 2008), and both sets are shifted by cross-correlation traveltimes to align with the respective phases (left: Pdiff, right: PKiKP). Traveltime shifts are about 2–6 seconds (see main text).

Figure 4.17.: A sensitivity kernel computed with wavefields from AxiSEM, time-integrated (time window: 20 s) over the arrival of the direct P-wave at 90° distance for a dominant period of 10 s. This denotes the “region of influence” in which this particular time-window in the seismogram may “see” compressional structure which deviates from the background model. Such kernels are not only the basis for waveform tomography, but may also aid in identifying obscure arrivals in the seismogram.
phases from the mantle transition zone (Stähler et al. 2012), core-mantle diffraction (Colombi et al. 2012), or caustics. Fig. (4.17) shows a sensitivity kernel for cross-correlation travel times with respect to compressional wavespeeds. This was computed with wavefields from AxiSEM, by time-integrating the velocity waveform of dominant seismic period 10 s within a 20 s time window around the $P$-wave arrival time at 90$^\circ$ epicentral distance. The kernel exhibits considerable heterogeneity (partly due to saturated colorscales to highlight its complexity), notably missing the “donut-hole” that is present for pure $P$-wave kernels (Hung et al. 2000). This stems from the fact that our wavefield-based approach honors the large time window, which obscures the purity of phase-based approaches, but correctly represents the measurement corresponding to the time window. Time-dependent sensitivity (i.e. without integrating over the time window) is useful not only as a basis for tomography, but also in a forensic sense to detect faint signals of sensitivity due to a given region or structure. Note that the (separate) calculation of sensitivity kernels is not part of the AxiSEM release, but will be added in the future as a separate package.

4.6. Conclusions

This paper presents a mature method and implementation for global seismic wave propagation across the seismic frequency spectrum by means of a diverse range of applications. It describes crucial extensions with respect to the initial papers (Nissen-Meyer et al., 2007b, 2008) such as the inclusion of anisotropy, attenuation, lateral heterogeneities, finite sources, the basis for sensitivity kernels, and innovative visualization. The method is, to our knowledge, the first time-domain local numerical method successfully benchmarked against independent solutions across the entire frequency band recorded in global seismology, and exhibits excellent scaling on large multi-core systems. The code offers a diverse range of realistic applications in forward and inverse modeling and showcases promising comparisons to recorded data. The moderate computational cost allows for reaching any desirable frequency with moderate resources, and storage of full space-time wavefields for sensitivity kernels.

The presented methodology is most accurate, efficient and useful in parameter regimes which are quite complementary to well-established, mature methods such as normal-mode summation (low-frequency seismology), 3D numerical methods (with local basis functions) such as SPECFEM3D_GLOBE (3D Earth models at intermediate frequencies), and asymptotic ray theory (high-frequency regime with potentially complex wavespeeds). As with any method, the realm of validity for AxiSEM is limited, approximative and blurred, and any application must be undertaken with
4.6. Conclusions

cautions despite the excellent and robust validation shown here and with the actual code available from http://www.axisem.info. This parameter space promises a diverse range of applications which were previously inconvenient, inexact, or unattainable due to limited computational resources or methodologies. Specifically, the main factor attributed to its efficiency in a 2D computational domain is the availability of space-time wavefields for axisymmetric, viscoelastic anisotropic media and realistic earthquake sources.

We have touched upon a few key applications, far and away from explaining or validating each one of them. Rather, the purpose of this paper is to present a new open-source methodology and scan its usability specifically in those directions that we deem most benefitting from this modeling tool. Details on specific applications and implementation are found in other publications to be submitted, and the state of reliable features in the code should always be consulted in its concurrent manual.

All limitations of the methodology are by construction related to the existence of the symmetry axis, which mainly translates into neglecting true 3D media (effects such as 3D off-plane scattering and focusing) and realistic Earth rotation. All other limitations (lack of ocean layer, gravity and topography) mentioned here or in the code reflect the current stage of the algorithm, but pose no fundamental restriction.

4.6.1. Future Additions

Current and future extensions of the presented methodology include low-frequency effects like gravitation (Chaljub and Valette 2004), internal and external topography, and a local-scale version of the method. Sensitivity kernels upon AxiSEM also deliver the basis for scattering solutions to wave propagation, which may then allow for considering mild effects of 3D (Born) scattering, which can be applied to both 3D volumetric and boundary topography. AxiSEM-generated wavefields may also be injected into a small 3D box of local 3D heterogeneities in a hybrid sense (Tong et al. 2014). This will allow for the consideration of teleseismic wavefields to locally travel through 3D heterogeneities (Masson et al. 2013), for instance beneath a dense seismic array above a tectonically active region such as USArray in Western USA or the Pyrenees (Monteiller et al. 2012). It may further be useful to attempt a cost-accuracy benefit analysis across various wave-propagation codes which cover a sensible overlapping parameter space. This is a non-trivial task, as efficiency highly depends on the actual problem at hand (frequency range, distance range, number of sources, number of receivers, multi-scale models, source complexity, solid-fluid domains etc).
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    git clone https://github.com/geodynamics/axisem.git

References


4. AxiSEM: Broadband 3D Seismic Wavefields in Axisymmetric Media


4. AxiSEM: Broadband 3D Seismic Wavefields in Axisymmetric Media


Chapter 5

*Instaseis*: Instant Global Seismograms Based on a Broadband Waveform Database

**Abstract**

We present a new method and implementation (*Instaseis*) to store global Green’s functions in a database which allows for near-instantaneous (on the order of milliseconds) extraction of arbitrary seismograms. Using the axisymmetric spectral element method (*AxiSEM*), the generation of these databases, based on reciprocity of the Green’s functions, is very efficient and is approximately half as expensive as a single *AxiSEM* forward run. Thus, this enables the computation of full databases at half the cost of the computation of seismograms for a single source in the previous scheme and allows to compute databases at the highest frequencies globally observed. By storing the basis coefficients of the numerical scheme (Lagrange polynomials), the Green’s functions are 4th order accurate in space and the spatial discretization respects discontinuities in the velocity model exactly. High-order temporal interpolation using Lanczos resampling allows to retrieve seismograms at any sampling rate. *AxiSEM* is easily adaptable to arbitrary spherically symmetric models of Earth as well as other planets. In this paper, we present the basic rationale and details of the method as well as benchmarks and illustrate a variety of applications. The code is open source and available with extensive documentation at [www.instaseis.net](http://www.instaseis.net).

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5. Instaseis: Instant Global Seismograms Based on a Broadband Waveform Database

5.1. Introduction

Despite the exponential growth of computational power and substantial progress of 3D numerical methods for seismic wave propagation in the last 15 years (Igel et al. 2000; Komatitsch and Tromp 2002b; Tromp 2007; Tromp et al. 2010), the simulation of the highest frequencies observed in seismic waves on the global scale remains a high-performance computing challenge and is not yet done routinely. This is why many seismologists still rely on approximate methods to compute and analyze high-frequency body waves such as ray-theoretical traveltimes (e.g. the TauP-toolkit described in Crotwell et al. 1999), WKBJ synthetics (Chapman 1978), the reflectivity method (Fuchs and Müller 1971) or the frequency-wavenumber integration method (Kikuchi and Kanamori 1982). More recently, several methods that include the full physics in solving the seismic wave equation while reaching the highest observable frequencies by assuming spherically symmetric models have become available, see Fig. 5.1 for an example. These methods include the direct solution method (DSM, Geller and Ohminato 1994; Kawai et al. 2006), the frequency domain integration method (GEMINI, Friederich and Dalkolmo 1995) and a generalization of it including self gravitation (Yspec, Al-Attar and Woodhouse 2008).

As detailed by Nissen-Meyer et al. (2007b), the main drawback of these methods when applied to computing wavefields rather than single seismograms, is their scaling proportional to the number of points in space where the wavefield is sampled. This motivated the development of a direct time-domain approach, where the displacement as a function of space and time is a natural field variable and only needs to be written to disk (Nissen-Meyer et al. 2007a, 2007b, 2008). The implementation of this axisymmetric spectral element method AxiSEM was recently extended to include anisotropy and attenuation (van Driel and Nissen-Meyer 2014b, 2014a), published under public license (Nissen-Meyer et al. 2014) and is available at www.axisem.info.

As computing full global waveforms especially at higher frequencies requires substantial computational resources, several initiatives serve to deliver waveforms by means of databases without having to run a full numerical solver. The ShakeMovie project (http://global.shakemovie.princeton.edu) provides synthetics for earthquakes from the CMT (Global Centroid-Moment-Tensor) catalogue (www.globalcmt.org) recorded at permanent GSN and FDSN stations in 1D and 3D velocity models (Tromp et al. 2010). The Pyrocko toolbox (http://emolch.github.io/pyrocko) provides a Python interface to generate and access Green’s function databases, which for the global case are based on GEMINI, several databases are offered for download. In this paper we present a method that uses AxiSEM to generate global Green’s
Figure 5.1.: Global stack of 1h seismograms accurate to a shortest period of 2 s for an earthquake in 27 km depth computed with Instaseis. The displacement is color-coded analogous to the IRIS global stack (Astiz et al. 1996), i.e. red = transversal component, green = radial component, blue = vertical component. An Automatic Gain Control (AGC) with a window of 100 s length is used to balance large amplitude variations between the various phases. Note that creating this plot does not require to define the source depth at the time of database calculation.
function databases and provides a Python interface for convenient extraction of seismograms. The advantage over ShakeMovie synthetics are the possible higher frequencies and arbitrary source and receiver combinations independent of catalogues and real stations. Compared to Pyrocko with GEMINI synthetics, AxiSEM is more efficient in generating the databases, allowing to routinely compute them for a large number of different background models or specialized applications (e.g. limited depth/distance ranges). Also, by using the Lagrangian polynomials in the SEM mesh as basis functions, it achieves higher spatial accuracy.

This paper is structured as follows. In section 5.2 we present the technical aspects and argue for the choices made in the spatial and temporal discretization. Section 5.3 gives a short overview of the Python interface. In section 5.4 we show the performance with respect to accuracy, speed and disk space requirements for the databases. Finally, we depict a variety of applications in section 5.5.

5.2. Methods

5.2.1. Computing Green’s Functions with AxiSEM

AxiSEM was designed from the beginning with the application of computing global wavefields rather then single seismograms in mind (Nissen-Meyer et al. 2007b). This becomes apparent in the following main advantages in this application: it uses a 2D discretization (Fig. 5.2), with an analytical decomposition of the 3D wavefield into several 2D wavefields. For moment tensor sources, four 2D wavefields are needed, for force sources, two. As it is a time domain method, the displacement field in space-time is a natural field variable of the numerical scheme and simply needs to be written to disk without any extra computational cost when larger regions of Earth are included in the database. AxiSEM uses a spectral element scheme for spatial discretization which lends itself well to parallelization on HPC systems. As it is based on the weak formulation of the wave equation, it naturally includes the free surface boundary condition and allows for highly accurate modeling of surface waves.

Nissen-Meyer et al. (2014) argued against using collective parallel I/O since the availability of the NetCDF libraries (Rew and Davis 1990) was not granted on all supercomputers. For that reason, we implemented a round robin I/O scheme, which remains advantageous when running AxiSEM on less than about 100 cores in parallel and to avoid installation problems on systems where NetCDF is not available as a pre-compiled package. On supercomputers however, the situation has since improved and NetCDF compiled with parallel support seems now to be widespread. For this
5.2. Methods

Figure 5.2.: The 3D wavefield is decomposed analytically into monopole, dipole and quadrupole radiation patterns (left) and the remaining 2D problem is solved on a D-shaped domain (right) using the spectral element method. While the forward databases require a total of four 2D computations, it is only two for the backward databases using reciprocity of the Green’s function: one for the vertical and one for the horizontal components. (modified from Nissen-Meyer et al. 2014)

reason, we implemented a collective parallel I/O scheme that performs well, even when running on more than 1000 cores, see Table 5.1. In this scheme, all processes that have to write data to disk communicate via the message passing interface (MPI) and then write collectively at the same time to the parallel file system. This way we achieved throughputs of up to 4 GB/s on SuperMUC.
5.2.2. Forward and Backward Databases

*Instaseis* has the capability of dealing with forward wavefields, i.e. the waves are propagated from a moment-tensor point source at fixed depth (i.e. receivers exist throughout the medium), as well as backward or reciprocal wavefields, where the wavefields are propagated from a single-force point source at fixed depth and recorded throughout the medium (i.e. sources exist throughout the medium).

Potential applications of forward databases are the generation of 3D wave-propagation movies (Holtzman et al. 2013), the computation of incoming teleseismic waves in 1D/3D hybrid methods (e.g. Monteiller et al. 2012; Masson et al. 2013) or the forward field in the computation of sensitivity kernels (Nissen-Meyer et al. 2007a) for seismic tomography. To generate a forward database, a total of four runs with *AxiSEM* are needed (Nissen-Meyer et al. 2007b).

