Full wave sensitivity of $SK(K)S$ phases to arbitrary anisotropy in the upper and lower mantle

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SUMMARY
Core-refracted phases such as $SKS$ and $SKKS$ are commonly used to probe seismic anisotropy in the upper and lowermost portions of the Earth’s mantle. Measurements of $SK(K)S$ splitting are often interpreted in the context of ray theory, and their frequency dependent sensitivity to anisotropy remains imperfectly understood, particularly for anisotropy in the lowermost mantle. The goal of this work is to obtain constraints on the frequency dependent sensitivity of $SK(K)S$ phases to mantle anisotropy, particularly at the base of the mantle, through global wavefield simulations. We present results from a new numerical approach to modelling the effects of seismic anisotropy of arbitrary geometry on seismic wave propagation in global 3-D earth models using the spectral element solver AxiSEM3D. While previous versions of AxiSEM3D were capable of handling radially anisotropic input models, here we take advantage of the ability of the solver to handle the full fourth-order elasticity tensor, with 21 independent coefficients. We take advantage of the computational efficiency of the method to compute wavefields at the relatively short periods (5 s) that are needed to simulate $SK(K)S$ phases. We benchmark the code for simple, single-layer anisotropic models by measuring the splitting (via both the splitting intensity and the traditional splitting parameters $\phi$ and $\delta t$) of synthetic waveforms and comparing them to well-understood analytical solutions. We then carry out a series of numerical experiments for laterally homogeneous upper mantle anisotropic models with different symmetry classes, and compare the splitting of synthetic waveforms to predictions from ray theory. We next investigate the full wave sensitivity of $SK(K)S$ phases to lowermost mantle anisotropy, using elasticity models based on crystallographic preferred orientation of bridgmanite and post-perovskite. We find that $SK(K)S$ phases have significant sensitivity to anisotropy at the base of the mantle, and while ray theoretical approximations capture the first-order aspects of the splitting behaviour, full wavefield simulations will allow for more accurate modelling of $SK(K)S$ splitting data, particularly in the presence of lateral heterogeneity. Lastly, we present a cross-verification test of AxiSEM3D against the SPECFEM3D_GLOBE spectral element solver for global seismic waves in an anisotropic earth model that includes both radial and azimuthal anisotropy. A nearly perfect agreement is achieved, with a significantly lower computational cost for AxiSEM3D. Our results highlight the capability of AxiSEM3D to handle arbitrary anisotropy geometries and its potential for future studies aimed at unraveling the details of anisotropy at the base of the mantle.

Key words: Planetary interiors; Numerical modelling; Computational seismology; Seismic anisotropy; Wave propagation.

1 INTRODUCTION
Seismic anisotropy, the property of elastic materials to manifest directionally dependent seismic wave speeds (e.g. Anderson 1989; Babuska & Cara 1991), occurs in many regions of the Earth, including the crust (e.g. Barruol & Kern 1996), the upper mantle (e.g. Silver 1996; Savage 1999), the transition zone (e.g. Foley & Long 2011; Yuan & Beghein 2013), the uppermost lower mantle (e.g. Lynner & Long 2015; Ferreira et al. 2019), the $D^\prime$ region at the base of the mantle (e.g. Nowacki et al. 2011; Creasy et al. 2017) and the inner core (e.g. Beghein & Trampert 2003). Because mantle anisotropy reflects deformation processes, knowledge of its
presence, style and strength yields insight into past and present mantle flow (e.g. Long & Becker 2010). The proper characterization of seismic anisotropy is therefore crucial for our understanding of the dynamics of Earth’s mantle. Our ability to completely characterize anisotropy in the mantle is limited, however, in part due to limitations imposed by seismic data coverage, and in part due to theoretical or computational limitations to relate observations to Earth structure. It is common in many global seismological studies to either neglect anisotropy entirely, and consider an isotropic approximation to Earth structure, or to consider only simple anisotropic geometries, such as radial anisotropy.

Elastic anisotropy manifests itself in the seismic wavefield in many ways, including the difference in propagation velocity between vertically polarized Rayleigh waves and horizontally polarized Love waves (e.g. Anderson 1961; Moulík & Ekström 2014), the splitting of normal modes (e.g. Anderson & Dziewonski 1982; Tromp 1995; Beghein et al. 2008), the directional dependence of traveltimes of body waves such as $P_n$ (e.g. Hess 1964; Buehler & Shearer 2017) or surface waves (e.g. Forsyth 1975; Schaeffer et al. 2016), the scattering of energy from Love waves to Rayleigh waves via the coupling of spheroidal and toroidal modes (e.g. Park & Yu 1993; Servali et al. 2020), the polarization of $P$ waves (e.g. Schulte-Pelkum et al. 2001) and directionally dependent $P$-to-$S$ conversions as manifested in receiver functions (e.g. Levin & Park 1998; Wirth & Long 2014). The most widely used technique for detecting anisotropy in the mantle, however, is shear wave splitting or birefringence (e.g. Silver 1996; Savage 1999; Long & Silver 2009). The splitting of $SKS$ and $SKKS$ phases is routinely measured to study anisotropy in both the upper mantle (e.g. Silver & Chan 1991; Wolfe & Silver 1998; Levin et al. 1999; Long & van der Hilst 2005; Long 2013; Roy et al. 2014) and in the lowermost mantle (e.g. Niu & Perez 2004; Restivo & Helffrich 2006; Long 2009; Roy et al. 2014; Long & Lynner 2015; Grund & Ritter 2018; Reiss et al. 2019). Core traversing phases such as $SKS$ and $SKKS$ have several distinct advantages for shear wave splitting analysis. These include the known initial polarization of the shear wave, controlled by the $P$-to-$S$ conversion at the core–mantle boundary (CMB), the lack of source-side effects, and the ability to observe clear $SK(K)S$ phases that are often easily identifiable on seismograms. Shear wave splitting analysis also has several shortcomings, however; chief among these is the lack of vertical resolution of anisotropy, since it is a path-integrated measurement, and the need to obtain splitting measurements from multiple azimuths in order to fully characterize the anisotropic structure.

While a full 21 elastic parameters are needed to fully describe arbitrary anisotropy, it is common to use simpler parametrizations of anisotropy that invoke assumptions about anisotropic symmetry. For example, in global tomographic inversions that include radial anisotropy, under the assumption of hexagonal symmetry (e.g. Auer et al. 2014; Tesoniero et al. 2015), it is typical to use 5 parameters to describe the model, rather than the 2 needed for the isotropic case (e.g. Ritsma et al. 2011). Similarly, inversions of $SKS$ splitting data for azimuthal anisotropy in the upper mantle typically rely on reduced parametrizations (e.g. Monteiller & Chevrot 2011; Lin et al. 2014a; Mondal & Long 2019). While such parametrizations may make sense in the context of practical limitations on observational data sets, they may not always be realistic for actual Earth materials. For example, olivine, the primary mineral constituent of the upper mantle and the major cause of upper mantle anisotropy, has orthorhombic symmetry, although deformed olivine aggregates may be approximated with higher symmetry classes (e.g. Karato et al. 2008). In any case, it is desirable to have computational tools that can simulate accurate wave propagation through anisotropic media of arbitrary symmetry efficiently; furthermore, azimuthal anisotropy is a well-known property of the upper mantle, so it is necessary for wavefield modelling schemes to be able to handle azimuthal anisotropy in addition to the more commonly invoked radial anisotropy.

Measurements of shear wave splitting are commonly interpreted in the framework of ray theory, either implicitly or explicitly. The most straightforward interpretation of $SKS$ splitting measurements, for example, invokes a single layer of azimuthal anisotropy beneath a station whose properties (symmetry axis orientation, strength of anisotropy and/or layer thickness) are related to the observed splitting parameters (typically fast splitting direction, $\phi$ and delay time, $\Delta t$) via a simple ray theoretical approximation. In some cases, complex patterns of $SKS$ splitting, in which apparent splitting parameters vary with backazimuth, are interpreted as reflecting multiple layers of anisotropy (e.g. Marson-Pidgeon & Savage 2004; Eakin & Long 2013), via analytical equations that were developed based on a ray theoretical approximation (Silver & Savage 1994). While there has been some work on the nature of the frequency dependent sensitivity of $SKS$ phases to upper mantle anisotropy (e.g. Favier & Chevrot 2003; Favier et al. 2004; Chevrot 2006; Long et al. 2008; Sieminski et al. 2008; Lin et al. 2014a; Mondal & Long 2019), only a few observational studies have actually used finite-frequency sensitivity estimates to interpret (or invert) actual data (Monteiller & Chevrot 2011; Lin et al. 2014b). Furthermore, the finite-frequency sensitivity of $SKS$ and $SKKS$ phases to anisotropy in the lowermost mantle remains poorly understood. Given the increasing use of $SK(K)S$ phases in studies of deep mantle anisotropy, it is crucial to understand the nature of this sensitivity.

