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AxiSEM: broadband 3-D seismic wavefields in axisymmetric media

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Abstract

We present a methodology to compute 3-D 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 ac-

- ⁵ commodated by mandating axisymmetric background models which allow for a multipole expansion such that only a 2-D 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 correspond-
- ing 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.

15 **1** Introduction

Seismology currently enjoys transformative progress upon a simultaneous surge in instrumention, 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 3-D wave propagation (e.g. Tromp et al., 2005).

Traditionally, global seismic tomography (e.g. Rawlinson et al., 2010) 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 et al., 2008), or instantaneous phase (Bozdag et al., 2011) are based on waveforms, and therefore necessitate full wavefield modeling. Moreover, high-frequency waveform modelling (e.g. Ni et al., 2005) is often employed to fit specific strong, often 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 3-D space and time (Nissen-Meyer et al., 2007a). For the purpose of this paper, let us postulate the desire for a method to deliver.
 - 1. 3-D wavefields for realistic sources and structures,
- 15 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.

20 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 1-D structures, but largely due to the fact that such averaged models represent and fit

²⁵ 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,

⁵ 3-D 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, 2013).

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

- ¹⁰ 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 captivating 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 bound-

aries and the Northern Hemisphere. It thus seems desirable to seek a compromise for modeling between broad frequency ranges, realistic effective Earth models, while captivating a maximal amount of usable data.

1.2 Numerical wave propagation

Unlike discplines subject to more complex, non-linear physical systems such as fluid dynamics, the availability of mature seismic wave-propagation codes (e.g. Komatitsch and Tromp, 2002b) has diminished the challenge of capturing the underlying physical system in a comprehensive manner. Instead, it appears to shift attention for achieving realistic wave propagation simulations towards



- 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 generally resolvable, the latter point is especially stringent. Worse still, for global seismology it will remain a dominant limitation on the maximally resolved frequencies (where computational cost scales with the fourth power) and exponentially increasing number of usable data with millions of recorded waveforms (IRIS annual report 2011, www.iris.edu) for years to come. Full 3-D 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., 2003). 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. This is unfortunate, as especially the domain of seismic periods below 10 s
 (see Fig. 1) offers both a wealth of seismic data and a resolution harboring many open geophysical questions. The plot in Fig. 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 s 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 con-
- straint on the global timestep. This is not seen in SPECFEM since intra-crustal layers are not explicitely meshed.

Considering desirable extensions for the inversion such as comprehensive modelsampling, uncertainty analysis, or probabilistic approaches, this represents not only a formidable challenge, but is essentially not computable for 3-D methods even with most optimistic estimates of the evolution of computation on a decadal time-scale. Several strategies of speeding up numerical methods exist, focused on either the physical system or the implementation. Code optimization may exploit dedicated hard-



ware 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 (which is effectively done by computationally expensive 3-D methods such as Komatitsch and Tromp, 2002a) or lower end (ray theory). Additionally, we commonly find cost reductions related to reduced dimensionality (e.g., 2-D, 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.

1.3 3-D 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-¹⁵ 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 be-

- ²⁰ come computationally more expensive if an entire wavefield as for sensitivity kernels is needed. Axisymmetric finite difference methods (Toyokuni and Takenaka, 2006; Jahnke et al., 2008) may accommodate this effectively, but suffer the shortcoming of approximate sources and high dispersion errors for large propagation distances of interfacesensitive phases such as surface or diffracted waves.
- ²⁵ The purpose of this paper is to introduce the axisymmetric spectral-element implementation *AxiSEM* as a new and publicly available, production-ready method 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 2-D semi-disk, and the azimuthal third dimension is computed analytically. Radiation pattern symmetries require all sources

- ⁵ to be located along the axis, and any lateral heterogeneities are translated into a 2.5dimensional ring-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 2-D parallelization, scalability to > 8000 cores, bench-
- ¹⁰ marks at 1 Hz 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. Section 3 describes those source types that may be simulated with AxiSEM, ranging from moment-tensors, single forces, to finite faults and stochastic sources. Section 4 similarly details a range of background models to

- ²⁰ be used in AxiSEM, covering anisotropy, intrinsic attenuation, classical 1-D Earth models, solar models, small-scale 2.5-D heterogeneities and tomographic cross-sections, random media and potentially explicit mesh representations of the crust and oceans. Section 5 shows simulation results for a selection of the previously mentioned ranges of applicability, covering the entire seismic frequency spectrum, 3-D wavefield visual-
- ization, lowermost mantle structures, simulations for 2.5-D 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 current release version for up-to-date features of the code.