In contrast, reciprocal databases utilize the reciprocity of the Green’s functions, and are useful in all cases where the receivers are at fixed depth, thus for instance mimicking earthquake catalogues recorded at stations along the surface. The source can be located anywhere in the region where the Green’s functions are recorded in the simulation, thus allowing for unlimited choices in the source-receiver geometry. To generate a reciprocal database, a total of two runs with *AxiSEM* are needed, one for the vertical component and one for both horizontal components of the seismogram (Nissen-Meyer et al. 2007b). It is also possible to compute a database for the vertical component seismograms only, which is then a factor of 3 faster and uses only about 40% of the disk space.

5.2.3. The Spatial Scheme

For the spatial discretization we choose to keep the same basis as used in *AxiSEM*. The displacement $u$ within each element is expanded in terms of Lagrangian polynomials $l_i$ (see Fig. 5.3) of order $N$ defined on the integration points of the spectral element scheme (see Fig. 5.4):

$$u(\xi, \eta, t) = \sum_{i,j=0}^{N} u_{ij}(t)l_i(\xi)l_j(\eta); \quad (5.1)$$

$\xi$ and $\eta$ are the reference coordinates of the element and $N$ typically has a value of 4. This approach has several advantages.

- The wavefield is represented by polynomials, typically of degree 4, interpolation is hence of 4th order accuracy.
5.2. Methods

**Figure 5.3.** Lagrangian basis polynomials $l_n(\xi)$ of fourth order in one dimension. At the collocation points, all but one are zero, such that the value of the interpolated function at this point coincides with the coefficient in this basis expansion.

**Figure 5.4.** Lagrange interpolation points inside an element (gray) and its neighbours. Coordinates $\xi$ and $\eta$ are the reference coordinates of the gray element. Points on the edges (black squares) are shared between neighbours and function values at these points need to be stored only once if the function is continuous (e.g. displacement). The number of global degrees of freedom per element of such functions is thus approximately 16 compared to 25 for discontinuous functions (e.g. strain).
5. Instaseis: Instant Global Seismograms Based on a Broadband Waveform Database

- The basis is local and only few coefficients are needed to represent the wavefield inside an element (typically 25), in contrast to e.g. global basis functions such as spherical harmonics.

- Discontinuities in the model that cause discontinuities in the strain Green’s functions are respected by the mesh.

- The strain tensor (representing the moment tensor in the reciprocal case) can be computed on the fly from the stored displacements at high accuracy. This reduces the storage by a factor of 2 as the displacement has 3 degrees of freedom, compared to 6 for the strain.

- Since the displacement is continuous also at model discontinuities and element boundaries, it needs to be stored only once at all Gauss-Lobatto-Legendre (GLL) points that belong to multiple elements, reducing the storage by another factor of $16/25 = 0.64$ (see Fig. 5.4).

- Storing the displacement allows to use force sources as well without any extra computation or storage requirements.

Fig. 5.5 visualizes the spatial representation for a long period mesh (50s) for the Rayleigh wave train and the $G_{rr,r}$ component of the strain Green’s tensor: the strain is smooth also across the doubling layer of the mesh where the background model (ak135f, Montagner and Kennett 1996) is smooth as well. Still, the discontinuities of the model and hence the strain are explicitly represented by this discretization and the resolution of the mesh is adapted to the local wavelength, as for instance in the crust. Figure 5.6 shows an example for 2 s shortest period and compares the SEM discretization to regular depth sampling. In the regular sampling case with nearest neighbour interpolation, the phase and envelope errors can be quite large, especially close to the model discontinuities (up to 80% envelope misfit and 4% phase misfit as defined by Kristekova et al. (2009)) and for very shallow sources (up to 40% envelope misfit and 14% phase misfit).

Finite Element Mapping

One performance-critical step in the spatial scheme is to find the reference coordinates $(\xi, \eta)$ inside the spectral element that includes a point given in global coordinates $(s, z)$. While the opposite mapping is trivial because this is how the elements of the SEM are defined (Nissen-Meyer et al. 2007a, appendix A1), it cannot be generally inverted easily. Hua (1990) presents an analytical inverse solution for
5.2. Methods

Figure 5.5.: Snapshot of one component of the Green’s tensor \( (G_{rr,r}) \) as represented in the SEM basis for a shortest period of 50s. Discontinuities such as caused by the crustal layers are exactly represented and the wavefield is smooth across doubling layers of the mesh.

We follow a two-step approach to finding the reference coordinates. First, we find the six closest element midpoints to limit the search to a small number of candidate elements in which the point could be. The number six is specific to the AxiSEM mesh, where each corner point can belong to a maximum of six elements in the doubling layers, see Fig. 5.7. This step can be seen as approximating the AxiSEM quadrilateral elements, which is quite involved and not easy to generalize for the semicircular elements used in AxiSEM.
Figure 5.6: One component of the strain Green’s tensor ($G_{rr,r}$) for a distance of 30° as a function of time and depth with a shortest period of 2 s. (a) SEM basis vs. (b) regular sampling with 1 km distance and (c) phase and envelope misfits (EM and PM in the legend, see Kristekova et al. 2009) caused by the regular sampling computed in the period range 1-20 s. Dashed lines in the left panel sketch the spectral elements. The crustal discontinuities of ak135f (Montagner and Kennett 1996) are indicated by solid lines and lead to discontinuities in $G_{rr,r}$, which are exactly represented in the SEM basis.
5.2. Methods

Figure 5.7.: Voronoi approximation (colored) of the AxiSEM mesh (black lines) using the midpoints of the elements (red circles) only, zoomed onto a doubling layer for a 50 s mesh. For most elements, the Voronoi cell coincides almost exactly with the AxiSEM element, note that most of the AxiSEM elements have edges of concentric circles while the edges of the Voronoi cells are all straight lines. In the worst case, six AxiSEM elements have to be tested whether a point is inside or not.

mesh with Voronoi cells. For most points, the closest midpoint will already indicate the correct element, in the worst case the second step has to be performed for all six candidates.

In a second step, the reference coordinates \((\xi, \eta)\) of the given point \((s_p, z_p)\) are computed for the six candidate elements sorted by the distance of the midpoints. If both \(\xi\) and \(\eta\) are in the interval \([-1, 1]\), the element is found. The coordinates \((\xi, \eta)\) are computed using an iterative gradient scheme adopted from SPECFEM3D (Komatitsch and Tromp 2002a). Starting from the midpoint of the candidate element, updated values are found by linear approximation of the inverse mapping:

\[
\begin{pmatrix}
\xi_{n+1} \\
\eta_{n+1}
\end{pmatrix} = \begin{pmatrix}
\xi_n \\
\eta_n
\end{pmatrix} + \mathcal{J}^{-1}(\xi_n, \eta_n) \cdot \begin{pmatrix}
s_p - s(\xi_n, \eta_n) \\
z_p - z(\xi_n, \eta_n)
\end{pmatrix}
\]

(5.2)
Figure 5.8.: Normalized amplitude spectra of the Gaussian source time function (sliprate) used at 2s mesh period and a vertical component synthetic seismogram recorded at 40° epicentral distance. The vertical lines denote the resolution of the mesh and the Nyquist frequency of the downsampling using 4 samples per mesh period.

with the Jacobian matrix defined as

$$\mathcal{J}(\xi, \eta) = \begin{pmatrix} \frac{\partial s}{\partial \xi} & \frac{\partial s}{\partial \eta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} \end{pmatrix},$$

(5.3)

and the mapping $s(\xi, \eta)$ and $z(\xi, \eta)$ depending on the element type as defined in Nissen-Meyer et al. (2007b). In the AxiSEM mesh, this iteration converges to numerical accuracy within less than 10 iterations and is not performance critical for Instaseis as it is only used on the few candidate elements. Also, this two-step approach requires only the midpoints of all elements in the mesh to be read from file on initialization and can be implemented efficiently using the kd-tree provided by the SciPy package (Jones et al. 2001).

5.2.4. The Temporal Scheme

The design of the temporal scheme is guided by a number of constraints on the spectrum of the source time function: the spectrum should decay steep enough above the highest frequency resolved by the mesh, such that the least number of samples according to the Nyquist criterion can be used without introducing aliasing. On the other hand, it should not decay too steeply, such that it is still possible to deconvolve and convolve with another source time function. Additionally, the spectrum should
5.2. Methods

Figure 5.9.: Lanczos kernels used for resampling. For large values of the parameter $a$, it converges towards the sinc function, which is the kernel that allows exact reconstruction for bandlimited signals as stated in the Nyquist sampling theorem (Nyquist 1928).

be as flat as possible within the usable frequency range and 'earthquake-like' without the necessity of deconvolving it when extracting a seismogram from the database. An actual delta function as would be required for true Green’s functions cannot be represented in a discrete approximation as it is not bandlimited.

We found a Gaussian source time function with $\sigma = \tau/3.5$ to fulfill these requirements, where $\tau$ is the shortest period resolved by the mesh. Fig. 5.8 shows the amplitude spectra of this source time function as well as a corresponding velocity seismogram at a distance of 40°. The two spectra have a very similar general shape and decay to $10^{-3}$ of the maximum at half the shortest period. This motivates that sampling with four samples per period will not introduce aliasing artifacts. It is desirable to retrieve seismograms from the database with arbitrary time steps, which requires interpolation or resampling. Popular time domain schemes such as interpolation by low-order polynomials or splines do not work well close to the Nyquist frequency. On the other hand, frequency domain resampling by zero-padding the discrete Fourier transform of the signal can only resample to rational multiples of the original sampling interval. Finally, the kernel from the theoretically exact reconstruction according to the Nyquist-Shannon sampling theorem (i.e. the sinc function) has infinite support which renders it impractical as well (see Burger and Burge 2009, section 10.3 for an extended introduction to interpolation).

Therefore, we adopt the Lanczos resampling scheme, which is popular in image processing and an approximation to the sinc-resampling with finite support. The Lanczos kernel is defined as the sinc function multiplied by the Lanczos window.
Figure 5.10.: Resampling using a Lanczos kernel with $a = 12$ of a P arrival velocity seismogram convolved with the source time function from Fig. 5.8 recorded at 40° distance, and the resampling error multiplied by a factor of 100. The relative error is on the order of 0.05% of RMS, see Fig. 5.11.

Figure 5.11.: RMS error of the resampling using the first 1800s of the seismogram from Fig. 5.10. Convergence is reached around $a = 20$. It does not converge to zero because some high-frequency energy was neglected in the downsampling, see Fig. 5.8.

function (Burger and Burge 2009):

$$L(t) = \begin{cases} \text{sinc}(t) \text{sinc}(t/a) & \text{if } t \in [-a, a] \\ 0 & \text{else,} \end{cases}$$  \hspace{1cm} (5.4)$$

where $a$ is a parameter to control the number of samples to be used in the interpo-
>>> import instaseis
>>> db = instaseis.open_db("./AK135")
>>> receiver = instaseis.Receiver(network="BW", station="ZUGS",
                                latitude=47.416, longitude=10.979)
>>> source = instaseis.Source(
    latitude=89.91, longitude=0.0, depth_in_m=12000,
    m_rr = 4.71e+17, m_tt = 3.81e+15, m_pp = -4.74e+17,
    m_rt = 3.99e+16, m_rp = -8.05e+16, m_tp = -1.23e+17)
>>> st = db.get_seismograms(source=source, receiver=receiver)
>>> print(st)

3 Trace(s) in Stream:
  BW.ZUGS..LXZ | 1970-01-01T00:00:00.00Z - ... | 2.1 Hz, 7746 samples
  BW.ZUGS..LXN | 1970-01-01T00:00:00.00Z - ... | 2.1 Hz, 7746 samples
  BW.ZUGS..LXE | 1970-01-01T00:00:00.00Z - ... | 2.1 Hz, 7746 samples

Figure 5.12: The Instaseis Python API demonstrated in a short interactive Python session. A Source and a Receiver object are created and then passed to the get_seismograms() method of an InstaseisDB object. This will extract the Green’s functions from the databases and perform all necessary subsequent steps resulting in directly usable three-component seismograms in form of an ObsPy Stream object. Please refer to the Instaseis documentation for details.

Interpolation and the sinc function is defined as

\[ \text{sinc}(t) = \frac{\sin(\pi t)}{\pi t} \]  \hspace{1cm} (5.5)

Interpolation is then performed by convolving the discrete signal \( s_i \) with this kernel and evaluating it at the new time samples \( t_j \) (Burger and Burge 2009):

\[
S(t_j) = \sum_{i=\lfloor t_j/\Delta t \rfloor-a+1}^{\lfloor t_j/\Delta t \rfloor+a} s_i L(t_j/\Delta t - i),
\]  \hspace{1cm} (5.6)

where \( \lfloor \cdot \rfloor \) denotes the floor function and \( \Delta t \) the sampling interval of the original signal. Figure 5.9 shows the Lanczos kernel for different values of \( a \), Fig. 5.10 shows a practical example of resampling a seismogram. In Fig. 5.11 we test a number of values for \( a \) for the first 1800 s of the same seismogram and we find \( a = 12 \) to be a reasonable compromise between cost (using 25 samples in the interpolation) and accuracy (RMS error of 0.03%).

