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# AxiSEM3D: efficient 3D wave propagation across scales and worlds

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## SUMMARY

We present a new, unified release of the AxiSEM3D seismic modelling code, which is able to rapidly and efficiently compute synthetic seismograms for the Earth and many other worlds. Over the past decade, separate and incompatible versions of AxiSEM3D's main branch have been developed and individually benchmarked, including new capabilities such as the inclusion of fluid oceans and atmospheres, full anisotropy, local- and regional-scale Cartesian domains, sensitivity kernels, and distributed (finite-fault) sources. This release (version 2.1) consolidates those previously disparate branches into a single, cross-compatible, community-maintained codebase. The release includes substantially expanded documentation with simplified end-to-end installation and use instructions; a suite of eleven ready-to-run templates for terrestrial, planetary, and stellar applications; and tools for producing wavefield visualisations and other derived products such as sensitivity kernels.

**Key words:** Seismology – Seismic modelling – Finite-element methods

## 1 INTRODUCTION

Both the volume and diversity of seismic data available to geophysicists have expanded dramatically in recent years (e.g., Cochran 2018; Yu et al. 2021; Arrowsmith et al. 2022). On the technological front, new and increasingly dense broadband seismic deployments have been accompanied by the rise of technologies including nodal systems, amateur/community networks, and distributed acoustic sensing (Clayton et al. 2011; Parker et al. 2014; Dean et al. 2018). Similarly, executed or planned deployments to Mars, the Moon, and Titan have offered exciting and novel geophysical insights into other worlds of our Solar System (Lorenz et al. 2019; Banerdt et al. 2020; Panning et al. 2021). These advances have offered a view into problems that are wide-ranging in both spatial and temporal scale: from global tomography to microphysical crack propagation, human behaviour to nuclear non-proliferation, and environmental monitoring to natural hazards (e.g.,

Rawlinson et al. 2010; Larose et al. 2015; Zhao et al. 2016; Lecocq et al. 2020; Caplan-Auerbach et al. 2023; Danciu et al. 2024; Steinmann et al. 2025; Fernando 2026).

A core driver of modern seismology is the existence of forward solvers for the elastodynamic and acoustic wave equations (Peter et al. 2011; Berkhout 2014; Tromp 2015; Lecoulant et al. 2022; Igel 2017). Solutions to the forward problem allow us to test our understanding of wave physics across both spatial and temporal scales, and to test the robustness of our models. Simultaneously, forward modelling is a key part of seismic inversion, wherein observational data are used to constrain source and structural models, most commonly by minimising the misfit between observed and predicted data (Russell 1988). Hence, advances in data collection and inversion strategies must necessarily be accompanied by advances in seismic modelling methods.

### 1.1 Full-waveform modelling and inversion

Full-Waveform Inversion (FWI) is in many ways the current state-of-the-art in seismology (Virieux & Operto 2009; French & Romanowicz 2014; Bozdağ et al. 2016). FWI attempts to use all of the available information included within a seismogram (i.e., the arrival times, amplitudes, and waveforms of all phases) to make inferences about the internal structure of the Earth or other planet, rather than relying on simplified measurements such as arrival time picks for a selected group of phases. FWI must necessarily be complemented by Full-Waveform Modelling (FWM), in which the amplitudes, spectral content, and arrival times of all corresponding seismic phases are predicted based upon a model of interior structure and source properties, and a computational representation of the relevant equations of motion.

A number of full-waveform modelling tools are already available to seismologists. Many of the most commonly used modelling tools rely on Spectral Element Methods (SEM,) Komatitsch & Tromp (2002a); Nissen-Meyer et al. (2014); Afanasiev et al. (2019)), wherein a specific choice of basis functions (high-order Lagrange polynomials) is utilised to ensure high accuracy and significant computational efficiency savings as compared to many finite-element or finite-difference based solvers (Komatitsch et al. 2005; Graves 1996; Dumbser & Käser 2006). The ability of SEMs to easily incorporate complex geometries and multi-media propagation, including fluid layers, has led to their widespread adoption in numerous areas of terrestrial seismology and acoustics (e.g., Peter et al. 2011; Bottero et al. 2016; Martire et al. 2018; Lecoulant et al. 2019).

One of the most widely used SEM FWM tools in seismology is SPECFEM (Komatitsch & Tromp 1999, 2002a). Nissen-Meyer et al. (2007, 2008) introduced AxiSEM as a complementary tool to SPECFEM, offering more computationally-efficient generation of synthetics at the cost of a restriction to axisymmetric media. The fundamental philosophy behind AxiSEM is that the lateral gradients in seismic properties within the solid Earth (or indeed any planetary or stellar body) are generally much smaller than the radial gradients. As a consequence, the seismic wavefield is generally ‘smoother’ (i.e. more weakly varying) in the two non-radial directions as compared to along the radial axis.

AxiSEM took advantage of this lateral smoothness to solve the equations of motion on a 2D planar grid with a pseudospectral expansion in the third direction, rather than using a 3D volumetric grid outright (Nissen-Meyer et al. 2007, 2008). The resulting increase in computational efficiency enabled synthetics to be generated at much higher frequency than would be possible with other methods (e.g., SPECFEM) given the same amount of computational resources, though with the additional restriction that the properties of the simulation (e.g., heterogeneities, boundary conditions, sources) all needed to be axisymmetric. This type of setup is often referred to as ‘2.5D’, as 3D wavefield character is permitted but the seismic structures represented are not fully 3D. For example, a spherical heterogeneity that does not intersect

the symmetry axis could only be represented axisymmetrically; that is, it could only be captured once swept through  $2\pi$  about the symmetry axis and hence would behave seismically as a ‘doughnut’ embedded within the Earth, rather than a sphere.