5 2 Methodology

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The mathematical foundation and validation of rudimentary 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 3-D wavefields in axisymmetric Earth models, and distinguishes itself by

- 1. decreasing the computational costs by orders of magnitude compared to 3-D method due to axisymmetry,
- 2. taking no limiting assumptions about wave-propagation physics (except for longperiod effects such as rotation) 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 3-D modeling, by not compromising on either essential wave-propagation physics or the coverage of the entire recorded frequency band between 0.001–1 Hz. The efficiency gain is grounded upon assuming axisymmetric background models, which reduces the numerical cost to a 2-D domain where 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.



2.1 Equations of motion

The 3-D integral (weak-form) elastodynamic equations of motion in the solid Earth \oplus read (Nissen-Meyer et al., 2007b)

$$\int_{\oplus} \rho \boldsymbol{w} \cdot \partial_t^2 \boldsymbol{u} d^3 \boldsymbol{x} + \int_{\oplus} \nabla \boldsymbol{w} : \mathbf{C} : \nabla \boldsymbol{u} d^3 \boldsymbol{x} = \int_{\oplus} \nabla \boldsymbol{w} \cdot \mathbf{f} d^3 \boldsymbol{x}$$
(1)

where the displacement solution vector \boldsymbol{u} is subjected to a test vector \boldsymbol{w} and \boldsymbol{f} is teh source. ρ is the mass density, and \boldsymbol{C} the anisotropic fourth-order elasticity tensor with 21 independent parameters. It may be time-dependent for intrinsic attenuation (in which case the double contraction : implies a convolution).

10 2.2 Axisymmetric dimensional collapse

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

$$\boldsymbol{u}_{m}(\boldsymbol{x}) = \begin{pmatrix} u_{s}(\tilde{\boldsymbol{x}})\cos m\phi \\ u_{\phi}(\tilde{\boldsymbol{x}})\sin m\phi \\ u_{z}(\tilde{\boldsymbol{x}})\cos m\phi \end{pmatrix},$$
(2)

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where m = 0, 1, 2 are monopole, dipole, quadrupole radiation types, respectively (Fig. 2), and $\tilde{x} = (s, z) = (r, \theta)$ spans a two-dimensional domain (Fig. 3) by cylindrical (s, ϕ, z) or spherical r, θ, ϕ coordinates, respectively. This relation is accurate for axisymmetry in source $f = f(\tilde{x})$ and structure $\rho = \rho(\tilde{x}), \mathbf{C} = \mathbf{C}(\tilde{x})$. Seismograms and wavefields at any location (s, ϕ, z) are obtained by multiplication with these azimuthal radiation factors in Eq. (2) during the post-processing stage (Sect. 2.5). Conceptually,



3-D integrals in \oplus over any integrand ψ that contains azimuthal dependencies such as in Eq. (2) are then collapsed to 2-D integrals in *D* as

$$\int_{\oplus} \psi(\mathbf{x}) \, d^3 \mathbf{x} \Rightarrow \int_{D} \psi(\tilde{\mathbf{x}}) \, d^2 \tilde{\mathbf{x}},$$

- ⁵ by evaluating integration over ϕ analytically. This delivers solutions for the 3-D displacement vector \boldsymbol{u} within a 2-D computational domain (Fig. 3). Axisymmetry (blue axis in Fig. 3) mandates all heterogeneities away from the symmetry axis to adopt a torus-shaped, azimuthally invariant elongation, whereas the point source remains along the axis. Such torus-shaped lateral heterogeneities are useful for studying many Earth-like structures especially at high frequencies (see Sect. 4.4), only precluding
- three-dimensional, off-plane back-scattering wave effects.