5.3. Python API

Instaseis is implemented as a library for the Python programming language with some performance critical parts written in Fortran. Furthermore it directly inte-
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...
### 5.4. Benchmarks

#### 5.4.1. Accuracy

As we already provided some rigorous validation comparing *AxiSEM* synthetics to a reference solution (*Yspec* Al-Attar and Woodhouse 2008) in van Driel and Nissen-Meyer (2014b, 2014a), the purpose of this section is only to confirm that using the new scheme with reciprocal computations, spatial interpolation and temporal resampling does not decrease accuracy. Fig. 2.4 shows a record section and some details for *Instaseis*, *AxiSEM* and *Yspec* seismograms computed in the anisotropic, visco-elastic PREM model for an event at 126 km depth beneath Tonga bandpass filtered to 50 s to 2 s period.

While this figure is similar and the *AxiSEM* and *Yspec* reference data actually the same as presented in van Driel and Nissen-Meyer (2014a, Fig. 11), it is important to note that they were generated in very different ways: here we computed a whole Green’s function database for all epicentral distances and down to 700 km source
Figure 5.14.: *continued from Fig. 5.13* The traces are recorded at the GSN stations indicated in the map. The zoom windows are depicted with gray rectangles in the record section and the time scale is relative to the ray-theoretical arrival. \( EM \) and \( PM \) (Kristekova et al. 2009) denote the envelope and phase misfit between Instaseis and Yspec traces in the corresponding time window.
depth and changing source or receivers would cost a few milliseconds only. In our previous approach, this would have required a full new AxiSEM simulation on the order of 10K CPU hours computational cost. Also, in contrast to van Driel and Nissen-Meyer (2014a), we used default mesh parameters for 2 s period and time step close to the stability limit of the 4th order symplectic time scheme (Nissen-Meyer et al. 2008). Still, the phase misfit (Kristekova et al. 2009) is well below 1% in all zoom windows and the maximum of the envelope misfit is 2% for the PPP phase on station ALE.

The fact that these traces are virtually indistinguishable for such a demanding setup of wave propagation over 800 wavelengths (waves at 2 s period traveling for 1600 s) verifies that the entire workflow of computing and querying the database are correctly implemented. In particular, numerical reciprocity (i.e. the different force and moment sources), on-the-fly calculation of the strain tensor as well as temporal and spatial sampling have no significant adverse effect on accuracy, i.e. any remaining errors vanish within numerical accuracy of the forward solver AxiSEM.

5.4.2. Database Size

One major constraint for computing a database beside the CPU cost is the permanent storage requirement. Here, we summarize the most important parameters and the related scaling of the required disk space. The amount of data scale with the third power of the highest frequency resolved by the mesh, but zip compression is slightly more efficient for longer traces, resulting in an empirical exponent of 2.7, see Fig. 5.15. Scaling with the length of the seismograms is slightly stronger than linear, again because the compression is more efficient on the zeros before the first P arrival. Scaling with depth and epicentral distance range is linear, where the prefactor for depth scaling is halved at each doubling layer of the mesh. The reciprocal databases for vertical (40%) and horizontal (60%) components are computed and therefore usable independently.

Several examples are shown in Fig. 5.15: for Earth, a complete reciprocal database including all three components, all epicentral distances and sources down to 700 km and one hour of seismogram length accurate down to 2 s period, is about 1 TB in size. Calculating such a database once and storing it on a central server will give any user arbitrary and immediate access to short period synthetic seismograms without any further cost. More specialized databases are possible: for example to study inner core phases for shallow events in an epicentral distance from 140° to 160°, 200 GB storage suffices to store a database with a frequency of 2 Hz.
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Figure 5.15.: Storage requirements of the reciprocal databases for PREM after zip compression for all three components and several parameter sets (maximum source depth, components, seismogram length and epicentral distance range). Dashed lines are fitted functions $g(f) = af^{2.7}$, where each point was weighted with the frequency $f$ to ensure better fitting at the higher frequencies. The exponent is slightly smaller than the expected 3, because the zip compression is more efficient for longer time traces. At long periods, element sizes are governed by the layer thickness rather than the wavelength, resulting in the discrepancy from the power law at long periods.

5.4.3. Performance

To evaluate the overall performance of Instaseis, two distinct parts have to be analyzed: First, the databases have to be generated with AxiSEM. Though very efficient, the database generation at short periods is a high-performance computing task. However, AxiSEM scales well on up to 10,000 cores such that global wavefields can be computed at the highest frequencies within hours on a supercomputer. Detailed performance and scaling tests of AxiSEM can be found in Nissen-Meyer et al. (2014), here we just show the total CPU time required to compute full databases (i.e. horizontal and vertical component) for 1 hour long seismograms for two different time schemes (2nd order Newmark and 4th order symplectic Nissen-Meyer et al. 2008) and two planets (Earth and Mars) at a variety of resolutions, see Fig. 5.16. The general scaling of AxiSEM is proportional to $T^{-3}$, where $T$ is the shortest period resolved by the mesh. The slight discrepancy from this power law at longer
5.4. Benchmarks

Table 5.1.: I/O performance for a typical setup of AxiSEM on SuperMUC. The simulation parameters were as follows: 2 s shortest period, 3600 s simulation length, model: ak135f, vertical component and maximum source depth 700 km. The resulting uncompressed wavefield file has a size of 675 GB. The I/O throughput is not affected much by the number of CPUs involved. The throughput between different runs varies, which is probably caused by the changing I/O load on the system.

<table>
<thead>
<tr>
<th>#CPUs</th>
<th>Runtime</th>
<th>I/O time</th>
<th>Throughput</th>
<th>rel. I/O time</th>
</tr>
</thead>
<tbody>
<tr>
<td>4624</td>
<td>1091 s</td>
<td>196 s</td>
<td>3.44 GB/s</td>
<td>18.0 %</td>
</tr>
<tr>
<td>2304</td>
<td>1802 s</td>
<td>281 s</td>
<td>2.40 GB/s</td>
<td>15.6 %</td>
</tr>
<tr>
<td>1152</td>
<td>2359 s</td>
<td>167 s</td>
<td>4.04 GB/s</td>
<td>7.0 %</td>
</tr>
<tr>
<td>576</td>
<td>4482 s</td>
<td>193 s</td>
<td>3.50 GB/s</td>
<td>4.3 %</td>
</tr>
</tbody>
</table>

Figure 5.16.: Computational cost in CPU hours (measured on Monte Rosa, a Cray XE6, for Earth and Piz Daint, a Cray XC30, for Mars) to generate full Instaseis databases with 1 hour long seismograms for two time schemes: 2nd order Newmark and 4th order symplectic.

periods is due to the thin crustal layers causing a smaller global time step in the simulation. Simulations for Mars are approximately a factor 5 faster than for Earth, due to the smaller radius.

The performance of the second part, the seismogram extraction, on the other
Figure 5.17: Results of benchmarks for four typical use cases run on different hardware with a variety of shortest periods. Each run calculates 1000 three-component seismograms for the same database, with the top and bottom values discarded, and the mean of the remaining values used in the benchmark. The graphs show the inverse time for the calculation of the three-component seismogram and illustrate the speed of the CPU and I/O bound scenarios, illustrating the efficiency of the buffer in the finite source scenario for the 2 second run and the efficiency of the buffer in the space source scenario for the 2 second run.
hand is rarely limited by raw computing power. It scales linearly with increasing frequency of the databases’ Green’s functions and can easily be accomplished on a standard laptop. The limiting factor in most cases is the latency of the storage system, e.g. the time until it starts reading from the database. To alleviate this issue we implement a buffering strategy on the functions reading data from the files: The Green’s functions from a whole element of the numerical grid are read once and cached in memory. If data from the same element is needed again at a later stage it will already be in memory thus avoiding repeated disc access. Once the cache memory limit is reached, the data with the earliest last access time is deallocated, effectively resulting in a priority queue sorted by last access time. This optimization is very effective for most common use cases as they oftentimes require seismograms in a small range of epicentral distances and depths.

*Instaseis* comes with a number of integrated benchmarks to judge its performance for a certain database on a given system. The benchmarks emulate the computational requirements and data access patterns of some typical use cases like finite source simulations and source parameter inversions. Finite sources within the benchmarks are simulated by calculating waveforms for moment tensor sources on an imaginary fault plane along the equator ranging from the surface to a depth of 25 km. One source is calculated for each kilometer in depth until the bottom of the fault is reached. This is repeated each kilometer along the fault’s surface trajectory until the benchmark terminates. A source parameter inversion is simulated by calculating seismograms from moment tensor sources randomly scattered within 50 km distance to a fixed point. Results for four runs are shown in Figure 5.17. As is the case with all benchmarks they have to be interpreted carefully, nonetheless they demonstrate the behaviour and performance characteristics of *Instaseis* on real machines.

### 5.5. Applications

In this section we depict several possible use cases of *Instaseis*. This list is not exhaustive and deliberately unconnected to provide a broad overview.

#### 5.5.1. Graphical User Interface

To prominently highlight the features and nearly instantaneous seismogram extraction for arbitrary source and receiver combinations of *Instaseis*, we developed a cross-platform graphical user interface (GUI), shown in Figure 5.18. It ships with
Figure 5.18: Screenshot of the Instaseis graphical user interface (GUI). Aside from quickly exploring the characteristics of a given Green's function database, it is a great tool for understanding and teaching many features of seismograms. The speed of Instaseis enables an immediate visual response to changing source and receiver parameters. The left-hand side shows three-component seismograms where the total traveltime is overlaid as vertical lines.
the standard Instaseis package and is written in PyQt, a Python wrapper for the Qt toolkit. Most evidently, this may be used for visual inspection and verification of any given AxiSEM Green’s function database. Instaseis’ performance permits an immediate visual feedback to changing parameters. This also delivers quantitative insight for an intuitive understanding of the features and parameter sensitivities of seismograms. Examples of this are the polarity flips of first arrivals when crossing a moment tensor’s nodal planes, the triplication of phases for shallow sources, the Hilbert transformed shape of reflected phases and the relative amplitude of surface waves (especially overtones) depending on the earthquake depth. Furthermore, the GUI allows the calculation of seismograms from finite sources and the exploration of waveform differences in comparison to best-fitting point sources.

5.5.2. IRIS Web-interface

To enable usage of Instaseis seismograms to a broader community, we aim to remove all hurdles of computing and storing large databases locally. To this end, and in collaboration with IRIS, we plan to establish a web interface to the Instaseis databases. In contrast to the ShakeMovie approach (Tromp et al. 2010), this interface will be able to handle arbitrary sources and receivers independent from catalogue data or other parameter limitations. The interface and databases will be described and benchmarked in detail in a separate publication, the status of this project can be viewed on http://ds.iris.edu/ds/products/ondemandsynthetics.

5.5.3. Finite-Frequency Tomography

In finite-frequency tomography (e.g. Nolet 2008) information is extracted from recorded seismograms by matched filters in multiple frequency bands (Sigloch and Nolet 2006; Colombi et al. 2014). A matched filter correlates a predicted signal with the measured signal to detect the predicted signal in the presence of noise. In the case of seismic tomography, a synthetic seismogram is necessary, which is usually created by convolving a Green’s function with an estimated source-time function. For body waves, short periods down to 1s are commonly used (e.g. Stähler et al. 2012; Hosseini and Sigloch 2015). Typical data sets contain thousands of earthquakes (e.g. Auer et al. 2014), each recorded at hundreds of stations, resulting in up to a million waveforms. For each of these waveforms, a separate Green’s function has to be calculated, which requires solving the seismic forward problem at the desired frequencies. For wave propagation methods that solve the forward problem
separately for each event, computing these reference synthetics presents a formidable computational challenge, which is why previous studies resorted to approximate solutions like WKBJ (Chapman 1978) or the reflectivity method (Fuchs and Müller 1971). The full method implemented in Yspec (Al-Attar and Woodhouse 2008) is about an order of magnitude faster than AxiSEM in computing seismograms for a single source. However, at least in the current implementation the cost scales linearly with the number of events.

As Instaseis takes advantage of reciprocity of the Green’s function, we can now build the whole database for all possible sources with only two runs of AxiSEM: one for the vertical and one for the horizontal components. Figure 5.19 compares the computational cost of computing the reference synthetics down to 2 s period assuming that each event was recorded at 1000 three-component stations. Ignoring the cost of computing the database, Instaseis is comparable in performance to WKBJ, but actually returns full seismograms including all phases, see Figure 5.20. In contrast
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Figure 5.20.: Comparison between observed seismograms (black) and Instaseis synthetics for the Sumatra earthquake on September 30, 2009 with magnitude Mw 7.5 at 82 km depth. Vertical axis labels are epicentral distances, horizontal is time relative to the ray-theoretical arrivals. A Gabor filter with 3.7 s central period is applied to all traces and the synthetics are convolved with an inverted source time function (Sigloch and Nolet 2006). The waveforms are aligned by computing relative time-shifts between data and synthetic seismograms using cross-correlation (similar to actual finite-frequency tomography).

to WKBJ, where each crustal reverberation has to be defined separately, it automatically calculates the full crustal response. Also, it appropriately models diffracted phases such as \( P_{\text{diff}} \) and triplicated phases from upper mantle discontinuities. If we include the database generation, Instaseis breaks even in computational cost with \( Y_{\text{spec}} \) already at about 14,000 waveforms, i.e. five events with 1000 three-component stations each. At about 5 \( \cdot 10^8 \) waveforms, the cost of extracting the seismograms from the database becomes dominant over the database generation. Assuming 2000 seismograms per event, this is equivalent to 10,000 earthquakes, i.e. in the order of available earthquake catalogues. However, generating seismograms with different source locations or moment-tensor radiation patterns, which is often necessary in tomography, does not require a new database generation.
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5.5.4. Probabilistic Source Inversion

Uncertainties in source parameters have been shown to have a strong influence on waveform tomography (Valentine and Woodhouse 2010). Probabilistic point source inversion estimates the uncertainties of source parameters and their correlation. From these, the effect on seismic tomography can be estimated (Stähler and Sigloch 2014). It requires the repeated calculation of synthetic waveforms for varying moment tensors, depths and source time functions to calculate the likelihood and posterior probability density of models in a Bayesian sense. Changing source time function and moment tensor is extremely efficient from an Instaseis perspective, and the limitation to a fixed epicenter means that the I/O buffering can be done very efficiently, which is reflected in the Source Inversion test case in the benchmark (Fig. 2.4).