For both upper and lowermost mantle anisotropy studies, it is desirable to have a computationally efficient tool to simulate global seismic wave propagation for $SK(K)S$ phases in anisotropic media with arbitrary symmetry. The popular spectral-element based community software package SPECfem3D_GLOBE (Komatitsch & Tromp 2002a,b) is capable of handling arbitrary anisotropy, but its significant computational requirements make global simulations at the periods relevant for $SK(K)S$ phases (down to $\sim 5$–$10$ s) impractical. In this study, we make use of the AxiSEM3D code (Leng et al. 2016, 2019), a coupled pseudospectral spectral element solver for 3-D global wavefield propagation in realistic 3-D earth models. While previously released versions of AxiSEM3D only handled radially anisotropic input models, the actual solver is capable of handling the full fourth-order elasticity tensor $C_{ijkl}$ with 21 independent coefficients. We have modified the formulation of the input models to handle arbitrary elasticity, and in this study we test and implement a range of anisotropic mantle models that include azimuthal anisotropy, relevant for $SK(K)S$ splitting. The AxiSEM3D code combines the advantages of a full 3-D spectral element method to model complex, 3-D structures with the computational efficiency of axisymmetric methods; this allows the user to model complex and realistic Earth structures with significant computational speedup and without significant loss of performance (Leng et al. 2019).

The goal of this study is to evaluate the frequency dependent effects of anisotropy of different symmetry classes (albeit in relatively simple, laterally homogeneous structures) on the splitting of $SK(K)S$ phases, via global wavefield simulations for seismic periods down 5 s. We generate synthetic seismograms for a suite of earth models with anisotropy in the upper and lowermost mantle, and analyse the synthetic $SKS$ and $SKKS$ waveforms by measuring shear wave splitting using both the traditional transverse component energy minimization method (Silver & Chan 1988) and the
splitting intensity method (Chevrot 2000). We present benchmark results for simple cases, including one based on the spherically symmetric PREM model (Dziewonski & Anderson 1981) and one that invokes vertically propagating shear waves travelling through a transverse isotropic medium with a horizontal axis of symmetry (HTI). We then model global wave propagation for more realistic upper mantle anisotropy scenarios, including approximations to olivine crystallographic preferred orientation (CPO) that invoke both hexagonal and orthorhombic symmetry. Next, we investigate the effects of anisotropy in the $D^\prime$ layer at the base of the mantle on $SKS$ splitting, via a series of global wavefield simulations for models that invoke CPO of lower mantle minerals such as bridgmanite and post-perovskite. In the last part we provide a verification of our implementation of full anisotropy via a benchmark solution against the full 3-D spectral element solver SPECFEM3D. We then discuss the implications of our results from relatively simple models for future work on the interpretation of shear wave splitting measurements in terms of mantle anisotropy, particularly as more complex models are considered.

## 2 Anisotropic Modelling Strategy with AxiSEM3D

AxiSEM3D (Leng et al. 2016, 2019) is a powerful hybrid spectral element solver for 3-D global wave propagation in realistic Earth structures. It aims to bridge the gap between computationally expensive simulation methods for 3-D Earth structure and faster simulation methods for spherically symmetric earth models. It is a fully convergent 3-D method not unlike other discrete full 3-D methods, for example SPECFEM3D. The method follows the axisymmetric spectral element solver AxiSEM which assumes spherically symmetric or axisymmetric structures. To accommodate arbitrary 3-D structures, AxiSEM3D is built upon a collection of coupled axisymmetric 2-D domains. This relies on the fact that wavefields in realistic 3-D structures are relatively smooth in the azimuthal direction (Leng et al. 2016), and can thus be accurately represented in the azimuthal direction by honouring this smooth complexity rather than a complexity-blind, fine discretization just as in the in-plane dimension or for conventional 3-D methods. AxiSEM3D couples the azimuthal dimension by Fourier series, which can assume arbitrarily low or high expansion orders for each patch in the source-receiver plane. This hybrid formulation combines the strength of a full 3-D discrete method to compute global wavefields with the significant speedup of computational time of 2-D methods. In other words, a 3-D global wavefield in complex earth models can be efficiently computed at a cost that scales almost as (multiple) 2-D simulations, allowing us to run simulations of global wavefield propagation over a large frequency range with relatively limited computer resources. This computational efficiency is coupled with the capability of AxiSEM3D to readily allow the usage of 3-D earth models based on global tomography, including those available from the Incorporated Research Institutions for Seismology (IRIS) Earth Model Collaboration (EMC) in netCDF format. Independent modules can be invoked to handle certain geometrical properties, such as surface topography or topography on boundaries such as the CMB (Leng et al. 2019). AxiSEM3D automatically handles radial anisotropy if the velocity structure of the underlying seismic velocity model is provided as horizontal and vertical compression and shear wave velocity values. Detailed descriptions of the theoretical formulation of AxiSEM3D and benchmark tests with independent, fully 3-D discrete spectral element solvers (e.g. SPECFEM3D) are given in (Leng et al. 2016, 2019).

For this study, we take advantage of the accuracy and efficiency of the method to solve the elastodynamic wave equation in global media, and implement a new independent module which introduces general anisotropy of arbitrary symmetry. The mathematical formulation of the three-dimensional wave equation is based on the generalized Hooke’s law, $\sigma_{ij} = C_{ijkl} \epsilon_{kl}$, which relates the components of the stress tensor $\sigma_{ij}$ to the strain tensor $\epsilon_{ij}$ through the fourth-order elasticity tensor $C_{ijkl}$. The elasticity tensor describes the elastic properties of the material, and in the most general case it can be fully described by 21 independent coefficients (see Malvern 1969; Babuska & Cara 1991, for details). In the new anisotropic module, the elastic properties of a specific anisotropic region in the domain are described by 21 independent elastic parameters, as opposed to the 2 Lamé constants ($\lambda$ and $\mu$) for the isotropic case or the 5 Love parameters ($A$, $C$, $L$, $N$, $F$, described further below) for the vertical transverse isotropy (VTI) case. In order to use the general anisotropy module in AxiSEM3D, the user must provide the solver with a netCDF file containing the information about the elasticity tensor and the anisotropic media’s geographical location within the model domain.

Introducing general anisotropy (an intrinsically 3-D property of the medium) usually only accounts for a relatively small increment of the total computational cost. However, similarly to the case for lateral heterogeneity in (isotropic) velocity structure, the user must ensure that the Fourier degree of expansion is larger than the size of the heterogeneous structure, in order to ensure a correct representation of the seismic wavefield. Moreover, the user must take particular caution in taking into account the geometrical properties of the elasticity tensor. This is usually defined in a local coordinate system such that certain crystallographic axes (or a strain directions) align certain geographic coordinates. However, AxiSEM3D works with a global spherical coordinate system. Therefore, except at the geographical poles (where the coordinate systems coincide), a rotation matrix must be applied to the elasticity tensor (specified by the user in a local coordinate system) to translate its orientation to the global domain of AxiSEM3D.

## 3 Benchmark Tests for Simple Anisotropic Models

We begin by running two different numerical tests with the intention to benchmark the new anisotropic module of AxiSEM3D against well-understood wave propagation behaviour for simple anisotropic models. In the first of these, we run a global wavefield simulation for the 1-D PREM model (Dziewonski & Anderson 1981), which includes radial anisotropy in the depth range between 25 and 220 km depth. In the second of these, we run wave propagation simulations for a simple, single layer of anisotropy with a horizontal axis of transverse isotropy (HTI), reproducing a synthetic test presented in Chevrot (2000).

### 3.1 Radially anisotropic PREM

In the first test, we run global wavefield simulations for PREM under two different conditions:

1. Using the traditional model input format of AxiSEM3D, in which radial anisotropy is specified via horizontal and vertical velocity values for both $P$ and $S$ waves and
Figure 1. Map showing the source–receiver configuration settings and the synthetic results for the self-benchmarking tests computed using AxiSEM3D with the anisotropic PREM model (black seismograms) and the solution obtained using a description of the anisotropic PREM as $C_{ijkl}$ (red seismograms). Three representative pairs of synthetic seismograms are plotted at three different locations. A close-up view of the synthetics is shown in the three boxes at the bottom of the figures for three different sections of the time-series.

(2) using the model input format of the new anisotropy module, in which anisotropy is specified via the full elasticity tensor.