2.3 Spatial discretization

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

$$\mathcal{J}(\boldsymbol{\xi}) = \left| \frac{\partial \tilde{\boldsymbol{X}}}{\partial \boldsymbol{\xi}} \right|,\tag{4}$$

where |.| is the determinant. This mapping is purely analytical for all element types of 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

$$\boldsymbol{u}(\boldsymbol{\xi}) \approx \sum_{i,j=0}^{N} \boldsymbol{u}_{ij} \boldsymbol{I}_{ij}(\boldsymbol{\xi}),$$

20

(3)

(5)

with two-dimensional Lagrange polynomials I_{ij} (Nissen-Meyer et al., 2007b). Partial derivatives $\partial_{\xi} u(\xi)$ are given by analytically differentiating I_{ij} along ξ . These derivative operations are responsible for the bulk of the computational cost in typical spectral-element methods. Having performed elemental derivatives and quadratures, individual

elemental contributions are summed to define the discrete global stiffness Ku and mass terms Mu. Our particular formulation using cylindrical coordinates leads to singularities in the gradients at the symmetry axis. This is accommodated by a different basis compared to the interior domain, l'Hospital's rule, and asymptotic expressions to accommodate boundary conditions (Nissen-Meyer et al., 2007b). By choice of either kind of basis function, the mass matrix is exactly diagonal.

2.4 Temporal discretization

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

 $\ddot{\boldsymbol{u}}(t) = \mathbf{M}^{-1} \left(\mathbf{f}(t) - \mathbf{K} \boldsymbol{u}(t) \right),$

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This system is solved by various time-evolution schemes such as second-order Newmark, or higher-order symplectic schemes (Nissen-Meyer et al., 2008) up to eighthorder accuracy. Note that for the case of solid-fluid domains, the time-stepping becomes a combined system of these two domains, and needs to be iterated appropriately across the solid–fluid interface (Nissen-Meyer et al., 2008).

2.5 Post-processing: summation, rotation, filtering

Unlike most seismic wave-propagation codes, AxiSEM requires a crucial sequence of post-processing steps to retrieve the full solution Eq. (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. For instance, one does not need to decide on the source mechanism, source-time function, filtering, instrument re-



sponse, and receiver components at the time of the actual simulation but can defer this to post-processing. Figure 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. Clicking on any receiver links to an image of the post-processed seis ⁵ mograms, and source information is provided as text (see Fig. 4). The only necessary geophysical choices at the time of the simulation are source depth, receiver distances, maximal frequency, and background model. Section 5.3 sketches a generalization of this post-processing that fully exploits its flexibility in the context of solving the forward

¹⁰ post-processing as well.

Recasting the 3-D equations of motion into axisymmetric solutions yields a system of four independent wave equations to represent all six elements of the moment tensor separately, where the two remaining elements only vary by the azimuthal dependence (Nissen-Meyer et al., 2007a). Consequently, AxiSEM simulations are by construction

problem once-and-for-all, by deferring the choice of the source-receiver geometry to

- ¹⁵ always given for each element of the moment tensor separately. The task to sum to a full moment-tensor is described in Sect. 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 3-D wavefield visualizations. In addition, users may specify rendering perspectives, wavefield components, 3-D cuts, hypersurface extractions within post-processing. In effect, this allows for in-situ visualization and merges seismic trace analysis with visualization on-the-fly.

2.6 Parallelization

²⁵ At frequencies around 1 Hz, the required run-time memory (roughly 20 GB) for 1 Million elements exceeds the typical memory of 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 2-D domain decom-



position into $2N_{\theta}N_{r}$ domains, where $N_{\theta}N_{r}$ represent positive integers for the number of latitudinal and radial slices, respectively. 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 excellent scaling in Sect. 2.7.

2.7 Performance and scaling

The reduction of 3-D wave propagation to a 2-D computational domain is reflected by the method's performance compared to 3-D methods (Fig. 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 kernels for the inverse problem, one needs to save the entire space-time wavefield everywhere,

- ¹⁵ and hence such dependencies become inefficient especially when moving to higher resolutions. Figure 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. Figure 6 shows the new implementation of 2-D parallelization
- and 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 akin to efficient memory usage. Weak scaling shows a slightly sub-optimal behavior at 95 % for > 8000 cores, still a remarkable figure indicating that message passing and parallelization is 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 3-D seismic methods which are often memory-bound. As in any (2-D) 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).

- ⁵ Figure 7 serves as a guidance for typical settings of a simulation for global wave propagation, cast in terms of external computational limitations such as available runtime memory, number of cores, or maximal simulation time. The input parameter files are kept at a generic, streamlined minimum such that these choices are easily applicable to running the code. As a rough estimate, each 2-D element occupies 1.5 wavelengths
- and about 2.5 kB, and for seismic periods of 5 s approximately 400 000 elements are needed. Figure 7 (right) provides a hint of the required CPU-cycles, which can be approximated as requiring about eight microseconds simulation time per time-step and element.