From a previous study (Stähler and Sigloch 2014), we assume that for an inversion for depth, the moment tensor and the source time function, a 20-dimensional model space has to be sampled, which requires to perform roughly 60,000 forward simulations. Using 100 seismic stations and three-component seismograms, this means that roughly $1.8 \cdot 10^7$ waveforms have to be calculated for one source inversion, costing on the order of 50-100 CPU hours (Fig. 5.19).

5.5.5. Finite Sources

Finite sources can be represented in Instaseis by a cloud of point sources without limitations on the fault geometry or source time functions. Each point source needs to be attached with a moment tensor, a sliprate function and a time shift relative to the origin time. These can for instance be retrieved from standard rupture format (*.srf) or subfault format (*.param) files as provided by the USGS for most events with $M > 6.5$. As a show case, we computed the seismograms for the source inversion validation (SIV) exercise #3 (http://equake-rc.info). The source is a $M 7.8$ strike-slip earthquake on the San Andreas Fault represented by $\approx 10^5$ point sources, where each source has a different mechanism and sliprate function. The 52 stations are in $30^\circ$ to $90^\circ$ epicentral distance (see Fig. 5.21), where the P wave arrival is supposed to be well separated (compare Fig. 5.1). Excluding the cost of generating the database, it cost a total of 12 CPU hours to compute the 52 one hour long three-component seismograms accurate down to 5 s.

Fig. 5.22 compares the Instaseis seismograms to P-phases computed with the frequency wavenumber integration method (fk) by Kikuchi and Kanamori (1982), where only direct and surface reflected phases where taken into account. While the
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Figure 5.21.: Stations used in the source inversion validation (SIV) exercise. Circles mark 30°, 60° and 90° epicentral distance. The source is a strike-slip earthquake in Southern California represented by $\approx 10^5$ point sources, the beachball represents the centroid moment tensor, i.e. the orientation and predominant direction of slip of the overall fault.

First arriving waves agree to certain extent with Instaseis providing systematically larger amplitudes, there are significant differences for later time windows. These are due to additional phase arrivals within the time window (especially triplicated PP, compare Fig. 5.1) and crustal reverberations not modeled by the fk method. For events with long rupture durations as in this example (200 s) this suggests that more accurate waveforms should be beneficial for finite source inversions.
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Figure 5.22: Seismograms for the SIV benchmark, Z-component aligned on the P arrival band-pass filtered between 5 and 100 s period. The labels denote the station code and epicentral distance. In the frequency-wavenumber integration ($fK$, Kikuchi and Kanamori 1982), only direct P and the depth phases were included, while Instaseis provides full seismograms, including PP, PcP and other phases. Especially for the stations in less than 40° distance, the effect is profound, since PP arrives as a triplicated complex wave train only 70-100 s after P. Due to the long source duration, the PP arrival overlaps with the direct P wave train for several stations.

5.5.6. Insight / Mars

The upcoming NASA-lead Mars Insight mission (Banerdt 2013), to be launched in March 2016 and scheduled to land September 2016, will deploy a single station with both a broad-band and a short-period seismometer on Mars. This will be the first extra-terrestrial seismic mission since the Apollo lunar landings (1969–1972) and Mars Viking missions (1975) with the goal of elucidating the interior structure of a planet other than Earth. The instrument will record local, regional, and more
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Figure 5.23.: Seismic waves traveling in Mars after a meteorite impact at its north pole computed with *AxiSEM*. P-waves are shown in blue and S-waves and surface waves in red.

distant marsquakes (including meteorite impacts) and send data back to Earth for analysis.

Our knowledge of the seismic structure of Mars is limited because of lack of resolution of currently available areophysical data (e.g., Khan and Connolly 2008) and the limited sensitivity of the Viking seismometers due to their installation on board of the lander. For this reason, we will generate databases of “reference” seismic waveforms for a comprehensive collection (order of magnitude 1000) of 1D Martian models to be used by modelers and analysts in preparation for the Insight mission. The models are constructed from current areophysical data (mean mass, mean moment of inertia, tidal Love number, and tidal dissipation) and thermodynamic modeling methods and summarize our current understanding of the internal constitution of the planet. *AxiSEM* and hence *Instaseis* can readily be used to propagate
waves on Mars, see Fig. 5.23, allowing us to build these databases very efficiently.

5.5.7. Synthetic Ambient Seismic Noise

As mentioned in section 5.2.3, seismograms generated by force sources can be extracted from the same reciprocal databases. This is particularly interesting for studying ambient seismic noise. By cross-correlating noise recorded at two stations, using long enough time series and under certain assumptions (uncorrelated, isotropically distributed white noise sources), it is possible to retrieve the Green’s function of the medium between the two stations (e.g. Sanchez-Sesma 2006; Gouédard et al. 2008). However, not all of these assumptions are met in nature, e.g. the noise sources are not evenly distributed (Tsai 2009; Froment et al. 2010; Basini et al. 2013). Also, the noise sources themselves are not yet well understood, especially with respect to the generation of Love waves in the microseismic band (Nishida et al. 2008).

Instaseis provides a basis to quickly generate noise synthetics to study such effects, which we illustrate in Fig. 5.24. We computed noise cross correlations, accurate down to a period of 5 s, for a total of 20 days of noise data generated with 100,000 noise sources. The calculation only took 1 CPU hour. In the first case, the noise sources consist of vertical forces with a random source-time function, all have the same amplitude and are distributed evenly on the globe. The resulting cross correlation is in good agreement with the Green’s function, which is obtained by introducing an impulse source at each of the stations in Zurich and Munich. In the second case, sources are located in the oceans only, their amplitude proportional to the significant wave height (Gualtieri et al. 2013). For the two stations located in Zurich and Munich the close sources are thus solely located in the west, which leads to strong asymmetry in the retrieved correlations (Stehly et al. 2006). Instaseis thus enables users to study noise on the global scale across the microseismic band, by generating realistic waveforms at negligible cost.

5.6. Conclusions & Outlook

In this paper we presented a readily available methodology and code to extract seismograms for spherical earth models from a Green’s function database. High efficiency in the generation of databases and very fast extraction (on the order of milliseconds per seismogram) of highly accurate seismograms (indistinguishable from conventional forward solvers) can then replace previously employed approximations such as WKBJ, reflectivity or frequency-wavenumber integration methods that were
used for computational reasons in many applications of global seismology. **Instaseis** is open source and available with extensive documentation at [www.instaseis.net](http://www.instaseis.net).

Future developments include Cartesian local domains with layered models, which are not yet supported by **AxiSEM**. As a large fraction of earthquakes are located below oceans and receivers on continents, it may be beneficial for body waves studies to take advantage of the axisymmetric capability of **AxiSEM** and place the receiver on a circular ‘island’ of continental crust within a global oceanic crustal model.

**Author contributions**

M. v. D. and L. K. implemented **Instaseis**, M. v. D., S. C. S. and T. N.-M. continuously develop **AxiSEM** and added the database output, and K. H. prepared the finite frequency example. M. v. D. prepared the manuscript with contributions from all co-authors.

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**References**


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![Graph of tsunami model results showing sources only in the oceans, amplitude proportional to significant waveheight (January 3rd 2015).]
Figure 5.24.: Synthetic ambient seismic noise cross correlations computed with *Instaseis*. Top: 100,000 vertical force sources located in the oceans and amplitude proportional to the significant wave height from the NOAA WAVEWATCH III model on Jan. 3rd, 2015 (Tolman 2009). Red crosses indicate the receivers located in Munich and Zurich. Middle: Cross correlations of 20 days of noise for evenly distributed noise sources and (bottom) the sources in the map, the traces are normalized to their maximum amplitude.


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Chapter 6
Conclusions & Outlook

As the most important output of this dissertation, we continued the development of the axisymmetric spectral element method (AxiSEM), which now allows to reach parameter regimes that were previously unattainable. This work included the addition of relevant physics, anisotropy and viscoelastic dissipation, as well as continued code development to make the codes reliable, robust and scale on modern supercomputers. These developments also lead to its open source release. The code is now featured by CIG (www.geodynamics.org), has been picked up by several working groups and is more and more becoming a standard tool in global seismology (Beller et al. 2014; Boué et al. 2013, 2014; Retailleau et al. 2014b; Retailleau et al. 2014a; Bharadwaj et al. 2013; Colombi et al. 2014, 2012; Holtzman et al. 2013). The Dissemination to the community is supported by training events on workshops such as the 2013 IRIS-CIG-QUEST workshop (Fairbanks, Alaska), the 1st ELSI summer school (Tokyo, Japan), the PhD workshop on "Advanced seismic imaging of the lithosphere" (Copenhagen, Denmark) and the upcoming TIDES Training School (Bertinoro, Italy).

Future Developments

External Meshes and Local/Regional Domains

The current implementation of AxiSEM is limited to spherical bodies such as whole planets with smooth perturbations of the seismic velocities. This is not a limitation of the theory or the method, but mostly the custom mesh builder. Using meshes built with external tools like cubit (https://cubit.sandia.gov/) and standard mesh decomposition methods based on graph partitioning such as scotch (http://glaros.dtc.umn.edu/gkhome/views/metis) ormetis (http://www.labri.fr/perso/pelegrin/scotch/) will allow to take the full structure in the source-receiver plane into account, including both topography and oceans (Fig. 6.1) and continental scale domains (Fig. 6.2). Obvious applications of these capabilities range from ocean acoustics and floating seismometers as in the MERMAID project (https://www.geoazur.fr/GLOBALSEIS/LatestNews/index.html) as well as seismic
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Figure 6.1.: An example of a local 2D domain that could be used with a future version of AxiSEM and Instaseis, including topography and oceans.

![Local 2D Domain](image1.png)

Figure 6.2.: An example of a continental domain that could be used with a future version of AxiSEM and Instaseis.

![Continental Domain](image2.png)

exploration to avoid 3D-to-2D data transformation (e.g. Takenaka et al. 2003; Auer et al. 2013). The local meshing capability also opens the door to a 1D-1D hybrid method (e.g. Masson et al. 2013) to replace crustal corrections as commonly used in finite-frequency tomography with the actual seismic response of the local crustal properties.
Applications

Instaseis

As an application building directly on AxiSEM, we published Instaseis, which uses AxiSEM to compute Green’s function databases from which seismograms can be extracted in a few milliseconds. Although only a few months old, a number of applications using Instaseis are already emerging: Hosseini and Sigloch (2015) are adapting their finite frequency measurement method to use Instaseis to compute reference synthetic seismograms. Building upon Stähler and Sigloch (2014), they are working on a production setup of their source inversion scheme which will also be using Instaseis. The newly forming Marsquake Service at ETH uses synthetic data computed with Instaseis to validate their processing tools (Boese et al. 2014) and will continue to use it to compute reference synthetics to locate events and infer information about Martian deep structure. IRIS is currently building a new data service product called ‘On Demand Synthetics’, that is a web service built on top of Instaseis to deliver seismograms for any source and receiver combination (http://ds.iris.edu/ds/products/ondemandsynthetics/).

Sensitivity Kernels for Finite-Frequency Tomography

A second application built on AxiSEM only mentioned marginally in this thesis is MC Kerner, a code that uses the same Green’s function databases as Instaseis to compute sensitivity kernels for finite-frequency tomography. The main new feature of this code is to use Monte Carlo integration and high order interpolation in the projection of the kernels onto arbitrary inversion grids: this is very efficient as it converges quickly where the kernels are zero without a priori knowledge about the shape of the kernel. On the other hand, it is accurate to a user defined level without ad hoc decision about the sampling (Fig. 6.3). This code is currently in basic testing and verification stage and should be published and used for a first tomography based on a newly collected dataset (Hosseini and Sigloch 2015) soon.

Insight Mars Mission

A particularly interesting application of Instaseis combined with the local and regional domains mentioned above is the upcoming NASA-lead Mars Insight mission (Banerdt 2013). The landing site is at the border of Mars’ dichotomy with pronounced topography nearby (Fig. 6.4). The new meshing capability would then allow to include topography and Moho topography (known from laser altimetry and
Figure 6.3.: A cross-correlation travel time kernel for a $P$-wave computed with $MC\ Kerner$ based on the same Green’s function databases computed with $AxiSEM$ as $Instaseis$. High order interpolation leads to a very smooth representation allowing for highly accurate orthogonal projection onto the inversion grid.