This allows us to test whether we have correctly implemented the specification of elasticity in the new module, and whether we have correctly implemented the tensor rotations needed to map the local coordinate system of the model input file to the global spherical coordinate system of AxiSEM3D. In order to parametrize the PREM model in the new input file, we replace the elastic constants in the depth range between 24 and 220 km with equivalent elastic coefficients of the $6 \times 6$ elasticity tensor that describes the radial anisotropy contained in anisotropic PREM. At other depths, we use the isotropic PREM values, which are specified via the Lamé constants $\lambda$, $\mu$ (and the density $\rho$). The relationship between the full elasticity tensor $C_{ijkl}$ and the Love parameters that describe radial anisotropy are given by the following relationships (e.g. Babuska & Cara 1991):

$$A = \rho V_{PH}^2$$
$$C = \rho V_{PV}^2$$
$$L = \rho V_{SV}^2$$
$$N = \rho V_{SH}^2$$
$$F = \eta(A - 2L)$$

(1)

$$C_{ijkl} = \begin{pmatrix}
A & A - 2N & F & \cdot & \cdot \\
A - 2N & A & F & \cdot & \cdot \\
F & F & C & \cdot & \cdot \\
\cdot & \cdot & \cdot & L & \cdot \\
\cdot & \cdot & \cdot & \cdot & N
\end{pmatrix}$$

(2)

with $A$, $C$, $L$, $N$ being the parameters associated to the horizontal and vertical compressional and shear seismic wave speed and $F$ being the parameter associated to seismic waves propagating in intermediate directions through the coefficient $\eta$. We run the simulation for a hypothetical earthquake in the South American subduction zone whose moment tensor is represented by the focal mechanism in Fig. 1, which also shows the two sets of synthetic seismograms for different components at three representative stations (FFC, GRFO and COCO). This test shows the general ability of our new anisotropy module to correctly specify the full elasticity tensor for models that include radial anisotropy, however, this test is not capable of capturing the effects that azimuthally dependent anisotropy have on the propagating wavefield.

3.2 Single anisotropic layer with vertical wave propagation

In order to test whether the new anisotropy model correctly represents the effects of azimuthal anisotropy for simple models, we...
In order to mimic the synthetic test of Chevrot (2000) closely, and induce perfectly vertical to avoid global waveform effects, we use a point source sitting shifted along the latitudinal direction by 0.01°. This minor deviation from the fast axis orientation (Fig. 2), and a maximum in transverse component energy when the initial polarization is 45° from the symmetry axis. Following eqs (7) and (A4) from Chevrot (2000), we measure the splitting intensity for each synthetic seismogram, which is defined as:

\[ SI = -2 \frac{T(t)R'(t)}{||R'(t)||^2}. \]

The splitting intensity measured as a function of backazimuth forms the splitting intensity vector which is shown in Fig. 3. Estimates of the splitting parameters \((\delta, \beta)\) can be derived from fitting a \(\sin(2\theta)\) curve to the splitting intensity vector shown in Fig. 3, using the relationship \(SI \approx -1/2\beta \sin 2(\beta)\), where \(\beta\) corresponds to the angle between the initial polarization direction and the azimuth of the fast symmetry axis. Our estimates of the splitting parameters derived from Fig. 3 are \(\phi = 45°\) and \(\delta t = 0.228 s\), which agree well with the values for the same test in Chevrot (2000).

### 4 Upper Mantle Anisotropy Simulations and Comparison with Ray Theory

#### 4.1 Background: upper mantle anisotropy and shear wave splitting

Seismic anisotropy in the upper mantle is generally interpreted in terms of the CPO of anisotropic upper mantle minerals, primarily olivine. The relationships between strain and the resulting CPO are complex and depend on many factors, potentially including stress, temperature, pressure, water content, deformation history and pre-existing fabric (e.g. Karato et al. 2008; Skemer & Hansen 2016). Despite these complications, however, a number of simplified relationships are often used to interpret SKS\((K)S\) splitting data, often with implicit assumptions made about the symmetry of the anisotropic medium. For example, upper mantle anisotropy is often modelled using a hexagonal approximation to the actual elastic tensor (e.g. Browaeys & Chevrot 2004; Becker et al. 2006), even though olivine itself is orthorhombic, and even though actual aggregates of mantle rocks may have even lower symmetry in practice. As discussed in the Introduction, the interpretation of SKS(K)S data is usually done in the context of ray theory, with only a few exceptions. While a few studies have examined the finite-frequency sensitivity of SKS(K)S splitting to upper mantle anisotropy (e.g. Favier & Chevrot 2003; Favier et al. 2004; Chevrot 2006; Long et al. 2008; Sieminski et al. 2008; Zhao & Chevrot 2011; Lin et al. 2014a), it is relatively uncommon to carry out global wavefield simulations to model the effects of upper mantle anisotropy on SKS(K)S splitting. The purpose of the tests presented in this section is to establish the new
anisotropy module of AxiSEM3D as a viable tool for doing so, and to explore how anisotropy models of increasing complexity in terms of their symmetry (from hexagonal to orthorhombic) affect SK(K)S waveforms.

A second goal of these tests is to understand to what extent shear wave splitting measurements performed on synthetic seismograms derived from global wavefield simulations depart from the predictions of ray theory. Work by Lin et al. (2014a) established that full-wavefield effects on SK(K)S phases can cause significant deviations from ray theoretical predictions of shear wave splitting, even for relatively simple (laterally homogenous) upper mantle anisotropy models. We aim to extend our understanding of this phenomenon here, particularly as it relates to the interpretation of SKS−SKKS splitting discrepancies. Relatively large discrepancies between the splitting of SKS and SKKS phases for the same event-station pair are typically interpreted as evidence for a contribution to the splitting of one or both phases from anisotropy in the lower mantle (e.g. Niu & Perez 2004; Long 2009; Lynner & Long 2014; Grund & Ritter 2018; Reiss et al. 2019). However, Lin et al. (2014a) showed that wavefield effects that depart from the predictions of ray theory can cause small discrepancies in splitting intensity values (up to ∼0.3 s) between SKS and SKKS phases for models that only include upper mantle anisotropy. The work of Lin et al. (2014a) used computations of finite-frequency sensitivity kernels based on the formulation of Zhao & Chevrot (2011). Here we build on this work using a complementary method (global wavefield simulations as opposed to explicit sensitivity kernel computations).

In order to compare the splitting of synthetic SK(K)S waveforms to the predictions of ray theory (and eventually to real data), we measure both the splitting intensity introduced by Chevrot (2000), as described in Section 3.2, and the traditional splitting parameters (ϕ, δt) using the transverse component minimization method of Silver & Chan (1991). We use the implementation of the Silver & Chan (1991) method in SplitRacer (Reiss & Rümpker 2017), a MATLAB-based graphical user interface for teleseismic shear wave splitting analysis. We compare the splitting measurements made on synthetic waveforms with predictions from ray theory, derived from the Python tool christoffel (Jäcken & Cottenier 2016), which solves the Christoffel equation to predict the polarizations and velocities of the quasi-S phases for waves propagating over a range of directions.

### 4.2 Upper mantle case #1: horizontal transverse isotropy (HTI)

We now introduce a global wavefield simulation for a case that includes azimuthal anisotropy, in the form of a (single, laterally homogenous) anisotropic layer in the upper mantle with HTI symmetry. We do this simply by modifying the radially anisotropic upper mantle layer in PREM from a VTI symmetry to an HTI symmetry by rotating the symmetry axis by 90°. The symmetry axis thus lies in the horizontal plane for this simulation. The properties of the anisotropic layer are shown visually in Fig. 4, which shows representations of the anisotropic properties of various scenarios tested in this paper. The VTI elastic tensor of PREM is represented in Fig. 4, top row, while the rotated HTI tensor used in this test is shown in Fig. 4, second row. In order to avoid waveform complexity due to structural heterogeneity, we use a laterally homogeneous, 1-D earth model that corresponds to PREM except for in the depth range between 24 and 220 km, where we impose the HTI elastic tensor described above. We neglect attenuation and ellipticity in the simulation, even though this can be simulated with AxiSEM3D in general. We use a source and receiver configuration shown in the 

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**Figure 3.** Result of the shear wave splitting intensity analysis performed on the synthetic seismograms of Fig. 2. The splitting intensity vector (blue dots) is computed following Chevrot (2000, eq. A4). The orange curve is the least square fit solution \( s = \sin 2\theta (\phi - \phi_0) \), calculated over possible pairs of splitting intensity parameters \( \phi \) and \( \delta t \), that minimizes the misfit between the synthetic and the theoretical splitting intensity solution. The amplitude of the curve is 0.228 s and its phase is 45°. Compare this figure with (Chevrot 2000, fig. 3).
Figure 4. Polar view representation of different elasticity tensors belonging to different symmetry classes (from top to bottom hexagonal (VTI, HTI) and orthorhombic (olivine, bridgmanite, post-perovskite) used to describe the elastic and geometrical properties of the anisotropic regions tested in the different simulation settings. The magnitude of the slow and fast shear wave velocity and its polarization direction (black thick marks) are shown on the left-hand side and middle plots, respectively. A measure of the anisotropy is shown on the right plot along with the fast shear wave polarization direction (black thick marks). The VTI, HTI, and olivine tensors are used in examples where the anisotropy is localized in the upper mantle whereas the bridgmanite and post-perovskite are used in the $D''$. The orientation of the orthorhombic crystals are specified by the 2 orthogonal crystallographic axes that lie in the horizontal plane. The dashed concentric circles in the HTI and olivine tensors mark the region of the piercing points for the $SKS$ (orange) and $SKKS$ (red) phases in the upper mantle, while the solid circles indicate the region of the piercing points for the bridgmanite and post-perovskite crystals in the $D''$ layer.
left-hand panel of Fig. 5, with the source located at the surface (to avoid depth phases resulting from reflections off the free surface). The receiver is located at the North Pole, while the sources are located at 15° azimuthal intervals at an epicentral distance of 120°, at which both SKS and SKKS phases should be visible (e.g. Long 2009). The moment tensor for each source is chosen to maximize the radiation of S wave energy in the direction of the receiver, as shown in Fig. 5. While our simulations reproduce the entire wavefield, we focus on the portions of the synthetic seismograms that show the SKS, SKKS and Sdiff phases; the ray-theoretical paths of these phases are shown in the right-hand panel of Fig. 5. The synthetic seismograms for the radial and transverse components plotted against the backazimuthal direction of the incoming wavefield are shown in Fig. 6 in a time-window that includes SKS, SKKS and Sdiff phases. We also show synthetic waveforms as a function of backazimuth for epicentral distances of 100° and 110° in the Supporting Information (Figs S1–S2).