2.8 Excessive input/output

- ¹⁵ Spectral-element methods of the kind presented here have excellent scalability properties in general (Fig. 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. 5.3), platform-independence of the
- ²⁰ data is needed. However, the storage format of Fortran binary files is not even compilerindependent. 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 (shu 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 ac-



cess 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 significant 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 Robinscheme 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.

2.9 Implementation and availability

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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, fftw (Frigo and Johnson, 2005) for post-processing in the frequency domain, taup (Crotwell et al., 1999) for traveltime picks, paraview for visual-ization of *vtk-* and *xdmf*-based wavefields, matlab for visualization of record sections, gnuplot for creating seismogram image files, Google Earth 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.

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 builts and tractable subversion control system as well as an existent userbase.

3 Seismic sources

In global seismology, it is customary to rely on the point-source approximation and corresponding moment tensors \mathbf{M}^{ρ} (not to be confused with mass matrix \mathbf{M} in Sects. 2.1 and 2.4). The implementation of indigenous earthquake sources or single forces located at \mathbf{x}_{ρ} is detailed in Nissen-Meyer et al. (2007b). We use temporal Dirac delta functions acting at time t_{ρ} in the simulations, with a displacement time series is obtained by convolving a source-time function $S^{\rho}(t)$, such that $\mathbf{M}^{\rho}(t) = \mathbf{M}^{\rho}S^{\rho}(t)$, and the Green's tensor solution \mathbf{G}^{ρ}

15
$$\boldsymbol{u}^{\boldsymbol{\rho}}(\boldsymbol{x},\boldsymbol{\omega}) = \mathbf{M}^{\boldsymbol{\rho}}(\boldsymbol{\omega}) : \nabla_{\boldsymbol{\rho}} \mathbf{G}^{\boldsymbol{\rho}}(\boldsymbol{x},\boldsymbol{\omega}),$$

20

where we reverted to frequency domain ω for concise notation, and ∇_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, helioseismology), and the problem of handling Dirac delta functions $\delta(\mathbf{x})$ in a discrete world.

3.1 Moment-tensor and single forces

To obtain the response to a full moment tensor (e.g., CMT catalogue, www.globalcmt. ²⁵ org), one applies posteriori summation honoring the respective radiation patterns along



(7)

the azimuth jointly with the convolution:

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$$\boldsymbol{u}^{\boldsymbol{\rho}}(\boldsymbol{x},\boldsymbol{\omega}) = \sum_{m=1}^{4} \tilde{M}^{\boldsymbol{\rho}}_{m}(\boldsymbol{\phi},\boldsymbol{\omega}) \tilde{\boldsymbol{\mathsf{G}}}^{\boldsymbol{\rho}}_{m}(\tilde{\boldsymbol{x}},\boldsymbol{\omega}),$$

where $\tilde{\mathbf{G}}_{m}^{p}$ represent 2-D vectorial Green's responses to each simulation *m* for point source *p*, and \tilde{M}_{m} read

$$\tilde{M}_1(\phi) = M_{rr},\tag{9}$$

$$\tilde{M}_{2}(\phi) = \left(M_{\theta\theta} + M_{\phi\phi}\right)/2,\tag{10}$$

$$\tilde{M}_{3}(\phi) = M_{r\theta}\cos\phi + M_{r\phi}\sin\phi, \qquad (11)$$

$$\tilde{M}_{4}(\phi) = \left(M_{\theta\theta} - M_{\phi\phi}\right)\cos 2\phi + M_{\phi\theta}\sin 2\phi.$$

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 (e.g., Lamb's problem, ambient noise, impacts, adjoint wavefields), require two simulations (monopole vertical force, dipole horizontal force) to account for the three components (Nissen-Meyer et al., 2007b).

Figure 8 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) in 33° distance. Note that the summed trace bears little resemblance with any of the generic solutions due to radia-

tion patterns Eqs. (9)–(12) highlighting the sensitivity due to the chosen source parameters.