Figure 6.4.: Topography of Mars and the Insight Landing Site at the border of Mars’ dichotomy. Image source: NASA, the Mars Orbiter Laser Altimeter (MOLA)
gravity data, e.g. Wieczorek and Zuber 2004) in the source receiver plane. Also, for local events the new meshes reduce the computational burden by orders of magnitude and this way allow to include higher frequencies. This is relevant e.g. to discriminate between impacts and earthquakes based on the spectral properties of the seismograms. As the mission only carries a single three component seismometer, reciprocity can still be used and a full Green’s function database for a fixed azimuth computed with only two AxiSEM runs.

References


Appendix A

Models and Fréchet Kernels for Frequency-(in)dependent $Q$

Abstract

We present a new method for the modelling of frequency-dependent and -independent $Q$ in time-domain seismic wave propagation. Unlike previous approaches, attenuation models are constructed such that $Q$ as a function of position in the Earth appears explicitly as a parameter in the equations of motion. This feature facilitates the derivation of Fréchet kernels for $Q$ using adjoint techniques. Being simple products of the forward strain field and the adjoint memory variables, these kernels can be computed with no additional cost, compared to Fréchet kernels for elastic properties. The same holds for Fréchet kernels for the power-law exponent of frequency-dependent $Q$, that we derive as well. To illustrate our developments, we present examples from regional- and global-scale time-domain wave propagation.

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A.1. Introduction

Seismic waves propagating through the Earth are attenuated due to a multitude of micro-scale processes including diffusion and dislocation creep of point defects, grain boundary sliding, and the viscous motion in (partially) molten material (e.g. Jackson 2007; Karato 2008, chapter 11). Commonly described macroscopically in terms of the quality factor $Q$, visco-elastic attenuation leads to seismic phase velocity dispersion and to an amplitude reduction of seismic waves (e.g. Dahlen and Tromp 1998; Kennett 2001; Aki and Richards 2002). Numerous laboratory experiments consistently revealed a temperature and frequency dependence of $Q$ for Earth materials that can be described phenomenologically by the Arrhenius-type equation

$$Q(\omega) = Q_0 \left( \frac{\omega}{\omega_0} \right)^\alpha e^{\alpha E/RT},$$  \hspace{1cm} (A.1)

where $E$ is the activation energy, $T$ is temperature, $R$ is the gas constant, and $\omega_0$ is a reference frequency (e.g. Goetze 1971; Goetze and Brace 1972; Gueguen et al. 1989; Karato and Spetzler 1990; Jackson 2000). Typical values for the constant $\alpha$, summarised for instance by Karato (2008), range between 0.2 and 0.4. Much of the seismological interest in $Q$ is related to its exponential dependence on $T$, which suggests that attenuation may serve as a proxy for temperature in the Earth. The frequency dependence of $Q$ found in laboratory studies has been confirmed by analyses of seismic data across the seismologically observable frequency band from $\sim 10^{-3}$ Hz to $\sim 1$ Hz (e.g. Anderson and Minster 1979; Sipkin and Jordan 1979; Flanagan and Wiens 1998; Cheng and Kennett 2002; Lekić et al. 2009). A review on the frequency dependence of $Q$ may be found, for instance, in Romanowicz and Mitchell (2007). Despite convincing evidence for a power-law dependence of $Q$ on frequency, the majority of seismic studies assume frequency-independent attenuation. This simplification can be justified by the sparsity and bandlimited nature of seismic observations that often prevent reliable estimates of $\alpha$.

With the advent of the numerical age, the proper modelling of seismic wave attenuation has received considerable attention. While the implementation of visco-elastic attenuation in frequency-domain numerical modelling is nearly trivial, attenuation is more difficult to implement in time-domain wave propagation schemes that are most frequently used in large-scale 3-D applications (e.g. Igel and Weber 1995; Komatitsch and Tromp 1999; Moczo et al. 2002; Dumbser et al. 2007; Chen et al. 2007; Fichtner et al. 2009; Tape et al. 2010). Following the seminal work of Emmerich and Korn (1987) and Carcione et al. (1988b), attenuation has been modelled almost exclusively by superpositions of rheological bodies of either Maxwell or Zener type that...
have been shown to be equivalent (Moczo and Kristek 2005). The discrete ensemble of relaxation mechanisms leads, by construction, to a numerically convenient set of equations (Robertsson et al. 1994; Blanch et al. 1995; van Driel and Nissen-Meyer 2014a). The rheological bodies are described in terms of relaxation variables that are determined such that a prescribed $Q(\omega)$ is matched as closely as possible. The concept of representing a broad absorption band by a superposition of individual relaxation mechanisms already appears in Liu et al. (1976), where it had, however, not been used for numerical modelling.

While the forward problem of visco-elastic wave propagation can be considered solved (at least when sufficient computational resources are available), the inverse problem remains technically challenging because $Q$ does not appear explicitly in the description of the rheological bodies used to model attenuation (see section A.2.1 for details). Instead, $Q$ is determined implicitly by the set of suitably chosen relaxation parameters. Furthermore, the relation between $Q$ and the relaxation parameters may vary from one location to another. The absence of an explicit $Q$ in the time-domain visco-elastic wave equation complicates the computation of Fréchet kernels that are needed to invert for the heterogeneous distribution of $Q$ in the Earth.

Based on the assumption of a frequency-independent $Q$, Tromp et al. (2005) proposed to circumvent this problem through the definition of additional adjoint sources for the computation of $Q$ kernels. This approach, adopted for instance by Bozdağ et al. (2011) and Zhu et al. (2013), yields correct kernels, but it also doubles the computational cost because an additional adjoint simulation must be performed. Furthermore, an extension to frequency-dependent $Q$ seems difficult.

Here we present a new approach to the time-domain modelling of visco-elastic wave propagation with frequency-dependent or -independent attenuation where $Q$ at a specified reference frequency appears explicitly in the equations of motion. In addition to improving computational efficiency, this approach allows us to compute Fréchet kernels for $Q$ and its frequency dependence without the requirement of additional wavefield simulations.

This paper is organised as follows: To introduce basic concepts without heavy notation, we start our developments in section A.2.1 using a one-dimensional scalar wave equation. In section A.2.1 we describe a novel parametrisation of attenuation models where $Q$ appears explicitly. Subsequently, in section A.2.2 we make the transition to the elastic case. A examples, we consider isotropic media, as well as full anisotropy with 21 independent elastic parameters. Section A.3 is dedicated to the derivation of shear and bulk $Q$ kernels, based on the previously derived $Q$ models. In the interest of a readable text, we defer the derivation of kernels for the power-law exponent $\alpha$ to Appendix A.6.1. Examples of synthetic seismograms for
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frequency-dependent $Q$ and corresponding Fréchet kernels are presented in section A.4.

A.2. Forward Modelling

A.2.1. The Scalar Wave Equation

For the purpose of illustration, we start our development with the scalar wave equation. Written in velocity-stress formulation, it consists of the momentum conservation law

$$\rho \ddot{v} - \partial_x \sigma = f, \quad \text{(A.2)}$$

and the visco-elastic constitutive relation defined by

$$\dot{\sigma}(t) = \int_{-\infty}^{\infty} \dot{C}(t - t') \dot{\epsilon}(t') \, dt'. \quad \text{(A.3)}$$

In eq. (A.3), $\sigma$, $C$ and $\epsilon = \partial_x v$ are representative components of the stress tensor $\sigma$, the elastic tensor $C$, and the strain tensor $\epsilon$, respectively.

Numerical Modelling of Visco-Elastic Attenuation

Taking inspiration from Blanch et al. (1995), we model the time-dependence of the elastic modulus $C$ by a superposition of $N \geq 1$ exponential functions with decay times $\tau_p \ (p = 1, \ldots, N)$ that phenomenologically mimick different relaxation mechanisms in the Earth:

$$C(t) = C^r \left[ 1 + \tau \sum_{p=1}^{N} D^{(p)} e^{-t/\tau^{(p)}} \right] H(t). \quad \text{(A.4)}$$

The symbol $C^r$ denotes the relaxed modulus, $D^{(p)}$ are the weights of the relaxation mechanisms, $H$ is the Heaviside function, and $\tau$ is a parameter that controls the strength of visco-elastic attenuation. As described in section A.2.1, the free parameters $D^{(p)}$, $\tau^{(p)}$ and $\tau$ must be determined such that $C(t)$ approximates a pre-defined behaviour. Differentiating (A.4) with respect to time $t$, and introducing the result into (A.3), yields
\[ \dot{\sigma} = C^r (1 + s\tau) \dot{\varepsilon} + C^r \tau \sum_{p=1}^{N} M^{(p)}, \quad \text{with} \quad s = \sum_{p=1}^{N} D^{(p)}, \quad (A.5) \]

where the memory variables

\[ M^{(p)}(t) = -\frac{D^{(p)}}{\tau^{(p)}} \int_{-\infty}^{\infty} e^{-(t-t')/\tau^{(p)}} H(t-t') \dot{\varepsilon}(t') \, dt' \quad (A.6) \]

satisfy the first-order differential equation

\[ \dot{M}^{(p)} = -\frac{D^{(p)}}{\tau^{(p)}} \dot{\varepsilon} - \frac{1}{\tau^{(p)}} M^{(p)}. \quad (A.7) \]

The combination of eq. (A.7), the momentum conservation law (A.2), and the constitutive relation (A.3), forms a complete set of equations that describes the propagation of a scalar visco-elastic wave.

**Constructing Q Models**

The quality factor \( Q(\omega) \) is defined as the ratio

\[ Q(\omega) = \frac{\text{Re} \, C(\omega)}{\text{Im} \, C(\omega)}, \quad (A.8) \]

where the complex modulus \( C(\omega) \) is given by

\[ C(\omega) = i\omega \int_{-\infty}^{\infty} C(t) e^{-i\omega t} \, dt. \quad (i = \sqrt{-1}) \quad (A.9) \]

When \( Q \) is sufficiently large, typically \( \gtrsim 100 \), it can be related to the fractional energy loss per oscillation cycle, i.e. \( \Delta E/E = -2\pi Q^{-1} \). For the specific form of \( C(t) \) defined in eq. (A.4), we find

\[ Q(\omega) = \left[ 1 + \tau \sum_{p=1}^{N} \frac{D^{(p)} \omega^2 \tau^{(p)} 2}{1 + \omega^2 \tau^{(p)} 2} \right]^{-1} \left[ \tau \sum_{p=1}^{N} \frac{D^{(p)} \omega \tau^{(p)}}{1 + \omega^2 \tau^{(p)} 2} \right]. \quad (A.10) \]

To construct \( Q \)-models that approximate a prescribed empirical frequency dependence of the form suggested already in eq. (A.1),

\[ Q_{\text{target}}(\omega) = Q_0 \left( \frac{\omega}{\omega_0} \right)^\alpha \quad (A.11) \]
A. Models and Fréchet Kernels for Frequency-(in)dependent $Q$

across the frequencies of interest, we proceed as follows:

(i) We define a set of $Q_0$ values, $(Q_0^{(1)}, ..., Q_0^{(M)})$, that span the range of $Q$ in our Earth model.

(ii) We set $\tau = Q_0^{(k)}$ for each $k = 1, ..., M$. This defines a collection of numerical $Q$ models, $Q(\omega, Q_0^{(k)})$, via eq. (A.10).

(iii) We find optimal values for $\tau^{(p)}$ and $D^{(p)}$ by minimising the cumulative difference between the numerical $Q$ models $Q(\omega, Q_0^{(k)})$ and the target $Q$ models $Q_{\text{target}}(\omega, Q_0^{(k)})$,

$$J(\tau_p, D_p) = \sum_{k=1}^M \left\| \frac{Q(\omega, Q_0^{(k)}) - Q_{\text{target}}(\omega, Q_0^{(k)})}{Q_0^{(k)}} \right\| \omega .$$  
(A.12)

The minimization of $J$ represents a non-linear optimisation problem in a low-dimensional parameter space that can be solved efficiently with Monte-Carlo-type techniques. Finding optimal $\tau_p$ and $D_p$ for a whole set of $Q_0$ values has the effect that the approximation

$$Q(\omega) = \left[ 1 + Q_0^{-1} \sum_{p=1}^N \frac{D^{(p)} \omega^2 \tau^{(p)} 2}{1 + \omega^2 \tau^{(p)} 2} \right] \left[ Q_0^{-1} \sum_{p=1}^N \frac{D^{(p)} \omega \tau^{(p)}}{1 + \omega^2 \tau^{(p)} 2} \right]^{-1} \approx Q_0 \left( \frac{\omega}{\omega_0} \right)^\alpha$$  
(A.13)

effectively holds for any $Q_0$ inside the range of $Q$’s in the Earth model. The proposed optimisation scheme for the relaxation parameters $\tau^{(p)}$ and $D^{(p)}$ explicitly introduces $Q_0$ into the equations of motion through the enforcement of $\tau = Q_0^{-1}$ for all relevant $Q_0$ values. There are two immediate advantages of this approach: (i) The search for optimal $\tau^{(p)}$ and $D^{(p)}$ only has to be performed once. Thus, once $\tau^{(p)}$ and $D^{(p)}$ are found, they can be used throughout the Earth model even when $Q_0$ is spatially variable. This statement holds provided that $\alpha$ is constant, which includes the frequency-independent case with $\alpha = 0$. (ii) The explicit appearance of $Q_0$ facilitates the computation of Fréchet kernels for $Q_0$ using standard adjoint techniques. The computation of Fréchet kernels for $Q_0$ and $\alpha$ will be described in section A.3 and illustrated in section A.4.