The splitting analysis results of this simulation are shown in Fig. 7, which shows the measured splitting intensity as a function of backazimuth from the synthetic seismograms for SKS and SKKS phases, along with the predictions from ray theory. The ray theoretical predictions were obtained by solving the Christoffel equation for an elasticity tensor that was averaged over the depth range of the anisotropic layer, with the SKS and SKKS propagation directions derived from TauP (Crotwell et al. 1999) for the PREM model. As expected, the measured splitting intensity values exhibit a variation with backazimuth that is close, but not identical, to that predicted by ray theory (solid orange and dashed red curves in Fig. 7). The full wavefield solution yields splitting intensity values that are systematically smaller, by up to ~0.25 s, than the ray theoretical predicted values. Similar to Lin et al. (2014b), we also find modest differences in SKS and SKKS splitting intensity, of up to ~0.2 s, at certain azimuths, with the difference being largest at a backazimuth that is 30° from the fast direction. We retrieve the best-fitting splitting parameters (φ, δt) for SKS and SKKS, respectively, by fitting a $\sin(2\theta)$ curve to the splitting intensity measurements in Fig. 7, and obtain values of $\phi = 90°$ and $\delta t = 0.780$ s for SKS and $\phi = 90°$ and $\delta t = 0.862$ s for SKKS. These values generally compare well to the ray theoretical values of $\delta t = 1.036$ s for SKS and $\delta t = 1.038$ s for SKKS, although again, ray theory overpredicts the amplitude of the splitting compared to the wavefield simulations. Finally, we compare the splitting parameters obtained from the splitting intensity curve to those obtained by the transverse component minimization method at two representative backazimuths, shown in Fig. 8. As with the splitting intensity measurements, there are modest differences in measured splitting parameters between SKS and SKKS phases at the same backazimuth, although in this case these differences are not significant considering the error estimates (Fig. 8).

4.3 Upper mantle case #2: orthorhombic symmetry

We now explore a case in which the upper mantle anisotropic layer has a lower symmetry class. Because CPO of olivine is generally understood to be the main cause of upper mantle anisotropy, and because single-crystal olivine has an orthorhombic symmetry, it is reasonable to test an orthorhombic model. Single-crystal olivine has a strong anisotropy, up to ~25 per cent for P waves and ~22 per cent for S waves, according to laboratory measurements (Babuska & Cara 1991; Isaak 1992; Abramson et al. 1997; Mao et al. 2015). The bulk anisotropy in deformed olivine aggregates, however, is significantly lower than the single-crystal anisotropy (e.g. Ben Ismaïl & Mainprice 1998, Karato et al. 2008). We constructed a model for upper mantle anisotropy by taking an averaging approach that preserves the symmetry class of the orthorhombic single crystal but decreases its anisotropy strength. We used the MSAT code (Walker & Wookey 2012) to calculate a linear mixture consisting of 30 per cent San Carlos single-crystal olivine at upper mantle conditions, as described by Abramson et al. (1997), and 70 per cent isotropic PREM. The resulting elasticity tensor (Fig. 4, third row) has a similar symmetry of a single crystal of olivine (we choose an orientation such that the [100] and [001] axes are in the horizontal direction, and the [010] axis is oriented vertically), but the
Figure 6. Synthetic seismograms computed for the PREM model with a HTI layer localized between 24 and 220 km plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 120°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and Sdiff are shown as the vertical orange, red and green bars, respectively.

anisotropy is substantially weaker (~5 per cent maximum). As in the HTI upper mantle simulation, the anisotropic layer is confined between 24 and 220 km depth.

We show the results of our wavefield simulation in Fig. 9, which is similar to Fig. 7 but for the orthorhombic symmetry case. Synthetic seismograms across a range of backazimuths at epicentral distances of 100°, 110° and 120° for this simulation are shown in the Supporting Information (Figs S3–S5). Because of the departure from hexagonal symmetry, the ray theoretical predictions (solid orange and dashed red lines in Fig. 9) are no longer perfect sin(2θ) curves, and in this case ray theory predicts some discrepancies between SKS and SKKS phases at certain azimuths. The measured splitting intensity values from the synthetic seismograms show some departures from the ray theoretical predictions, as in the HTI simulation, but for the orthorhombic case the departures are more pronounced (compare Fig. 9 with Fig. 7). As with the HTI case, there are a few azimuths for which we find discrepancies in SKS–SKKS splitting intensities; somewhat surprisingly, this discrepancy is quite large (difference in splitting intensity of ~0.4 s) at backazimuths that lie 45° away from the fast splitting direction. An examination of the transverse component minimization measurements at selected backazimuths (Fig. 10) shows that the SKKS splitting measurement at a backazimuth of 45° is poorly constrained due to a stronger interference of a not well identifiable phase on the radial component that leads to the contamination of the splitting measurements.

5 LOWERMOST MANTLE ANISOTROPY SIMULATIONS AND COMPARISON WITH RAY THEORY

5.1 Background: lowermost mantle anisotropy and shear wave splitting

We now turn our attention to seismic anisotropy in the lowermost mantle, which has been the subject of a great deal of recent observational work (e.g. Wookey et al. 2005a; Long 2009; Nowacki et al. 2010; Cottaar & Romanowicz 2013; Lynner & Long 2014; Ford et al. 2015; Creasy et al. 2017; Grund & Ritter 2018; Reiss et al. 2019), but which is substantially more challenging to observe than upper mantle anisotropy. As summarized in Nowacki et al. (2011) and Creasy et al. (2019), there are a variety of possible mechanisms that may contribute to anisotropy in the D′ layer, including CPO of bridgmanite or post-perovskite (depending on which mineral dominates, which may in turn depend on the temperature in a given region of D′ (Houser 2007)), CPO of ferropericlase, or shape-preferred orientation (SPO) of elastically distinct material such as partial melt. We do not test all of these possible mechanisms in this paper; instead, we test models of aligned post-perovskite and aligned bridgmanite, one of which is expected to be the most volumetrically important phase in any given region of D′. Testing of other models for D′ anisotropy will be left to future work.

There are a variety of strategies for measuring D′ anisotropy using body waves, only some of which rely on SK(K)S phases. One common approach is to measure the differential splitting of S–ScS phases [introduced by Wookey et al. (2005a); see also Wookey & Kendall (2008); Ford et al. (2015); Rao et al. (2017)] or to examine the waveform behaviour of phases such as Sdiff (e.g. Cottaar & Romanowicz 2013). The identification of significant discrepancies between the splitting of SKS and SKKS phases for the same event–station pair, first documented by James & Assumpção (1996), have been attributed to anisotropy at the base of the mantle beginning with Niu & Perez (2004) and Restivo & Helffrich (2006). The measurement of SKS–SKKS splitting discrepancies to study D′ anisotropy is becoming more common (e.g. Long 2009; He & Long 2011; Roy et al. 2014; Lynner & Long 2014, 2015; Grund & Ritter 2018), although there is some debate about the extent to which SKS–SKKS splitting discrepancies require a contribution to the lowermost mantle. Some studies (Monteiller & Chevrot 2011; Lin et al. 2014a) have argued that SKS–SKKS splitting discrepancies can be explained solely in terms of upper mantle anisotropy. Recently, some studies of SKS–SKKS splitting discrepancies have come to rely on the measurement of splitting intensity, rather than the traditional splitting parameter estimation methods, on the grounds that the splitting intensity is a more robust and stable measurement (Deng et al. 2017; Reiss et al. 2019). Despite ample observational evidence that SK(K)S phases can indeed be affected by anisotropy in the lowermost mantle, there is still no consensus in the literature about how strong the frequency-sensitivity of these phases is to anisotropy in D′ (Sieminski et al. 2008; Zhao & Chevrot 2011). Furthermore, there are disagreements in the literature about to what extent documented SKS–SKKS splitting discrepancies reflect a contribution to splitting from lowermost mantle anisotropy to one or
Figure 7. Shear wave splitting intensity analysis performed on the synthetic seismograms evaluated for the PREM model with HTI (see Fig. 4, second row) localized between 24 and 220 km depth. Values of the splitting intensity vector calculated for SKS are shown as orange circles while for SKKS are shown as red squares. The black solid and dashed curves represent the two least square fit solutions for SKS and SKKS, respectively. The orange solid and dashed red lines are the ray-theoretical predicted splitting intensity vectors for SKS and SKKS respectively, evaluated by solving the Christoffel equation for an elasticity tensor that was averaged over the depth range of a ∼200-km-thick anisotropic layer in the upper mantle.

both phases (e.g. Niu & Perez 2004; Restivo & Helffrich 2006; Long 2009), or whether such discrepancies can mainly be attributed to upper mantle anisotropy (e.g. Monteiller & Chevrot 2011; Lin et al. 2014a). There is, therefore, a need for global wavefield simulations that include lower mantle anisotropy.