(8)

(12)

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. AxiSEM

⁵ 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^{ρ}

$$\boldsymbol{u}(\boldsymbol{x},t) = \sum_{\boldsymbol{\rho}} \boldsymbol{u}^{\boldsymbol{\rho}}(\boldsymbol{x},t).$$

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Note that the dependence on the point-source locations \mathbf{x}^{ρ} exists for moment-tensor \mathbf{M}^{ρ} (by means of radiation pattern and source-time function), and Green tensor \mathbf{G}^{ρ} in Eq. (7), requiring separate solutions to the wave equation for each location \mathbf{x}^{ρ} . 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 \mathbf{x}^{ρ} 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 cer-

- tain 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. 5.3), such that existent AxiSEM databases can
 simply be applied to finite sources as well, and finite faults can be naturally embedded
- within any application of AxiSEM with little additional computational effort.



(13)

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 earthquake coda (e.g. Boué et al., 2013), or random pressure fluctuations in the Sun's inte-

⁵ rior (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 a single force only at the surface) 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 ambientnoise source locations.

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 distribution, which, from a rigorous perspective, is ¹⁵ 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 characteris-²⁰ tics and (2) sufficient sampling below Nyquist frequency. This is automatically computed in the code, depending on the sampling and period ranges.

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 vs. smooth variations,

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- regional 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 finiteelement 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, or 2.5-D structures that are invariant in the azimuthal direction are then superimposed onto the background mesh on-the-fly in the solver. These structures can be of pre-defined shape types, or arbitrarily superimposed by interpolation of discrete external grids (see Sect. 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 1-D
 structures in the meshing process, such that other Earth models such as those based on mineral physics can be easily accommodated. One can also apply the methodology to other planetary bodies 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 varia tions readily discretized by our methodology, we reach out for our central star: The sun



is a giant fluid sphere subject to violent 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 wavespeeds. 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. 9. Surface boundary conditions for acoustic waves pose no technical difficulty, but are not yet included in the first code release and shall be added in a timely future version.

4.2 Crustal variations

¹⁰ 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 2-D 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 can be discretized by actual fluid-domain elements, instead of resorting to a loading equiva-

²⁰ lent (Komatitsch and Tromp, 2002b) or a homogenized crust (Fichtner and Igel, 2008). Similar to axisymmetric structures, this divides the sphere into oceanic and continental pole-centric rings. This feature is not implemented in the first code release, but will be added in the future.

4.3 Random media

²⁵ 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 suffi-



ciently smooth and mildly deviatoric. In Fig. 10, we show two types of such random variations, perturbing either radial structure (left), or 2.5-D 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 and Dahlen, 2003).

4.4 Localized heterogeneities

The next level of complexity in structural properties is represented by 2.5-D axisymmetric media, which may have arbitrary variations in the source-receiver plane, but are invariant in the azimuthal, perpendicular direction. Especially in high-frequency regimes, 3-D effects from large-scale structures become less important given the decreased ratio between seismic and structural wavelength. Axisymmetry can then represent a tangible basis for waveform modelling of unknown arrivals, precursors, undetected arrival delays, oblique reflectors. This covers a diverse number of scenarios to extend our understanding of seismograms and wave propagation. The only neglected part of the wavefield compared to 3-D background models are 3-D wave effects from off-plane structures such as 3-D elastic lense focusing and off-plane back-scattering. All other scenarios in which structures vary preferentially in the source-receiver direction are re-

- spected, as for instance wave propagation through subduction zones, or forward scat tering of small-scale lowermost mantle structures. Figure 11 shows one example of lateral heterogeneities implemented in AxiSEM, including a Large Low-Shear Velocity Province (LLSVP) or "Superplumes" (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 func-
- tions 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 abritrary models are incorporated via KD-tree (Kennel, 2004) search for nearest neighbors and interpolation, and therefore allow for any shape



and complexity. The accuracy of wave propagation through such models is governed by the scale of heterogeneity vs. finite-element size, in that strong variations at short spatial scales tend to be smoothed in the discrete model.

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 log-ically 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 (2014a) 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.

4.6 Attenuation

Intrinsic attenuation or visco-elastic damping is a natural property of bulk real-Earth materials at frequency ranges of seismic wave propagation. However, models for the quality factor *Q* (inverse damping) of the mantle show little agreement, and the inseparable trade-off with elastic small-scale scattering may cause intrinsic damping not to be visible at the resolving power of teleseismic waves. We implemented an improved methodology based on coarse-grain methods which add little computational cost compared to purely elastic wave propagation and work well for strong attenuation. Details



on this new implementation, which is applicable to any finite-element method, are described in a separate paper (Van Driel and Nissen-Meyer, 2014b).