A numerical example for the case of $N = 3$ relaxation mechanisms and a frequency range from 0.02 to 0.2 Hz is shown in Fig. A.1. We determined the parameters $\tau^{(p)}$ and $D^{(p)}$ for $Q_0 = (0.1, 0.2, 0.3)$.
and $D^{(p)}$ using Simulated Annealing (Kirkpatrick et al. 1983). With $\alpha = 0.3$, $Q(\omega)$ deviates from $Q_{\text{target}}(\omega)$ by less than 3% for values of $Q_0$ between 50 and 500. While fully sufficient for practical purposes, the accuracy can be improved by using more than 3 relaxation mechanisms.

### A.2.2. Extension to the Elastic Case

Following the illustrative example for the scalar wave equation in the previous section, we now transition to the fully elastic 3-D case. We consider both general anisotropy (section A.2.2) and the practically most relevant isotropic scenario (section A.2.2).

#### General Anisotropy

In analogy to eq. (A.2) and (A.3), the momentum conservation and visco-elastic stress-strain relation for generally anisotropic media can be written as

$$ \rho \dot{v}_i - \partial_j \sigma_{ij} = f_i \quad (A.14) $$

and

$$ \dot{\sigma}_{ij}(t) = \sum_{k,l=1}^{3} \int_{-\infty}^{\infty} \dot{C}_{ijkl}(t-t') \dot{\epsilon}_{kl}(t') \, dt'. \quad (A.15) $$

respectively. The stress-strain relation (A.15) allows different elastic coefficients $C_{ijkl}$ to be subject to different forms of visco-elastic dissipation. These differences may result in anisotropic attenuation that has been predicted for finely layered media (Carcione 1992; Zhu et al. 2007) and observed in both laboratory and field experiments (e.g. Tao and King 1990; Bao et al. 2012). Anisotropic attenuation in the inner core, with stronger attenuation for waves propagating parallel to the Earth’s spin axis, is also well documented (Creager 1992; Song and Helmberger 1993). Generalising eq. (A.4) for the time dependence of elastic parameters, we have

$$ C_{ijkl}(t) = C_{ijkl}^r \left[ 1 + \tau_{ijkl} \sum_{p=1}^{N} D^{(p)} e^{-t/\tau^{(p)}} \right] H(t). \quad (A.16) $$
A. Models and Fréchet Kernels for Frequency-(in)dependent $Q$

Figure A.1.: Black curves show $Q(\omega)$ for $Q_0$ equal to 50, 100 and 500 (from left to right) for $N = 3$ relaxation mechanisms. $Q_{\text{target}}(\omega) = Q_0(\omega/\omega_0)^\alpha$ with $\alpha = 0.3$ and $\omega_0 = 2\pi \cdot 0.05$ Hz is shown in red. The optimal relaxation times and weights are $\tau_1 = 0.14$, $\tau_2 = 1.40$ s, $\tau_3 = 9.46$ s, $D_1 = 1.23$, $D_2 = 0.91$, and $D_3 = 2.07$. Within the target frequency range 0.02 to 0.2 Hz, $Q(\omega)$ matches $Q_{\text{target}}(\omega)$ to within 3% of the respective $Q_0$. 

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A.2. Forward Modelling

Following the developments in section A.2.1, we can eliminate the numerically inconvenient convolutional integral in (A.15) with the help of memory variables: Introducing the time derivative of (A.16) into the stress-strain relation (A.15), yields

\[
\dot{\sigma}_{ij} = \sum_{k,l=1}^{3} C_{ijkl}^r (1 + \tau_{ijkl}s) \dot{\epsilon}_{kl} + \sum_{k,l=1}^{3} C_{ijkl}^r \tau_{ijkl} \sum_{p=1}^{N} M^{(p)}_{kl}. \tag{A.17}
\]

The memory variables \(M^{(p)}_{kl}\), defined as

\[
M^{(p)}_{kl} = -\frac{D^{(p)}}{\tau^{(p)}} \int_{-\infty}^{\infty} e^{-(t-t')/\tau^{(p)}} H(t-t') \dot{\epsilon}_{kl} dt', \tag{A.18}
\]
satisfy the first-order differential equation

\[
\dot{M}^{(p)}_{kl} = -\frac{1}{\tau^{(p)}} M^{(p)}_{kl} - \frac{D^{(p)}}{\tau^{(p)}} \dot{\epsilon}_{kl}. \tag{A.19}
\]

Combined, eqs. (A.14), (A.15) and (A.16) constitute a complete set of equations that describes the propagation of dissipative waves in anisotropic media.

The Isotropic Case

Isotropic media described in terms of the bulk modulus \(\kappa\) and the shear modulus \(\mu\) are the simplest special case of the general visco-elasticity captured in eq. (A.15). The isotropic elastic tensor is given by

\[
C_{ijkl} = \left(\kappa - \frac{2}{3} \mu\right) \delta_{ij} \delta_{kl} + \mu \left(\delta_{ik}\delta_{jl} + \delta_{jl}\delta_{ik} - \frac{2}{3} \delta_{ij} \delta_{kl}\right). \tag{A.20}
\]

Using the fact that the relaxation parameters \(\tau^{(p)}\) and \(D^{(p)}\) are determined such that the \(\tau_{ijkl}\) from eq. (A.16) are equal to the inverses of their corresponding \(Q_0\)'s, we can write the time-dependent \(C_{ijkl}\) as

\[
C_{ijkl}(t) = \kappa^r \delta_{ij} \delta_{kl} \left[1 + Q_0^{-1} \sum_{p=1}^{N} D^{(p)} e^{-t/\tau^{(p)}}\right] H(t)
+ \mu^r \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3} \delta_{ij} \delta_{kl}\right) \left[1 + Q_0^{-1} \sum_{p=1}^{N} D^{(p)} e^{-t/\tau^{(p)}}\right] H(t). \tag{A.21}
\]
Inserting the time derivative of (A.21) into the stress-strain relation (A.15) yields the modified stress-strain relation

\[
\dot{\sigma}_{ij} = \kappa_r \left[ 1 + Q_{0 \kappa}^{-1} s \right] \dot{\epsilon}_{kk} \delta_{ij} + 2 \mu_r \left[ 1 + Q_{0 \mu}^{-1} s \right] \dot{\epsilon}_{ij}
+ \kappa_r Q_{0 \kappa}^{-1} \sum_{p=1}^{N} M_{kk}^{(p)} \delta_{ij} + 2 \mu_r Q_{0 \mu}^{-1} \sum_{p=1}^{N} \tilde{M}_{ij}^{(p)}.
\] (A.22)

where \( \epsilon_{kk} \) and \( \tilde{\epsilon} \) denote the trace and the deviator of the strain tensor \( \epsilon_{ij} \). Similarly, \( M_{kk}^{(p)} \) and \( \tilde{M}_{ij}^{(p)} \) are the trace and the deviator of the memory variable tensor \( M_{ij}^{(p)} \), defined as in eq. (A.18). The first two terms in eq. (A.22) represent a purely elastic stress-strain relation. The last two terms involving the memory variables account for visco-elastic dissipation.

### A.3. Sensitivity Kernels

In section A.2, we established forward problem equations that link visco-elastic parameters to the seismic wavefield. In what follows, we will use this link in order to derive expressions for Fréchet kernels with respect to \( Q \) and \( \alpha \). For this, we assume that a measurement, encoded in the measurement functional \( \chi(u) \), has been made. Possible measurements include \( L_1 \) and \( L_2 \) waveform differences (Brossier et al. 2009; Brossier et al. 2010), cross-correlation traveltimes (Luo and Schuster 1991), generalised seismological data functionals (Gee and Jordan 1992), or various time-frequency misfits (Fichtner et al. 2008). Our analysis rests on the adjoint method, described, for instance, by Tarantola (1984), Tromp et al. (2005), Fichtner et al. (2006a, 2006b) or Chen (2011).

#### A.3.1. Adjoint Equations and Adjoint Memory Variables

Invoking the adjoint method, the variation \( \delta \chi \) of the measurement functional can be written in terms of the forward wavefield \( u \), the forward strain tensor \( \epsilon \), the adjoint wavefield \( u^\dagger \), the adjoint strain tensor \( \epsilon^\dagger \), the variation in density \( \delta \rho \), and the variation of the elastic tensor \( \delta C \):
A.3. Sensitivity Kernels

\[
\delta \chi = - \int_{-\infty}^{\infty} \int_{V} \delta \rho \dot{u}_i^*(t) \dot{u}_i(t) \, dx \, dt + \int_{-\infty}^{\infty} \int_{V} \left[ \int_{-\infty}^{\infty} \varepsilon_{ij}^*(t) \delta \dot{C}_{ijkl}(t - t') \varepsilon_{kl}(t') \, dt' \right] \, dx \, dt. \tag{A.23}
\]

The adjoint field is governed by the adjoint equations that may be written in velocity-stress formulation, consisting of the momentum conservation equation

\[
\rho \dot{u}_i^* - \partial_j \sigma_{ij}^* = f_i^* \tag{A.24}
\]

and the stress-strain relation

\[
\dot{\sigma}_{ij}^* = \int_{-\infty}^{\infty} \dot{C}_{ijkl}(t' - t) \varepsilon_{kl}^*(t') \, dt'. \tag{A.25}
\]

The adjoint source \(f_i^*\) is determined by the definition of the measurement, i.e. by the specific form of \(\chi\) (see section A.4 for examples). Visco-elastic dissipation in the adjoint stress-strain relation is time-reversed, meaning that current stresses depend on future strains. Since the adjoint equations are, however, solved in reverse time, numerical stability is ensured (Tarantola 1988; Fichtner 2010). Again following the developments in section A.2.1, we eliminate the convolutional integral in (A.25) by defining adjoint memory variables \(M_{kl}^{(p)}\) as

\[
M_{kl}^{(p)} = - \frac{\mathcal{D}_{kl}^{(p)}}{\tau_{kl}^{(p)}} \int_{-\infty}^{\infty} e^{-\tau_{kl}^{(p)}(t') \varepsilon_{kl}^*(t')} \, dt' \tag{A.26}
\]

Differentiating eq. (A.26) with respect to time \(t\), it follows that the adjoint memory variables satisfy the first-order differential equation

\[
M_{kl}^{(p)} = \frac{1}{\tau_{kl}^{(p)}} M_{kl}^{(p)} + \frac{\mathcal{D}_{kl}^{(p)}}{\tau_{kl}^{(p)}} \varepsilon_{kl}^*. \tag{A.27}
\]

The resulting modified stress-strain relation for the adjoint field is

\[
\dot{\sigma}_{ij}^* = C_{ijkl}^r (1 + \tau_{ijkl}s) \varepsilon_{kl}^* + \sum_{k,l=1}^{3} C_{ijkl}^r \tau_{ijkl} \sum_{p=1}^{N} M_{kl}^{(p)}. \tag{A.28}
\]
Equipped with the complete set of adjoint equations, consisting of equations (A.23), (A.27) and (A.28), we can proceed with the calculation of sensitivity kernels for $Q$ and $\alpha$. In the interest of a lighter notation, we will consider shear and bulk $Q$ separately, and we transfer the detailed derivation of $\alpha$ kernels to Appendix A.6.1.