Another argument for the study of full-wave effects of $D''$ anisotropy on SK(K)S phases comes from recent work that has sought to carry out forward modelling of $D''$ anisotropy, relying on results from mineral physics (e.g. Walker et al. 2011; Cottaar et al. 2014; Ford et al. 2015; Ford & Long 2015; Creasy et al. 2017, 2019; Walker et al. 2018; Tommasi et al. 2018). These types of modelling studies tend to rely exclusively on ray theory, with very few exceptions (e.g. Nowacki & Wookey (2016), who looked at full-wave effects for complex anisotropic models but who only considered ScS phases). Given the popularity of these types of modelling approaches, it is crucial to understand how well the ray theoretical approximation captures the true behaviour of SK(K)S waves.

5.2 Lowermost mantle case #1: bridgmanite crystallographic preferred orientation

We first consider a case that invokes a laterally homogeneous, 250-km-thick $D''$ layer at the base of the mantle, with elasticity that is designed to capture the first-order characteristics of aligned bridgmanite. Because the dominant slip systems at lowermost mantle conditions remain uncertain, we follow the strategy of recent modelling studies (e.g. Ford et al. 2015; Creasy et al. 2017) and consider tensors based on single-crystal elasticity. We chose an orientation such that the [100] and [010] axes of bridgmanite are oriented in the horizontal direction, while the [001] axis is vertical. We create an elastic tensor via a linear mixture of 30 per cent single crystal anisotropy of post-perovskite, using the elastic constants from Wookey et al. (2005b), with 70 per cent of isotropic PREM at $D''$ depths. This mixing ratio yields an elastic tensor with an orthorhombic symmetry and with a maximum anisotropy of 6 per cent, as shown in Fig. 4, fourth row. As with the upper mantle cases, we propagate the seismic wavefield through this model using the source and receiver geometries shown in Fig. 5, and measure the splitting intensity, as well as the traditional shear wave splitting parameters, as a function of backazimuth. Also as with the upper mantle cases, we compare the synthetic splitting measurements with predictions from ray theory. In contrast to the upper mantle case, in the lowermost mantle the SKS and SKKS phases under study have significantly different ray propagation paths. Using TauP (Crotwell et al. 1999), we calculated nominal propagation angles (from the horizontal) through the $D''$ region of 67° for SKS and 42° for SKKS.

Results from our bridgmanite simulation are shown in Figs 11 and 12. Synthetic seismograms across a range of backazimuths at epicentral distances of 100°, 110° and 120° for this simulation are shown in the Supporting Information (Figs S6–S8). Because the ray paths of SKS and SKKS phases depart so significantly from the vertical, we no longer expect a simple sin 2(θ) variability in the splitting intensity curve, and this is borne out by the measurements on synthetic seismograms. For this reason, we do not fit a sin 2(θ) curve to our measurements, as we did for the upper mantle cases. We do predict the ray theoretical splitting intensity curves, as shown on Fig. 11; these are based on the predicted apparent splitting parameters at each azimuth, visualized in Fig. 4, fourth row. As with the upper mantle cases, particularly the HTI simulation, we find that the full-wavefield simulations predict splitting intensity behaviour that is generally similar to the ray theoretical predictions, but not identical to it. We see deviations of up...
Figure 8. Shear wave splitting analysis performed using the transverse component minimization method (Silver & Chan 1991) on the SKS (left-hand panel) and SKKS (right-hand panel) phases for 2 representative backazimuthal propagation directions of the incoming seismic energy (45° and 150°). The synthetic seismograms are evaluated for a PREM model with a HTI layer localized between 24 and 220 km as in Fig. 7. Each panel is composed by 3 plots: On the top left a 120 s long time-window with the radial (black) and transverse (red) component synthetic seismograms. The vertical red bars mark the phases on which the analysis is performed. On the top right corner we show the original and the corrected particle motion. In the bottom plot we show the energy map with the calculated splitting parameters and the 95 per cent confidence interval as the shaded black area. For this configuration SKS and SKKS yield a comparable results for both fast direction axis and delay-time.

to ~0.2 s in splitting intensity values between the ray theoretical predictions and the synthetic seismogram measurements at certain azimuths, again similar to what is observed for the upper mantle cases. Importantly, the bridgmanite model predicts splitting intensities of up to ~0.8 s for SKS and SKKS phases, nearly as large as the maximum values predicted from ray theory, indicating that these phases have significant sensitivity to anisotropy at the base of the mantle. Notably, both the synthetic seismogram measurements and the ray theoretical predictions indicate that at certain azimuths, significant discrepancies between SKS and SKKS splitting intensities are expected, even though the underlying model is laterally homogeneous.

5.3 Lowermost mantle case #2: post-perovskite crystallographic preferred orientation

Finally, we test a model that invokes aligned post-perovskite as the cause for $D''$ anisotropy. The phase transition from bridgmanite to post-perovskite, which was discovered experimentally by Murakami et al. (2004), is thought to be the cause of the $D''$ discontinuity, and is expected to dominate in relatively cold regions of the lowermost mantle (e.g. Hernlund et al. 2005), and perhaps throughout (e.g. Koelemey et al. 2018). Post-perovskite is generally favoured as the most likely mechanism for $D''$ anisotropy by many authors (e.g. Nowacki et al. 2010; Walker et al. 2011; Cottaar et al. 2014; Ford et al. 2015). Similar to our test for bridgmanite, we create an
elastie tensor that is a linear mixture of 30 per cent single crystal anisotropy, using elastic constants for post-perovskite from Wooley et al. (2005b), and 70 per cent isotropic PREM. In this scenario, we assume that the [100] and [010] axes are oriented in the horizontal directions, while the [001] axis is vertical. Predicted ray theoretical splitting patterns for this tensor are shown in Fig. 4, bottom row.

Results from our post-perovskite wavefield simulation, along with ray theoretical predictions for this scenario at the relevant azimuths, are shown in Figs 13 and 14 shows representative transverse component minimization splitting measurements at two azimuths. Synthetic seismograms across a range of backazimuths at epicentral distances of 100°, 110° and 120° for this simulation are shown in the Supporting Information (Figs S9–S11). Interestingly, for this orientation of the post-perovskite elasticity tensor, SKS phases are split only very weakly, with maximum splitting intensities of ~0.2 s. This is consistent with the ray theoretical prediction for SKS splitting behaviour (Fig. 13; see also Fig. 4, bottom row). The behaviour of SKKS phases provides a striking contrast; for the propagation angles relevant for SKKS, this elastic tensor scenario predicts strong splitting, with maximum splitting intensities of ~2.5 s. The azimuthal variation in the SKKS splitting intensities measured from the synthetic seismograms is to first order captured by the ray theoretical prediction (Fig. 13), although the synthetic splitting intensities are generally lower (sometimes by as much as ~1.0 s) than the values predicted by ray theory. For the traditional splitting measurements (Fig. 14), the splitting of SKS phases is so slight that there is not enough transverse component energy to obtain a stable measurement; as expected, these measurements do not yield meaningful splitting parameter estimates. For the SKKS phases, in contrast, the transverse component minimization method yields robust measurements with strong splitting, consistent with the splitting intensity measurements (Fig. 13) and as predicted by ray theory.

### 6 CROSS-VERIFICATION AGAINST AN INDEPENDENT 3-D SPECTRAL ELEMENT SOLVER

Here we present a verification of our implementation of full anisotropy in AxiSEM3D by a benchmark solution against SPECFEM3D GLOBE (Komatitsch & Tromp 2002a,b). It is important to point out that the following benchmark test should be regarded as a cross-verification rather than a validation per se, as SPECFEM3D GLOBE has not yet been benchmarked for global wavefield propagation in arbitrary anisotropic earth models. We use the global-scale 3-D anisotropic model of Montagner (2002), based on surface wave tomography, which includes both radial and azimuthal anisotropy. This model spans between the Moho (24 km) and the 670 km discontinuity and has a 5° horizontal resolution. Its elasticity tensor is determined by 13 independent parameters, numerically implemented as a fully anisotropic tensor with 21 independent parameters in both SPECFEM3D GLOBE and AxiSEM3D.