4.7 Lack of ellipticity and rotation

The Earth's radius differs, depending on latitude, by up to 40 km between poles and
 ⁵ equator. For reasons of axial symmetry, AxiSEM does not allow waves to propagate from a non-polar source through a pole-centric ellipsoid. It is therefore necessary to apply phase-specific ellipticity corrections to any traveltime measured with AxiSEM such as shifting receiver coordinates to account for the difference between purely spherical and ellipsoidal geometries, similar to the standard method in traditional tomography
 ¹⁰ (Kennett and Gudmundsson, 1996). Rotation of the polar axis can in principle be in-

- corporate 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 s), 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
- ¹⁵ of further study and implementation. In summary, such effects grow into a visible and recordable first-order concern for specific cases of seismic data analysis concerned with pathological body-wave paths and very long-period seismology.

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, 3-D 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.



5.1 High-frequency body waves

Previous publications on a rudimentary early version of this method showcasted the accuracy by comparison against normal-mode summation (Nissen-Meyer et al., 2008). Normal-mode summation is difficult to achieve at high frequencies due to the compu-

- tational cost in generating mode catalogues, as well as numerical issues related to determining the eigenfrequencies. We use an alternative frequency-domain reference solution YSpec (Al-Attar and Woodhouse, 2008) capable of covering the entire relevant frequency band from 0.001 Hz to 1 Hz. Figure 12 shows a record section and some details for both AxiSEM and YSpec 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 inconsistencies are amplitude differences, and most probably due to a cut-off in the summation done in YSpec. To our knowledge, this
- ¹⁵ is the first accurate validation of two completely independent methods for anisotropic, viscoelastic media at such high resolution.

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 h, 1.7 Million time steps, against YSpec in Fig. (13). The fit is again excellent, which is not trivial considering that time-domain numerical methods are subjected to significant dispersion errors for wave propagation
 over that many 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, agravic Earth model.



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. (2), such that seismograms only need to be stored along the distance range 0–180° for sources at a range of depths. This is computable. 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 3-D 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.
- ²⁵ parameters such as source inversion problems.



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 3-D space-time wavefield, for both research and teaching purposes

- ⁵ (Thorne et al., 2013). This is possible only due to the collapse to 2-D at run-time and the convenience of on-the-fly extraction of the 3-D radiation upon azimuthal factors. In practice, this means that one may save the entire 2-D wavefield in space and time, and then subsequently decide on any moment tensor, summation, source-receiver geometry, and rendering choices. Figure 14 depicts a snapshot of a typical simulation of
- a strike-slip event in Italy with a dominant period of 10 s and isotropic, anelastic PREM background model. Note the characteristic dispersion in the surface wave train, the large amplitudes in the PP phase, and the 3-D radiation pattern. A movie of this setting is available in the Supplement. 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.

5.5 Wave propagation in 2.5-D media

Multi-scale structures in the lowermost mantle have long been favourite objects for waveform modelling (Mégnin and Romanowicz, 2000). Constraining constituents of
 these abundant, dominant structures is critical for understanding the thermo-chemical dynamical regime of the Earth's deep interior. In many previous applications, such structures have been modelled as 2-D or 2.5-D-structures with source-receiver-plane heterogeneity using approximations at frequencies below 0.07 Hz suitable for available computational ressources (Thomas et al., 2000). Figure 15 displays seismograms and
 wavefield snapshots for the model in Fig. 11 for ULVZs flanking a LLSVP. The record sections highlight phases and distances at which the existance 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.

In general, such 2.5-D modeling taps into a regime of wave propagation that offers a realistic grasp of wave effects at resolution and computational cost that is difficult to achieve with alternative methods.

5.6 Tomographic models

Global models derived from tomography can equally be honored by a 2.5-D rendition with AxiSEM, in that they usually deviate only mildly and smoothly from spherically symmetric Earth models. The actual incorporation of tomographic models is trivial in AxiSEM for any model given by either discrete cartesian, spherical grids as well as spherical harmonics. Wavefield effects captured by this methodology are those that obey forward scattering, whereas true 3-D-medium effects such as off-plane scattering are neglected. Of course, this 2.5-D assumption does not represent our nature's dimensionality, but mimics 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 3-D domain. Figure 16 shows a comparison between synthetic modeling through a PREM, a 2.5-D section of tomographic model S40RTS (Ritsema et al., 2011), and SPECFEM synthetics for S40RTS and CRUST2.0 (Bassin et al., 2000). As seen by the waveforms in Fig. 16, many phases are largely insensitive
- to 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 completely overrides that of the tomographic model. The
- neglected effects such as 3-D back-scattering 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, or modify local properties for a given source-receiver geometry.