### A.3.2. Shear $Q$

Restricting ourselves to an isotropic medium with $C_{ijkl} = (\kappa - \frac{2}{3}\mu)\delta_{ij}\delta_{kl} + \mu\delta_{ik}\delta_{jl} + \mu\delta_{il}\delta_{jk}$ and variations in the shear modulus $\mu$, eq. (A.23) condenses to

$$\begin{align*}
\delta \chi &= 2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^\dagger(t) \delta \mu(t - t') \, dt \right] \tilde{\epsilon}_{ij}(t') \, dx \, dt',
\end{align*}$$

where $\tilde{\epsilon}_{ij}$ and $\tilde{\epsilon}_{ij}^\dagger$ are the deviatoric parts of $\epsilon_{ij}$ and $\epsilon_{ij}^\dagger$, respectively. Invoking the chain rule, we can express $\delta\mu$ in (A.29) in terms of variations in $Q_{0\mu}$:

$$\delta \mu = \frac{\partial \mu}{\partial Q_{0\mu}} \delta Q_{0\mu}. \tag{A.30}$$

The partial derivatives $\partial \mu / \partial Q_{0\mu}$ follows from the definition of the time-dependent elastic modulus in (A.4), with the general relaxed modulus $C^r$ set equal to the relaxed shear modulus $\mu^r$:

$$\frac{\partial \mu(t)}{\partial Q_{0\mu}} = -\mu^r Q_{0\mu}^{-2} \left[ \sum_{p=1}^{N} D^{(p)} e^{-t/\tau^{(p)}} \right] H(t). \tag{A.31}$$

Using (A.30) and (A.31), we can reformulate the integral over $\tilde{\epsilon}_{ij}^\dagger(t) \delta \mu(t - t')$ that appears in eq. (A.29):

$$\begin{align*}
\int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^\dagger(t) \delta \mu(t - t') \, dt &= \int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^\dagger(t) \delta \mu(t - t') \, dt \\
&= -\mu^r Q_{0\mu}^{-2} \sum_{p=1}^{N} \int_{-\infty}^{\infty} D^{(p)} e^{(t-t')/\tau^{(p)}} H(t - t') \tilde{\epsilon}_{ij}^\dagger(t) \delta Q_{0\mu} \, dt.
\end{align*} \tag{A.32}$$
A.3. Sensitivity Kernels

Identifying copies of the adjoint memory variables $M_{k_l}^{(p)\dagger}$, defined in (A.26), we can condense (A.32) into

$$\int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^\dagger(t) \delta \hat{\mu}(t - t') \, dt = \mu^r Q_0^{-2} \sum_{p=1}^{N} \tau^{(p)}(t) \tilde{M}_{ij}^{(p)\dagger}(t') \, \delta Q_0 .$$

(A.33)

We can now combine (A.29) with (A.33) in order to write $\delta \chi$ in terms of the volumetric Fréchet or sensitivity kernel $K_{Q_0 \mu}$:

$$\delta \chi = \int_V K_{Q_0 \mu}(x) \delta \ln Q_0 \mu(x) \, dx ,$$

(A.34)

where $K_{Q_0 \mu}$ can be explicitly computed from the interaction of the forward strain deviator $\tilde{\epsilon}_{ij}$ and the deviator of the adjoint memory variables, $\tilde{M}_{p,ij}$:

$$K_{Q_0 \mu} = 2 \mu^r Q_0^{-1} \sum_{p=1}^{N} \tau^{(p)}(t) \int_{-\infty}^{\infty} \tilde{M}_{ij}^{(p)\dagger} \tilde{\epsilon}_{ij} \, dt .$$

(A.35)

Equation (A.35) reveals that the kernel for $Q_0 \mu$ can be computed in a similar fashion as kernels for elastic parameters, velocity and density; without any additional computational requirements. The adjoint equations are solved in reversed time which automatically yields the adjoint memory variables needed to evaluate the time integrals in (A.35). For comparison, the sensitivity kernel for the shear modulus $\mu$ in a non-dissipative medium is given by (e.g. Tromp et al. 2005; Fichtner 2010)

$$K_{\mu} = 2 \mu \int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^\dagger \tilde{\epsilon}_{ij} \, dt .$$

(A.36)

Thus, for the computation of the $Q$ kernel $K_{Q_0 \mu}$, the term $Q_0^{-1} \sum_{p=1}^{N} \tau^{(p)} \tilde{M}_{ij}^{(p)\dagger}$, involving the deviator of the adjoint memory variables, simply takes the place of the adjoint strain tensor $\tilde{\epsilon}_{ij}^\dagger$ in eq. (A.36). Following similar steps as above, we show in Appendix A.6.1 that the Fréchet kernel $K_{\alpha}$ for the exponent $\alpha$ in the power-law frequency dependence of $Q_\mu$ (eq. A.11), is given by

$$K_{\alpha} = -2 \mu^r \alpha Q_0^{-1} \sum_{p=1}^{N} \frac{\tau^{(p)}}{D^{(p)}} \frac{\partial D^{(p)}}{\partial \alpha} \int_{-\infty}^{\infty} \tilde{M}_{ij}^{(p)\dagger} \tilde{\epsilon}_{ij} \, dt .$$

(A.37)
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### A.3.3. Bulk $Q$

Considering only variations in the visco-elastic properties related to the bulk modulus $\kappa$, the variation of the elastic tensor $C_{ijkl}$ reduces to $\delta C_{ijkl} = \delta \kappa$. The variation of the misfit or measurement functional $\chi$ can then be written in terms of the traces $\epsilon_{kk}$ and $\epsilon_{kk}^\dagger$ of the forward and adjoint strain tensors:

$$
\delta \chi = \int_\infty^{-\infty} \int_V \left[ \int_\infty^{-\infty} \epsilon_{kk}^\dagger(t) \delta \dot{\mu}(t - t') \, dt \right] \epsilon_{kk}(t') \, dx \, dt'.
$$

(A.38)

Following exactly the same steps as in section A.3.2 on shear $Q$, we can transform (A.38) into

$$
\delta \chi = \int_V K_{Q_0 \kappa}(x) \delta \ln Q_0 \kappa(x) \, dx,
$$

(A.39)

with the sensitivity kernel

$$
K_{Q_0 \kappa} = \kappa^r Q_0^{-1} \kappa \sum_{p=1}^{N} \tau^{(p)} \int_{-\infty}^{\infty} M_k^{(p)} \epsilon_{kk} \, dt.
$$

(A.40)

In eq. (A.40), $M_k^{(p)}$ denotes the trace of the memory variable tensor $M_k^{(p)}$. Just as the kernel for shear $Q$ in eq. (A.35), the kernel for bulk $Q$ can be computed from the forward strain and the adjoint memory variables that are a natural by-product of the adjoint solution. Again, for comparison, we note the kernel for the bulk modulus $\kappa$ in a non-dissipative medium is given by (e.g. Tromp et al. 2005; Fichtner 2010)

$$
K_\kappa = \kappa \int_{-\infty}^{\infty} \epsilon_{kk}^\dagger \epsilon_{kk} \, dt.
$$

(A.41)

It follows that a simple replacement of $\epsilon_{kk}^\dagger$ by $Q_0^{-1} \kappa \sum_{p=1}^{N} \tau^{(p)} M_k^{(p)}$ in eq. (A.40) yields $Q$ instead of $\kappa$ kernels.

In Appendix A.6.1 we demonstrate that the Fréchet kernel for the power-law exponent of bulk $Q$ is given by
A.4. Examples

To illustrate the practical implementation of frequency-dependent $Q$ and its effect on seismic waveforms, as well as the computation of $Q$ and $\alpha$ kernels, we present various examples from global- and regional-scale wave propagation.

A.4.1. Global Wave Propagation

In order to model global seismic wave propagation in a broad frequency range, while keeping the computational requirements at a manageable level, we limit ourselves to the radially symmetric Earth model PREM (Dziewoński and Anderson 1981). Being a special case of an axisymmetric medium, the equations of motion for PREM can be reduced to a system of PDE’s in two space variables, and solved efficiently by the time-domain spectral-element code AxiSEM (Nissen-Meyer et al. 2007, 2014; van Driel and Nissen-Meyer 2014b).

We consider three different $Q$ models, summarised in the left panel of Fig. A.2: The original, frequency-independent $Q$ of PREM (black curve), a frequency-dependent $Q$ with $\alpha = 0.3$ and reference frequency 1 Hz (red curve), and a frequency-dependent $Q$ with $\alpha = 0.3$ and reference frequency 0.1 Hz (blue curve). The phase velocities are matched to the phase velocities of PREM at the central period of the numerical simulation, which is 22 s. The resulting phase velocity dispersion curves are shown in the right panel of Fig. A.2.

The frequency dependence of $Q$ and the different choice in reference frequency lead to notable differences in synthetic seismograms, a small collection of which is presented in Fig. A.3 for a period band ranging from 2 to 200 s. The example illustrates that the frequency-dependence of $Q$ is generally not a small effect because realistic values of $\alpha$ between 0.2 and 0.4 (e.g. Karato 2008) can lead to substantial modification of $Q$ away from the reference frequency.

A.4.2. Regional-Scale Wave Propagation

In our next example, we consider wave propagation at regional scales, i.e. over distances of few hundred kilometres. Our computational domain, shown in the
Figure A.2.: (a) $Q$ as a function of frequency as approximated with linear solids and used in the global example shown in figure A.3. The original frequency-independent $Q$ of PREM (Dziewoński and Anderson 1981) is shown in black. Two frequency-dependent versions of $Q$ are shown in red (reference frequency 1 Hz) and blue (reference frequency 0.1 Hz). (b): Phase velocity dispersion relative to the phase velocity of PREM for $Q_0 = 1000$ and the $Q$ models shown to the left. Velocities are fixed to PREM velocities at the central period of the simulation (22 s) causing the red model to produce smaller travel times at short periods. The frequency range used in the example is indicated by grey shading.
A.4. Examples

Figure A.3.: Comparison of vertical-component displacement seismograms (band pass filtered between 2 and 200 s period) for a moment magnitude $M_w = 5.0$ event in 126 km depth under the Tonga islands, computed with AxiSEM in the anisotropic PREM model without ocean with the three different attenuation models shown in figure A.2. The traces are plotted for the GSN stations indicated in the map. The zoom windows are indicated with red rectangles in the record section and the time scale is relative to the ray-theoretical arrival.

upper right panel of Fig. A.5, is centred on Turkey. We locate the earthquake in eastern Turkey and choose an explosion as source mechanism in order to exclude radiation pattern effects on the sensitivity kernels computed in the following sections. As Earth model we again use PREM (Dziewoński and Anderson 1981), modified such that $Q_\mu$ and $Q_\kappa$ are frequency dependent as shown in Fig. A.1. For the simulation of 3-D seismic wave propagation, we use the spectral-element solver SES3D, described in Fichtner and Igel (2008) and Fichtner et al. (2009).

A comparison of synthetic seismograms with and without attenuation is shown in Fig. A.5 for station ADVT, located in western Turkey at an epicentral distance of $9^\circ$. As a result of the short epicentral distance and the short dominant period of 8 s, the wavefield mostly senses crustal and uppermost mantle structure where $Q_\mu$ and $Q_\kappa$ in PREM range around 600 and 58,000, respectively. It follows that the effects on phase and amplitude are small, but noticeable. The amplitudes of both body and surface waves are reduced by around 5 %. The time shifts induced by the
A. Models and Fréchet Kernels for Frequency-(in)dependent $Q$

For the calculation of Fréchet kernels we limit ourselves to two types of measurements: (1) Relative $L_2$ amplitude differences are defined as

presence of visco-elastic attenuation range around 1 s.
Figure A.5.: Comparison of vertical-component synthetic seismograms without (black) and with (red) viscoelastic dissipation for a dominant period of 8 s. The source-receiver configuration is shown to the right, with the computational domain shaded in light grey. As Earth model, we use the spherically symmetric PREM (Dziewoński and Anderson 1981) with a frequency-dependent $Q$ constructed as in Fig. A.1. The zoom into the P wave and surface wave trains (lower left and lower right, respectively), reveals time shifts of around 1 s and amplitude variations on the order of 5 %.
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\[ \chi = A = \frac{\int u^2 \, dt - \int u_0^2 \, dt}{\int u_0^2 \, dt}, \quad (A.43) \]

with $u$ and $u_0$ denoting synthetic and observed seismograms, respectively. For our examples, we restrict ourselves to the vertical components, i.e. $u = u_z$. (2) Correlation traveltime shifts are defined as the time $T$ where the correlation between observed and synthetic waveforms reaches its maximum (e.g. Luo and Schuster 1991; Dahlen et al. 2000):

\[ \chi = T = \arg \max \int u(\tau) u_0(t + \tau) \, d\tau. \quad (A.44) \]

The adjoint sources $f^\dagger$ for these measurements, i.e. the right-hand sides of the adjoint eq. (A.24), are given by

\[ f_A^\dagger(t) = \frac{2u(t)}{\int u^2 \, dt} e_z, \quad (A.45) \]

and

\[ f_T^\dagger(t) = -\frac{\ddot{u}(t)}{\int \dddot{u}^2 \, dt} e_z, \quad (A.46) \]

respectively (e.g. Luo and Schuster 1991; Fichtner 2010). Equipped with eqs. (A.45) and (A.46), we can solve the adjoint equations that provide the adjoint memory variables needed to compute Fréchet kernels for visco-elastic parameters, according to eqs. (A.35) and (A.40).

Fréchet Kernels for $Q$ at the Reference Frequency

Figure A.6 displays horizontal slices through Fréchet kernels for $Q_{0\mu}$, i.e. the shear $Q$ at the reference circular frequency $\omega_0$. Kernels are computed based on eq. (A.35) and for measurements performed in three different time windows. While the time window from 246-333 s mostly contains higher-mode Rayleigh waves, the time window from 362-400 s is dominated by the fundamental-mode Rayleigh wave. Acknowledging that more elaborate measurements – based for instance on multi-tapers or various time-frequency transforms (e.g. Laske and Masters 1996; Zhou et al. 2004; Fichtner et al. 2008) – are possible, we do not apply additional filters or time windows in order to keep the examples illustrative and repeatable. Kernels for amplitude and
traveltime measurements are shown in the second and third rows of Fig. A.6, respectively. All kernels are plotted at the depth where they attain their maximum values.

Being a composite of various higher modes, the time window from 246-333 s yields Fréchet kernels that deviate from the simple cigar shape produced by the fundamental-mode Rayleigh wave in the 362-400 time window. The comparatively high frequencies in the time window from 333-362 s lead to a thinner Fresnel zone than for the other time windows where the dominant frequencies are lower. Generally, amplitude and traveltime measurements have similarly strong sensitivity to relative perturbations in $Q_{0\mu}$, as previously noted, for instance, by Zhou (2009).