The benchmark problem, shown in Fig. 15, is based upon simulating an earthquake source located in Virginia at a depth of 12 km, corresponding to the 2011 Mw = 5.8 earthquake in Mineral, VA. The source time function is an error function with half-duration of 10 s. The synthetic seismograms are computed at 129 stations of the Global Seismographic Network (GSN) distributed across the Earth’s surface (Fig. 15). Attenuation is turned off and the record length of the seismogram is 3600 s. A nearly perfect agreement has been achieved between SPECFEM3D GLOBE and AxiSEM3D in this simulation.

In Fig. 16, we show the vertical components of a set of synthetic seismograms for stations (blue triangles in Fig. 15) in the ~90–130° range of epicentral distance. In this set of synthetic traces, which show a range of body wave arrivals as well as surface waves, the
Figure 10. Same as Fig. 8 but with the anisotropic region in the upper mantle between 24 and 220 km being described with an elasticity tensor of orthorhombic class which mimics the elastic properties of a horizontally strained olivine (see Fig. 4, third row). The splitting parameter estimates are less well constrained, with larger formal errors, than for the hexagonal upper mantle simulation shown in Fig. 8.

SPECFEM3D_GLOBE and AxiSEM3D traces are virtually indistinguishable. For reference, we also show corresponding synthetic seismograms computed for the radially anisotropic PREM, demonstrating the effect of the anisotropic structure in the Montagner (2002) model on the waveforms. Because the Montagner (2002) model only includes structure in the upper mantle, the major differences with PREM manifest in the upper mantle phases (SS, SSS) and the surface waves.

In Fig. 17, we show the same set of synthetics, but we zoom in on the time window shown in Fig. 16, to highlight the SKS and SKKS arrivals. We show both radial (top panel) and transverse (bottom panel) component records; the latter shows the effect of azimuthal anisotropy in the Montagner (2002) model. The same version of this figure for the vertical component is shown in the Supplementary Information (Fig. S12). For the transverse component traces in Fig. 17 (bottom panel), the PREM model predicts no energy associated with the SKS or SKKS time window; because PREM does not include azimuthal anisotropy, no splitting of SK(K)S phases is predicted. The SPECFEM3D_GLOBE and AxiSEM3D synthetics, in contrast, show significant transverse component SK(K)S energy at several of the selected stations. Again, the SPECFEM3D_GLOBE and AxiSEM3D traces are virtually indistinguishable in the time windows associated with SK(K)S arrival.

We also report in the Supporting Information the full record section for the radial, transverse and vertical component of all the stations localized in the ∼90–130° range of epicentral distance (Figs S13–S15). We do note some extremely small differences on the transverse components between the SPECFEM3D_GLOBE and AxiSEM3D traces in PS and PPS phases at some stations (e.g. II.MSVF). These differences are not visible on the corresponding
radial components. These small differences are due to the fact that in general, phases with small amplitudes are more vulnerable to numerical errors (such as floating point errors and discretization errors). Because the two different methods have entirely different discretization schemes, some small differences for low-amplitude phases are expected.

Compared to a fully discretized 3-D method such as SPECFEM3D_GLOBE, AxiSEM3D has only one more parameter: the Fourier expansion order of the solution $n_u$ (Leng et al. 2016, 2019). This parameter controls both the accuracy and the computational cost of AxiSEM3D. For a spherically symmetric earth model such as PREM, we have $n_u = 2$ everywhere in the 2-D computational domain of AxiSEM3D; in this case, AxiSEM3D degenerates to a pure axisymmetric spectral element method (Nissen-Meyer et al. 2014). For a 3-D model, the AxiSEM3D solution converges to the real 3-D solution as $n_u$ increases, and its value for solution convergence is always much smaller (usually by orders of magnitude) than a fully discretized one for global wave propagation in a realistic 3-D earth models (Leng et al. 2016). It is most efficient to vary $n_u$ with depth and epicentral distance to maximize the performance of AxiSEM3D. Convergence tests are common practice in AxiSEM3D and are thoroughly explained in Leng et al. (2016, 2019). We refer the reader to (e.g. Leng et al. 2016, fig. 11) and to Fig. S16 in the Supporting Information for a visual illustration of the convergence behaviour. In order to achieve the agreement demonstrated in Fig. 16 with SPECFEM3D_GLOBE, we have used $n_u = 400$ in the uppermost 200 km and $n_u = 100$ elsewhere. We enlarge $n_u$ near the surface to have better accuracy for surface wave propagation. Such $n_u$ field leads to highly accurate waveforms for all the phases at all the stations in Fig. 15. In terms of computer performance, with this $n_u$ field, we have obtained a speedup of $\sim 6$

compared to SPECFEM3D_GLOBE. This speedup can be further increased in case neither surface waves nor multiple bouncing body waves (SSS, SSSS) are of interest. The technique of wavefield scanning (Leng et al. 2019) can be used to fully optimize $n_u$ for better performance.

A key aspect of AxiSEM3D is its ability to correctly account for off great-circle scattering at minimal computational cost, via the Fourier expansion approach. This capability has been extensively discussed in previous papers (Leng et al. 2016, 2019), which include previous benchmark tests of the AxiSEM3D code against SPECFEM3D_GLOBE. Because the Montagner (2002) model involves strong upper mantle heterogeneity, and thus causes strong scattering from out-of-plane structure, the benchmark test presented here provides a clear demonstration of the ability of AxiSEM3D to capture the complex properties of scattering by anisotropic heterogeneities in 3-D.

7 DISCUSSION

7.1 A tool for efficient global wavefield modelling in arbitrary anisotropic media

The series of benchmark tests and global wavefield simulations presented in this paper establishes the AxiSEM3D code as an efficient tool for modelling of the global wavefield in earth models that include anisotropy with arbitrary symmetry. In contrast to other 3-D wavefield simulation methods, AxiSEM3D simulations can be run at periods that are relevant for studies of $SK(\bar{K})S$ splitting (down to $\sim 5−10 \text{ s}$ period) at relatively modest computational cost due to the sparse sampling of smoothness in the azimuthal wavefield. For
Figure 12. Same analysis presented in Fig. 8 but with orthorhombic style anisotropy in the form of a bridgmanite crystal localized in a 250-km-thick $D''$ layer.

As for the splitting intensity analysis, we can see a similar result for $SKS$ and $SKKS$ in the case of seismic energy coming from 150$^\circ$ backazimuthal direction and discrepant results for 45$^\circ$. We caution, however, that for the 45$^\circ$ backazimuth the $SKKS$ splitting measurement is not well constrained.

example, the computational requirements for the global simulations presented in this paper involved about 3 hr and 30 min (wall-clock time) on 40 cores to produce 2000-s-long synthetic seismograms that can resolve seismic periods of 5 s.

The benchmarking tests presented in Section 3 serve to validate the implementation of arbitrary anisotropy in AxiSEM3D. In the first case, we ran a global simulation for the PREM model, including radial anisotropy, in two ways: one in which the model was specified in terms of vertical and horizontal wave velocities in the anisotropic layer, and one in which the same model was specified in terms of the equivalent full elastic tensor $C_{ijkl}$. The two solutions were found to be numerically identical, as expected. In the second test, we replicated a synthetic test presented in Chevrot (2000) that included azimuthal anisotropy. This test successfully demonstrated the azimuthal dependence of transverse component waveforms, with the expected waveform shape, and reproduced the expected splitting parameters (as measured via the splitting intensity) found by Chevrot (2000) for this model case. The simulations for upper and lowermost mantle anisotropy presented in Sections 4.1 and 5 demonstrate the feasibility of interrogating wavefield behaviour due to anisotropy effects in the context of global models using AxiSEM3D, and the cross-validation tests with SPECFEM3D GLOBE presented in Section 6 yield a remarkable agreement between the two solutions, with a significant computational advantage obtained by AxiSEM3D.

7.2 Full wave sensitivity of $SK(K)S$ phases to upper and lowermost mantle anisotropy

The upper mantle anisotropy models presented here build on previous work on the finite-frequency sensitivity of $SK(K)S$ phases to azimuthal anisotropy in the upper mantle by a number of authors (e.g. Favier & Chevrot 2003; Favier et al. 2004; Lin et al.
Figure 13. Same as Fig. 11 but with an elasticity tensor describing a post-perovskite mineralogy (see Fig. 4, bottom row). Strong discrepancies between SKS and SKKS are observed in this case for all the backazimuthal propagation directions with a very strong splitting observed for the SKKS and no splitting (null measurement) observed for the SKS.