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 s) to observed data. This resolution is at the cutting edge of supercomput-

- ing with 3-D methods (see Fig. 1), 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 s (top), and 15–45 s. In the lat-
- ter case, we included SPECFEM synthetics for the S362ANI tomographic model (Kus-10 towski et al., 2008) and CRUST2.0 (Bassin et al., 2000) which are accurate to about 17 s (Tromp et al., 2010). AxiSEM synthetics are based on an inverted moment tensor and depth, whereas SPECFEM synthetics are taken from the IRIS database, i.e. calculated for GCMT. All synthetics have been convolved with an inverted source-time func-
- tion. The phases have been aligned by frequency-dependent cross-correlation, form-15 ing 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:

filter [s]	method	Δt (Pdiff) [s]	$\Delta t(PKiKP)$ [s]
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5–15	AxiSEM	2.5 ($\sigma^2 = 0.99$)	$2.3(\sigma^2 = 0.5)$
15–45	AxiSEM	$4.0(\sigma^2 = 0.89)$	$3.4(\sigma^2 = 0.3)$
15–45	SPECFEM	$3.7(\sigma^2 = 0.6)$	$6.0(\sigma^2 = 0.37)$

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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 s.

SED 6, 265-319, 2014 Paper **AxiSEM** T. Nissen-Meyer et al. **Discussion** Paper **Title Page** Abstract Introduction Conclusions References Figures Tables Discussion Paper Back Close Full Screen / Esc Printer-friendly Version **Discussion** Paper Interactive Discussion

Discussion

5.8 Time-frequency 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 presence of said space-time wavefields makes it principally trivial to compute time-dependent sensitivity kernels as a comprehensive basis for mapping seismogram to Earth structure, and the **G** matrix 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, by incorporating complete seismograms, arbitrary time- and frequency-windows as well as arbitrary wave effects such as triplicated phases from the mantle transition zone (Stähler et al., 2012), core-mantle diffraction (Colombi et al., 2012), or caustics. Figure 18 shows a snapshot of a time-dependent kernel roughly near the theoretical PP-traveltime. Such an animated sensitivity 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 first AxiSEM release, but will be added in the future.

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 theoretical papers

- ²⁰ 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
- ²⁵ a diverse range of realistic applications in forward and inverse modeling and showcasts promising comparisons to recorded data. The considerably cheap 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), 3-D numerical methods (with local basis functions) such as SPECFEM (complex 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 caution despite the

- excellent and robust validation shown here. 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 2-D computational domain is the availability of space-time wavefields for axisymmetric, viscoelastic anisotropic media and realistic earthquake
- 15 SOURCES.

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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 opensource 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 3-D media (effects such as 3-D off-plane scattering and focusing) and realistic Earth rotation. All other limitations

²⁵ (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.



6.1 Future additions

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 3-D (Born) scattering. AxiSEM-generated wavefields may also be injected into a small 3-D box of local 3-D heterogeneities in a hybrid sense (Tong et al., 2013). This will allow for the consideration of teleseismic wavefields to locally travel through 3-D heterogeneities, 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).

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SED 6, 265-319, 2014 **AxiSEM** T. Nissen-Meyer et al. **Title Page** Abstract Introduction Conclusions References Figures Tables Back Close Full Screen / Esc Printer-friendly Version Interactive Discussion

Discussion Paper

Discussion Paper

Discussion Paper

Discussion

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Figure 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 3-D domains (SPECFEM, 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 10⁶ 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.





 $u_l = u_l(s, z) \cdot f_l(\sin\phi, \cos\phi)$



 $u_l = u_l(s, z) \cdot f_l(\sin(2\phi), \cos(2\phi))$

Figure 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} depend on multipole order *m* as well as component *l*, that is, no summation is implied by the above products.





Figure 3. The 2-D 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 20 s. Zoom panels show a higher-resolution version (5 s) with upper-mantle discontinuities honored by the mesh (b), as well as the peculiar meshing below the inner-core boundary (ICB).





Figure 4. A Google-Earth rendition of the source-receiver geometry used in an AxiSEM simulation. A generic output of the post-processing embedded within AxiSEM, this *kml*-file contains earthquake parameters (red dot), and actual seismogram images as links at the station locations (yellow pins).