Fréchet kernels for $Q_{0\kappa}$, i.e. bulk $Q$ at the reference frequency, can be computed using eq. (A.40). Kernels for the same measurement windows and measurements as in Fig. A.6 are shown in Fig. A.7. As expected for surface waves with little sensitivity to the bulk modulus, sensitivities for bulk $Q$ are several orders of magnitude smaller than for shear $Q$. The overall geometrical pattern, however, remains unchanged.

## Fréchet Kernels for the Power-Law Exponent $\alpha$

The computation of Fréchet kernels for $\alpha$, i.e. the power-law exponent in the frequency dependence of $Q$, requires knowledge of the partial derivatives $\partial D^{(p)}/\partial \alpha$ (see eqs. (A.37) and (A.42)). Since the weights $D^{(p)}$ are computed by numerical optimisation as outlined in section A.2.1, their partial derivatives are not explicitly available. They can, however, be approximated by computing weights $D^{(p)}(\alpha + \delta\alpha)$ for a slightly perturbed power-law exponent $\alpha$:

$$\frac{\partial D^{(p)}}{\partial \alpha} \approx \frac{D^{(p)}(\alpha + \delta\alpha) - D^{(p)}(\alpha)}{\delta\alpha}.$$  \hspace{1cm} (A.47)

For our example with three relaxation mechanisms, the finite-difference approximation (A.47) yields the values $\partial D^{(1)}/\partial \alpha = -3.06$, $\partial D^{(2)}/\partial \alpha = -1.54$, and $\partial D^{(3)}/\partial \alpha = 2.56$ for shear $Q$.

Fréchet kernels for fractional perturbations in shear $\alpha$, displayed in Fig. A.8 for the previously used time windows and measurements, are orders of magnitude smaller than kernels for fractional perturbations in shear $Q$. While more targeted measurements are possible (e.g. Cheng and Kennett 2002; Lekić et al. 2009; Kennett and Abdullah 2011), this result still reflects that the frequency-dependence of $Q$ in the Earth is difficult to constrain.
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Figure A.6: Horizontal slices through Fréchet kernels for relative perturbations in $Q_0$ for measurements in different time windows on the vertical-component velocity seismogram from station ADVT (see Fig. A.5). The time windows are indicated in the top row by grey shading. Kernels for amplitude and traveltime measurements are shown in the second and third row, respectively. All kernels are plotted at the depth where they attain their largest values. Note the different colour scales.
Figure A.7.: The same as Fig. A.6 but for relative perturbations in the bulk quality factor $Q_0\kappa$. 
Figure A.8: The same as Fig. A.6 but for relative perturbations in the exponent $\alpha$ of the shear quality factor $Q$. The kernels are shown for traveltime and amplitude perturbations.
A.5. Discussion and Conclusions

We presented a novel method for the modelling of frequency-dependent and -independent $Q$ in time-domain numerical wave propagation. In contrast to previous approaches (e.g. Emmerich and Korn 1987; Carcione et al. 1988b, 1988a; Blanch et al. 1995), $Q$ as a function of position in the Earth is introduced explicitly into the equations of motion.

A key element of our method is the determination of only one set of relaxation parameters $\tau^{(p)}$ and $D^{(p)}$ from eq. (A.4) that is valid for the full range of $Q_0$ values in the Earth model. This is different from more classical approaches where a set of relaxation parameters is determined individually for each $Q_0$ value (e.g. Emmerich and Korn 1987; Blanch et al. 1995; van Driel and Nissen-Meyer 2014a). A direct consequence of working with one universal set of relaxation parameters are larger discrepancies between the target $Q$ model and the actual numerical $Q$ model. For most practical purposes, however, these errors are hardly relevant. Using, for instance, $N = 3$ relaxation mechanisms for frequencies between 0.02 and 0.2 Hz, and $Q_0$ between 50 and 500, the relative errors between the target $Q$ and the numerical $Q$ shown in Fig. A.1 are below 3%. This error is well below lateral variations of shear $Q$ in global models that are on the order of $\pm 100\%$ (e.g. Romanowicz 1995; Warren and Shearer 2002; Selby and Woodhouse 2002; Gung and Romanowicz 2004; Dalton et al. 2008). Differences between 1-D $Q$ models typically range between 10 and 100% (e.g. Dziewoński and Anderson 1981; Widmer et al. 1991; Durek and Ekström 1996; Resovsky et al. 2005; Trampert and Fichtner 2013).

The most relevant tuning parameters in our approach are the number and values of the target $Q_0^{(k)}$, as well as the number of relaxation parameters. While one should ideally give a generally valid recipe for the perfect distribution of the target $Q_0^{(k)}$, we think that carefully conducted numerical experiments with different choices for $Q_0^{(k)}$ are more likely to provide good results for specific applications with their specific requirements. The same holds for the number of relaxation mechanisms. The approximation can be improved through the incorporation of additional relaxation mechanisms, though at the expense of increase computational costs.

The $\alpha$ kernels derived in Appendix A.6.1 and computed in section A.4.2 for example measurements, in principle provide a tool that enables inversions for the frequency-dependence of $Q$ as a function of position. Since $Q$ itself tends to be poorly resolved (e.g. Resovsky et al. 2005), a good spatial resolution of $\alpha$, that is comparable to the spatial resolution of seismic velocities, seems unlikely. Model basis functions for $\alpha$ will thus need to have a broader spatial extent, or even be constant for the whole Earth - depending on the resolving power of a specific data
set. In our description of $Q$, we so far assumed a constant $\alpha$ throughout the Earth. In the case of spatially variable $\alpha$, this aspect would need to be relaxed, and position dependent weight factors $D^{(p)}$ would need to be determined.

The most important advantage of our approach lies in the computationally efficient calculation of Fréchet kernels that does not require additional computational costs, compared to the calculation of Fréchet kernels for elastic properties. Fréchet kernels for anelastic properties can generally be expressed in terms of the forward strain field and the adjoint memory variables that are a by-product of any adjoint calculation in a visco-elastic medium.

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References


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Megies, T., M. Beyreuther, R. Barsch, L. Krischer, and J. Wassermann. 2011. “Ob-
sPy - What Can It Do for Data Centers and Observatories?” Ann. Geophys. 54 (1).


heterogeneous staggered-grid finite-difference modeling of seismic motion with
volume harmonic and arithmetic averaging of elastic moduli and densities”. Bull.

element method for computing spherical-earth seismograms - I. Moment-tensor


ence modeling”. Geophysics 59 (9): 1444–1456.

Romanowicz, B. 1995. “A global tomographic model of shear attenuation in the
upper mantle”. J. Geophys. Res. 100 (B7): 12375.

from Crust to Core”. In Treatise on Geophysics, 731–774.

Selby, N., and J. H. Woodhouse. 2002. “The Q structure of the upper mantle: Con-


Tao, G., and M. King. 1990. “Shear-wave velocity and Q anisotropy in rocks: A
361.


Tarantola, A. 1984. “Inversion of seismic reflection data in the acoustic approxima-
A.6. Appendix


A.6. Appendix

A.6.1. Computing $\alpha$-Kernels

In this Appendix, we provide a detailed derivation of the Fréchet kernels for the exponent $\alpha$ in the power-law frequency dependence of $Q$, as defined in eq. (A.11). For this we first note that for $Q_0 \gg 1$, eq. (A.13) can be transformed to

$$\sum_{p=1}^{N} \frac{D_p \omega T^{(p)}}{1 + \omega^2 T^{(p)} \tau^{(p)}} \approx \left( \frac{\omega_0}{\omega} \right)^\alpha. \quad (A.48)$$

Keeping the relaxation times for a specific target frequency range fixed, eq. (A.48) implies that the vector of weights $\mathbf{D} = (D^{(1)}, \ldots, D^{(N)})^T$ only depends on $\alpha$ and not on $Q_0$, i.e. $\mathbf{D} = \mathbf{D}(\alpha)$. Equipped with this result, we now proceed with the
calculation of $\alpha$ kernels. In the interest of a lighter notation, we again consider shear and bulk attenuation separately.

**Shear Attenuation**

In isotropic media with $C_{ijkl} = (\kappa - \frac{2}{3}\mu)\delta_{ij}\delta_{kl} + \mu\delta_{ik}\delta_{jl} + \mu\delta_{il}\delta_{jk}$ and variations in the shear modulus $\mu$, the variation of the measurement functional (eq. A.23) takes the form

$$\delta \chi = 2 \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[ \int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^\dagger(t) \delta \mu(t-t') dt \right] \tilde{\epsilon}_{ij}(t') dx dt', \quad (A.49)$$

where $\tilde{\epsilon}_{ij}$ and $\tilde{\epsilon}_{ij}^\dagger$ are the deviatoric parts of $\epsilon_{ij}$ and $\epsilon_{ij}^\dagger$, respectively. In the next step, we express $\delta \mu$ in (A.29) in terms of variations in $\alpha$. For this, we invoke the chain rule and the previously noted fact that the weights $D_p$ only depend on $\alpha$ (eq. A.48):

$$\delta \mu = \sum_{p=1}^{N} \frac{\partial \mu}{\partial D^{(p)}} \frac{\partial D^{(p)}}{\partial \alpha} \delta \alpha. \quad (A.50)$$

The partial derivatives $\partial \mu/\partial D_p$ follow from the definition of the time-dependent elastic modulus in (A.4), with the general relaxed modulus $C^r$ set equal to the relaxed shear modulus $\mu^r$:

$$\frac{\partial \mu(t)}{\partial D^{(p)}} = \mu^r Q_0^{-1} e^{-t/\tau^{(p)}} H(t). \quad (A.51)$$

Using (A.50) and (A.51), we can reformulate the integral over $\tilde{\epsilon}_{ij}^\dagger(t)\delta \mu(t-t')$ that appears in eq. (A.49):

$$\int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^\dagger(t) \delta \mu(t-t') dt = \int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^\dagger(t) \delta \mu(t-t') dt$$

$$= \mu^r Q_0^{-1} \mu \sum_{p=1}^{N} \int_{-\infty}^{\infty} \frac{\partial D^{(p)}}{\partial \alpha} e^{-(t-t')/\tau^{(p)}} H(t-t') \tilde{\epsilon}_{ij}^\dagger(t) \delta \alpha dt.$$

$$\quad (A.52)$$
Substituting the adjoint memory variables $M_{kl}^{(p)\dagger}$, defined in (A.26), we can simplify (A.52) into
\begin{equation}
\int_{-\infty}^{\infty} \tilde{\epsilon}_{ij}^{\dagger}(t) \delta \hat{\mu}(t - t') \, dt = -\mu^r Q_{0\mu}^{-1} \sum_{p=1}^{N} \frac{\partial D^{(p)}}{\partial \alpha} \frac{D^{(p)}}{\tau^{(p)}} \bar{M}_{ij}^{(p)\dagger}(t') \delta \alpha. \tag{A.53}
\end{equation}

Combining eqs. (A.49) with (A.53) we can write the variation of the measurement functional $\delta \chi$ in terms of a volumetric Fréchet or sensitivity kernel:
\begin{equation}
\delta \chi = \int_V K_\alpha(x) \delta \ln \alpha(x) \, dx, \tag{A.54}
\end{equation}
where the kernel $K_\alpha$ is given in terms of the forward strain deviator $\tilde{\epsilon}_{ij}$ and the deviator of the adjoint memory variables, $\bar{M}_{p,ij}$:
\begin{equation}
K_\alpha = -2\mu^r Q_{0\mu}^{-1} \sum_{p=1}^{N} \frac{\tau^{(p)}}{D^{(p)}} \frac{\partial D^{(p)}}{\partial \alpha} \int_{-\infty}^{\infty} \bar{M}_{ij}^{(p)\dagger} \tilde{\epsilon}_{ij} \, dt. \tag{A.55}
\end{equation}
This proofs eq. (A.37).

**Bulk Attenuation**

For variations in the visco-elastic properties related to the bulk modulus $\kappa$, the variation of the elastic tensor $C_{ijkl}$ condenses to $\delta C_{ijkl} = \delta \kappa$. The variation of the measurement functional $\chi$ can then be written in terms of the traces $\epsilon_{kk}$ and $\epsilon_{kk}^{\dagger}$ of the forward and adjoint strain tensors:
\begin{equation}
\delta \chi = \int_{-\infty}^{\infty} \int_V \left[ \int_{-\infty}^{\infty} \epsilon_{kk}^{\dagger}(t) \delta \hat{\mu}(t - t') \, dt \right] \epsilon_{kk}(t') \, dx \, dt'. \tag{A.56}
\end{equation}
Following exactly the same steps as in section A.6.1, we transform (A.56) into
\begin{equation}
\delta \chi = \int_V K_\alpha(x) \delta \ln \alpha(x) \, dx, \tag{A.57}
\end{equation}
with the Fréchet kernel
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$$K_{\alpha} = -\kappa^r \alpha Q_0^{-1} \sum_{p=1}^{N} \frac{\tau^{(p)}(p)}{D^{(p)}} \frac{\partial D^{(p)}}{\partial \alpha} \int_{-\infty}^{\infty} M^{(p)}_{kk} \epsilon_{kk} dt. \quad (A.58)$$

This is the result previously stated without proof in eq. (A.42).