These other seismic phases coming in between SKS and SKKS correspond to PPPP phases: it can be observed from the seismograms directly that this phase is not split (no energy on the transverse component), consistent with it being a P phase. The amplitude of this phase is strongly attenuated in real data seismograms, but since attenuation is turned off in our simulations they show up with high amplitude in our synthetics.

In general, while ray theory is generally an adequate approximation for SK(K)S splitting due to upper mantle anisotropy, it is more likely to be inadequate when the anisotropic models under study are complicated (either in terms of their symmetry, as in this study, or when there are lateral variations in anisotropic structure, which was not considered here but which will be considered in future works). Similar to Lin et al. (2014a), we found that modest differences in splitting intensity for SKS versus SKKS phases (up to ∼0.2 s, with values up to ∼0.4 s for specific symmetries and at certain azimuths) for the same event-station pair can be caused by waveform effects for models that include upper mantle anisotropy only. We note, however, that the SKS–SKKS discrepancies due to upper mantle anisotropy documented in this study are modest compared to the larger discrepancies observed for the lowermost mantle cases (Section 5). For example, for the bridgmanite case, discrepancies larger than 0.5 s and up to ∼1 s are observed in the 30°–75° (105°–135°) backazimuthal range (Fig. 11), while discrepancies as high as ∼2.5 s are obtained for post-perovskite models (Fig. 13). Our findings reinforce the need for SKS–SKKS discrepancy studies of mantle anisotropy to exercise caution when interpreting weakly discrepant splitting, and to only attribute strong differences in splitting intensity values to anisotropy in the lowermost mantle (e.g. Deng et al. 2017; Reiss et al. 2019).
Figure 14. Same as Fig. 8 but with the anisotropy localized in a 250-km-thick $D''$ layer. The elasticity tensor used for this test is the one shown in Fig. 4, bottom row. Also in this case we note a strong discrepancy between SKS and SKKS, with the SKS yielding null measurements.

For the lower mantle, our results have shown that lowermost mantle anisotropy can have a significant effect on the splitting of SKS and SKKS phases, in agreement with the sensitivity kernel computations of Zhao & Chevrot (2011). A comparison between our shear wave splitting measurements on synthetic waveforms and the predictions of ray theory (for models that represent bridgmanite and post-perovskite elasticity) reveals that, as for the upper mantle models, ray theory generally correctly captures the first-order aspects of the splitting behaviour. However, ray theory typically slightly overpredicts the magnitude of shear wave splitting when compared to the behaviour of the full waveform. From these results, we conclude that forward modelling approaches for lowermost mantle anisotropy models that rely on ray theory (e.g. Walker et al. 2011; Cottaar et al. 2014; Ford et al. 2015; Ford & Long 2015; Creasy et al. 2017, 2019; Tommasi et al. 2018) are generally valid, but are less accurate than full-wavefield simulations. This implies that moving to approaches that consider the full waveform behaviour is desirable in future modelling work aimed at $D''$ anisotropy problems, as also suggested by Nowacki & Wookey (2016).

7.3 Limitations and future work

While this study has established the feasibility of full-wave solutions using AxiSEM3D for earth models that include anisotropy of arbitrary symmetry, it is important to highlight some caveats and limitations. One area in which particular concern must be taken in future studies of mantle anisotropy has to do with the design of the mesh and the size of anisotropic regions. In spectral element methods, the domain is subdivided into a number of non-overlapping quadrangular shaped elements, and on each element the nodes are chosen to be the Gauss–Lobatto–Legendre (GLL) points where the wave equation is evaluated (Peter et al. 2011). A good mesh design
must consider this characteristic and allow for seismic discontinuities to lie on the GLL points. This will make sure that the points at the discontinuity have the elastic properties of both materials, which in turn will allow for the correct partitioning of seismic energy at the interface and avoid contamination of the numerical solution by artefacts due to staircase sampling effects. A proper mesh design is an essential requirement for all spectral element methods and not just AxiSEM3D. It is indeed a more complex task to achieve for 3-D discrete methods as 3-D meshes that honour these conditions have to be generated, while for AxiSEM3D this condition applies to 2-D meshes. With this in mind, in future studies that interrogate anisotropic earth models, it will be important to ensure that anisotropic discontinuities are also honoured by the mesh design. This is relatively easy to accomplish in the case of vertical stratification of anisotropy (that is, horizontal interfaces), but it turns out to be more complex for cases of lateral variation in anisotropic properties, which are likely relevant for many regions of the Earth.

Consideration of laterally heterogeneous anisotropic structures has been intentionally neglected in this study, whose main purposes are to establish AxiSEM3D as a tool for modelling seismic waveforms in arbitrary anisotropic global earth models and to interrogate the behaviour of relatively simple anisotropy scenarios. However, more realistic models that include lateral heterogeneity are needed to more fully explore the origin of SKS−SKKS splitting discrepancies and the possible contributions of lowermost mantle anisotropy to SK(K)S phases in the real Earth. This is particularly true given that in the lowermost mantle, the length scale of anisotropic heterogeneity may be smaller than the Fresnel zone of SK(K)S phases; in practice, therefore, it is not clear how large the contribution to SK(K)S splitting may be for realistic models of lowermost mantle anisotropy. Now that AxiSEM3D has been established as a computationally efficient tool for modelling wave propagation in an anisotropic Earth, work to understand the full-wave sensitivity of SK(K)S phases to anisotropy in more realistic, heterogeneous Earth models is ongoing. In the case of 1-D anisotropic models, such as those considered in this study, the Fourier spectral order required for a correct approximate solution to the 3-D wave equation is dependent on the complexities of the underlying seismic velocity model. For a fully 3-D anisotropic model, it is crucial to ensure that the Fourier spectral order of expansion is large enough to correctly account for the geometrical properties of the anisotropic model. As the cost of 3-D anisotropic wavefield simulations increase with growing Fourier order, careful attention must be paid to the geographic dimensions of anisotropic domains in 3-D models in order to preserve the computational advantages of the method with respect to 3-D discrete spectral element methods.

7.4 Implications for the interpretation of SKS−SKKS splitting discrepancies

Observations of discrepant SKS−SKKS splitting for pairs of phases from the same event-station pair have been puzzling to shear wave splitting analysts since they were first documented by James & Assumpção (1996). A global study by Niu & Perez (2004) found that 95 per cent of SKS−SKKS observations globally were non-discrepant; that is, the SKS and SKKS phases showed similar splitting behaviour. In the remaining 5 per cent of cases, however, the pairs exhibited discrepant splitting. Niu & Perez (2004) argued that because SKS and SKKS phases have nearly identical ray paths in the upper mantle but diverge significantly in the lower mantle, discrepancies in SKS−SKKS splitting should be attributed to anisotropy in the lower mantle. Restivo & Helffrich (2006) suggested that anisotropy in the $D^\prime$ layer is the most likely explanation for such discrepancies, and argued that topography on structures at or near the CMB may generate polarization anomalies, and thus splitting anomalies. A key aspect of the argument made by Restivo & Helffrich (2006) is that lateral gradients in structure at the base of the mantle are responsible for SKS−SKKS splitting discrepancies. This notion was invoked by subsequent studies of SKS−SKKS splitting discrepancies and lowermost mantle structure (e.g. Wang & Wen...
Figure 16. Comparison of synthetic waveforms computed by SPECFEM3D_GLOBE (black) and AxiSEM3D (dashed red) for the tomographic model of Montagner (2002), which includes 3-D anisotropy. Synthetic seismograms for the radially anisotropic PREM model are shown in light grey for comparison. We show vertical displacements for all three cases. The receiver locations are shown with blue triangles in Fig. 15. Radial and transverse components are shown in Fig. 17 in the time-window bounded by the dashed black line that includes SKS and SKKS phases.

2007; Long 2009), who argued that SKS–SKKS splitting discrepancies should be interpreted in terms of a lateral gradient in seismic anisotropy at the base of the mantle (that is, with the SKS and SKKS phases sampling a different geometry and/or strength of lowermost mantle anisotropy). More recent papers that have been informed by forward modelling studies (e.g. Ford et al. 2015; Creasy et al. 2019) have explicitly acknowledged the possibility that SKS–SKKS splitting discrepancies can arise from homogenous anisotropy at the base of the mantle (e.g. Long & Lynner 2015; Deng et al. 2017; Wolf et al. 2019; Reiss et al. 2019). In this case, the anisotropy must be present in a geometry that splits SKS and SKKS phases differently.