Figure 5. A typical mesh decomposition for the PREM model running at dominant period of 9 s on 96 cores. Load balancing is exact, and the permissible arbitrary multiplicative between number of horizontal and radial slices guarantees flexibility for adapting numerical settings to existent hardware infrastructures.





Figure 6. Scalability of AxiSEM on a Cray XE6 at CSCS (Switzerland). Left: strong scaling, i.e. fixed global problem size (8 Million 2-D elements) as a function of the number of used cores communicating via the message–passing interface, for 12 000 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 where communication is not entirely hidden behind the computation of the stiffness terms.





Figure 7. A practical guide to usage of AxiSEM in terms of desired resolution (seismic period) and available resources (runtime, number of cores, RAM). Top: computational cost associated with the meshing process, which is primarily constrained by available run-time memory. The mesher code itself runs within minutes for typical resolutions. Bottom: computational cost for wave propagation simulations as a function of seismic period. Numbers along the function denote the necessary amount of CPU cores to achieve the corresponding wallclock time for a given period.





Figure 8. Left quadrant: the four time series upon the generic moment-tensor types (see Eqs. 9-(12)). Right: Summation to the full seismogram for the 2011 M9 Tohoku (point-source) event. Plotted is the displacement in the *s*-direction, with a dominant period of 10 s recorded at station BILL (East Siberia) at 33° distance.



Discussion Paper



Figure 9. 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.





Figure 10. Two examples of random wavespeed variations superimposed on PREM. Left: variations with depth only. Middle: variations in 2.5-D. Right (top): zoom into the crust for the 2.5-D random medium. Right (bottom): radial profile of these two realizations with respect to PREM.





Figure 11. An example of various lateral heterogeneities, representing realistic deep-mantle structures in the 2.5-D approximation. The large volume in yellow denotes a Large Low Shear Velocity Province (LLSVP), flanked by two ultra-low velocity zones (50 km height), 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.

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Figure 12. 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 Kristeková et al. (2009).





Figure 13. Amplitude spectra simulated by AxiSEM and YSpec for the PREM model (Dziewonski and Anderson, 1981) for frequencies below 0.02 mHz. The time-domain solution provided by AxiSEM extended over 48 h 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.





Figure 14. Snapshot of a 3-D wavefield emanating from a strike-slip event in Italy after 400 s. The background model is isotropic, anelastic PREM, and the simulation done at a dominant period of 10 s. Note the effect of the radiation pattern on the wavefield in 3-D. Similar snapshots are automatically generated in the post-processing of AxiSEM. A movie is available as Supplement.





Figure 15. A forensic application of AxiSEM on the detectability of ULVZs near LLSVPs (see model in Fig. 11). Left: seismograms for a model with a ULVZ as in Fig. 11 (black traces), and one exactly the same but without the ULVZ (red traces). The underlying Earth model is isotropic PREM (Dziewonski and Anderson, 1981), dominant period 2 s. The *N*-displacement record sections are at considerably large epicentral distance ranges. Right: wavefield snapshot of the same simulation with ULVZ, at time 604 s. 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).





Figure 16. Modelling 3-D wave propagation through a 2.5-D version of tomographic model S40RTS (Ritsema et al., 2011) (bottom left) for an event near Antarctica (left top). Right: seismograms filtered at 10 s from the receivers denoted on the cross section (bottom left) for 1-D model, 2.5-D tomographic model, and SPECFEM synthetics through S40RTS and CRUST2.0 (Bassin et al., 2000), aligned with the *P* wave arrival time.





Figure 17. A comparison of AxiSEM synthetics with recorded data and SPECFEM synthetics (Tromp et al., 2010) for a Mw7.5 2009 event in Southern Sumatra at 82 km 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 s (top), and 15–45 s (bottom). In the latter case, SPECFEM synthetics are included which are accurate down to 17 s. Bottom right: the same for PKiKIP. AxiSEM synthetics are simulated through a viscoelastic, anisotropic PREM model, SPECFEM 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 s (see main text).





Figure 18. A snapshot of a time-dependent sensitivity kernel, denoting the "region of influence" in which this particular instance in the seismogram may "see" structure which deviates from the background model. The plot shows an instance within the PP surface multiple for P wavespeeds. Such kernels are not only the basis for waveform tomography, but may also aid in identifying obscure arrivals in the seismogram.