While many authors have interpreted SKS–SKKS splitting discrepancies as reflecting a contribution from anisotropy in the lower(most) mantle, other workers have questioned the extent to which anisotropy in the upper mantle may give rise to such discrepancies (or to discrepancies in splitting between SKS phases measured at the same station at similar backazimuths and incidence angles). For example, Monteiller & Chevrot (2010) documented differences in transverse component waveforms for pairs of SKS and SKKS phases from nearby earthquakes, and pointed out that the variability between phases coming from nearby directions is of similar magnitude to the variability documented in previous studies of SKS–SKKS splitting discrepancies that invoked D″ anisotropy as an explanation. Monteiller & Chevrot (2010) suggested that noise on the transverse component waveforms was the most likely explanation for these discrepancies, although other workers have argued that strong discrepancies measured on seismograms with relatively low noise levels cannot be due (solely) to noise (Long 2009; Lynner & Long 2014; Long & Lynner 2015). In a later paper, Monteiller & Chevrot (2011) documented differences in estimated SKS splitting parameters for stations in southern California between their measurements, obtained with the splitting intensity method, and previously published measurements; again, they attributed these discrepancies to the presence of noise and to differences in processing and measurement methods. Finally, Lin et al. (2014a) showed that full-wave effects can cause splitting discrepancies between SKS and SKKS phases for the same event-station pairs of up to ~0.3 s at certain azimuths for models that only include homogeneous upper mantle anisotropy, as discussed in Section 4.1.

What insights do our simulations give us into the interpretations of SKS–SKKS splitting discrepancies? Our documentation of
predicted SKS–SKKS splitting discrepancies for both upper and lowermost mantle anisotropy models demonstrates that such discrepancies can arise from a physical cause, although of course the effects of noise must be considered for actual data. Similar to Lin et al. (2014a), we found that modest splitting intensity discrepancies (typically up to 0.2 s, with a few values up to 0.4 s) can arise from homogeneous upper mantle anisotropy models, possibly influenced by the interference of other phases in the
SK(κ)S time window. Our simulations showed that much larger SKS–SKKS splitting intensity discrepancies can arise from lowermost mantle anisotropy models (up to ~1.0 s or greater for post-perovskite; see Fig. 13). Therefore, our work shows that both upper and lowermost mantle anisotropy may potentially contribute to SKS–SKKS splitting intensity discrepancies for simple, homogeneous anisotropic models. Ongoing work that extends to models that include realistic 3-D heterogeneity in anisotropic structure will answer the question of whether our general finding that lowermost mantle anisotropy models predict substantially stronger SKS–SKKS splitting discrepancies than upper mantle models holds for more complex models. Particularly because SK(κ)S phases have large zones of sensitivity at the base of the mantle (e.g. Zhao & Chevrot 2011), and because there may be heterogeneity in lowermost mantle anisotropy on length scales shorter than the Fresnel zones of the SK(κ)S waves under study, lowermost mantle anisotropy may contribute less to the splitting of SK(κ)S phases in practice than the results from laterally homogeneous models suggest. Furthermore, for actual, noisy data that reflects complex Earth structure, the effects of noise, phase interference, and complex wave propagation effects on apparent splitting parameters must be carefully considered.

Our lowermost mantle simulations also reinforce the notion that discrepant splitting behaviour between SKS and SKKS phases can arise even in models that feature laterally homogeneous anisotropic structure in the lowermost mantle. While SKS − SKKS splitting discrepancies are often taken to imply a contribution to splitting from anisotropy sampled by one SK phase and SKKS phases can interpret shear wave splitting measurements, particularly due to D′ anisotropy.

8 CONCLUSION

We have presented a new wavefield modelling strategy to introduce the effects of general anisotropy in global models using the pseudodisplacial element code AxiSEM3D. The implementation of arbitrary anisotropy is accomplished by describing the elastic properties of the seismic domain in terms of the full elastic tensor with 21 independent coefficients. We have carried out global wavefield simulations for models that include anisotropy in the upper and lowermost mantle, reaching frequencies as high as 0.2 Hz with relatively modest computational resources. We benchmarked our implementation against known reference solutions for simple upper mantle models, and then investigated the behaviour of SK(κ)S phases for models that include upper mantle anisotropy (in HTI and orthorhombic geometries) as well as those that include anisotropy at the base of the mantle (for possible bridgmanite and post-perovskite CPO scenarios). We carried out shear wave splitting analysis (both the traditional transverse component minimization method and the splitting intensity method) on synthetic waveforms for the suite of global anisotropic models. These tests revealed that shear wave splitting, as manifested in the full-wavefield simulations, behaves similarly to the predictions of ray theory to first order, but some departures from ray theoretical behaviour (due to full waveform effects) are found.

Our results indicate that although some SKS–SKKS splitting intensity discrepancies arise from anisotropic upper mantle models, particularly when low symmetry classes (e.g. orthorhombic) are considered, these are of modest amplitude (generally less than 0.2 s, with a few discrepancies up to 0.4 s). On the other hand, we find that realistic lowermost mantle anisotropy scenarios can cause significant splitting (up to ~1 s) of SK(κ)S waveforms when full wave propagation is taken into account, with SKS–SKKS splitting intensity discrepancies up to ~1 s or greater. The cross-validation test with the discrete spectral element solver SPECFEM3D_GLOBE further highlights the capability of AxiSEM3D to handle increasingly complex earth models, including those with arbitrary anisotropic symmetry, without loss of accuracy and with accessible computing resources. In the future, AxiSEM3D will be used to investigate the behaviour of SK(κ)S phases in the presence of lateral heterogeneity in anisotropic structure, paving the way for more realistic consideration of full wavefield effects when interpreting shear wave splitting measurements, particularly due to D′ anisotropy.

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REFERENCES


**SUPPORTING INFORMATION**

Supplementary data are available at *GJI* online.

**Figure S1.** Synthetic seismograms computed for the PREM model with a HTI layer localized between 24 and 220 km plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 100°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and ScS are shown as the vertical orange, red and blue bars respectively.

**Figure S2.** Synthetic seismograms computed for the PREM model with a HTI layer localized between 24 and 220 km plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 110°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and $S_{d if f}$ are shown as the vertical orange, red and green bars, respectively.

**Figure S3.** Synthetic seismograms computed for the PREM model with olivine style anisotropy localized between 24 and 220 km plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 100°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and ScS are shown as the vertical orange, red and blue bars, respectively.

**Figure S4.** Synthetic seismograms computed for the PREM model with olivine style anisotropy localized between 24 and 220 km plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 110°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and $S_{d if f}$ are shown as the vertical orange, red and green bars respectively. Phases with large amplitude arriving in the 1450−1500 s range correspond to $PPPP$. For this particular symmetry class they are strongly affected by the anisotropy in the backazimuthal range 45−135°.

**Figure S5.** Synthetic seismograms computed for the PREM model with olivine style anisotropy localized between 24 and 220 km plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 120°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and $S_{d if f}$ are shown as the vertical orange, red and green bars, respectively. Phases with large amplitude arriving between SKS ans $SKKS$ correspond to $PPPP$. For this particular symmetry class they are strongly affected by the anisotropy in the backazimuthal range 45−135°.

**Figure S6.** Synthetic seismograms computed for the PREM model bridgmanite style anisotropy localized at the base of the base of the lower mantle in a 250-km-thick $D^\prime$ plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 100°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and ScS are shown as the vertical orange, red and blue bars respectively.

**Figure S7.** Synthetic seismograms computed for the PREM model a bridgmanite style anisotropy localized at the base of the base of the lower mantle in a 250-km-thick $D^\prime$ plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 110°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for $SKS$, $SKKS$ and $S_{d if f}$ are shown as the vertical orange, red and green, respectively.

**Figure S8.** Synthetic seismograms computed for the PREM model bridgmanite style anisotropy localized at the base of the base of the lower mantle in a 250-km-thick $D^\prime$ plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 120°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and $S_{d if f}$ are shown as the vertical orange, red and green, respectively.

**Figure S9.** Synthetic seismograms computed for the PREM model with post-perovskite style anisotropy localized at the base of the base of the lower mantle in a 250-km-thick $D^\prime$ plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 100°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and ScS are shown as the vertical orange, red and blue, respectively.

**Figure S10.** Synthetic seismograms computed for the PREM model with post-perovskite style anisotropy localized at the base of the base of the lower mantle in a 250-km-thick $D^\prime$ plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 110°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and $S_{d if f}$ are shown as the vertical orange, red and green, respectively.

**Figure S11.** Synthetic seismograms computed for the PREM model with post-perovskite style anisotropy localized at the base of the base of the lower mantle in a 250-km-thick $D^\prime$ plotted against the backazimuth of the incoming seismic energy. The epicentral distance is 120°. The radial component is shown in black and the transverse is shown in red. Predicted arrival time for SKS, SKKS and $S_{d if f}$ are shown as the vertical orange, red and green respectively.

**Figure S12.** Same as Fig. 17 of the main manuscript but for the vertical component.

**Figure S13.** Comparison of synthetic waveforms computed by SPECFEM3D_GLOBE (black) and AxiSEM3D (dashed red) for the benchmark test presented in Section 6 of the main text. The record section shows the radial component for all the stations mapped in Fig. 15 of the main text located in the 90−130° range of epicentral distance.

**Figure S14.** Same as Fig. S13 but for the transverse component.

**Figure S15.** Same as Fig. S13 but for the vertical component.

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