## 1.2 AxiSEM3D: Motivation

AxiSEM3D built upon the original ‘2.5D’ AxiSEM method, but extended it to include fully 3D Earth models (including truly 3D heterogeneities) and undulating discontinuities (Leng et al. 2019). AxiSEM3D thus maintains many of the computational advantages of the original AxiSEM, but enables more realistic physical situations to be modelled. Since its initial introduction, AxiSEM3D’s functionality has been expanded to include surface oceans (Fernando et al. 2020), anisotropy of arbitrary symmetry (Tesoniero et al. 2020; Wolf et al. 2022b), kernel computation (Szenicer et al. 2020), and local- and regional-scale simulations (in spherical or Cartesian geometry; Haindl et al. 2021). Each of these steps has been individually verified in the published literature; this verification heritage is summarised in Section 2.6 (Table 1). Similarly, AxiSEM3D has been used to simulate acoustic, seismoacoustic, and seismic wave propagation on other worlds. These include Mars, the Moon, and asteroids (Nissen-Meyer et al. 2019; Saade et al. 2019; Nishiyama et al. 2021; Nunn et al. 2024).

## 1.3 AxiSEM3D: New developments

Each of these new features was developed on a separate branch of the code, as a consequence of AxiSEM3D having become a community code that is used and developed by a number of different research groups. An unfortunate consequence of this is that the different branches have differing standards of documentation, are not fully cross-compatible, and are not all described to the degree needed for another user to implement similar problems without starting from scratch.

Addressing these issues is the motivation for the current release, `version 2.1`, the corresponding codebase for which may be cited as Leng et al. (2026). This release offers a modernised codebase, updated dependencies, and streamlined installation. To assist in reproducibility and to showcase the code’s functionality, we present here a suite of eleven ready-to-run examples that support the generation of high-frequency synthetics for complex geometries in heterogeneous multi-media on the Earth, on other planetary bodies, and even within stars.

Additionally, we highlight the new community-support infrastructure built around the code, including standardised documentation, improved processing/visualisation tools, and version control. End-to-end installation and use instructions for both stand-alone machines and high-performance computing (e.g. cluster and supercomputer) architectures are also provided. This paper is not intended to be a manual for use (the AxiSEM3D Manual having recently been released online; Section 2.5), but rather an overview of the features, functionality, and performance of this latest version of AxiSEM3D.

# 2 METHODOLOGY

## 2.1 Equations of motion

To begin, we briefly summarise the mathematics underlying the AxiSEM3D approach. Complete (but disparate) derivations may be found in Leng et al. (2016, 2019), Fernando et al. (2020), and Haindl et al. (2021); our purpose here is to summarise the relevant mathematics in a unified form.



We begin by considering a spherical Earth model that consists of solid domains  $\Omega_S$  (with spatially-varying mass density  $\rho$  and elasticity tensor  $\mathbf{C}$ ) and fluid domains  $\Omega_F$  (with a similar non-constant mass density  $\rho$  and bulk modulus  $\kappa$ ). An arbitrary number of solid-fluid interfaces, collectively denoted  $\Sigma$ , separate these regimes and in our initially spherical model, each interface is at a constant radius.

As AxiSEM3D is optimised for the computation of high-frequency synthetics, we neglect long-period effects such as rotation and gravitation throughout. The quantities we solve for are the time-dependent displacement field  $\mathbf{u}(\mathbf{x}, t)$  in the solid domain and the fluid potential  $\chi(\mathbf{x}, t)$  in the fluid domain, starting from a quiescent state at  $t = 0$  and marching forward in time over a user-specified record length; in the equations as presented here the material properties ( $\rho$ ,  $\mathbf{C}$  and  $\kappa$ ) are time-independent (see the remark on attenuation below). The weak formulation of the equations of motion reads:

$$\begin{aligned} \int_{\Omega_S} \rho \mathbf{w} \cdot \partial_t^2 \mathbf{u} d^3 \mathbf{r} + \int_{\Omega_S} \nabla \mathbf{w} : \mathbf{C} : \nabla \mathbf{u} d^3 \mathbf{r} \\ = \int_{\Omega_S} \mathbf{w} \cdot \mathbf{f} d^3 \mathbf{r} - \int_{\Sigma} \partial_t^2 \chi \hat{\mathbf{n}} \cdot \mathbf{w} d^2 \mathbf{r}, \end{aligned} \quad (1)$$

where  $\hat{\mathbf{n}}$  is the unit normal of each solid-fluid interface, oriented to point from the fluid domain  $\Omega_F$  into the solid domain  $\Omega_S$  (the same  $\hat{\mathbf{n}}$  appears in Eqns. 1 and 2),  $\mathbf{f}$  is a body force source,  $\mathbf{u}$  is the displacement vector,  $\chi$  is the fluid potential (defined below), and  $\mathbf{w}$  is an arbitrary, vector-valued test function. AxiSEM3D works in Hooke's linear stress-strain regime, appropriate to the vast majority of seismology problems. Terms representing attenuation effects are not included in the above equations for simplicity of presentation, but are included in the actual code and the fuller description of Leng et al. (2016, 2019). The fluid potential  $\chi$  is defined such that  $\mathbf{u} = \rho^{-1} \nabla \chi$  in  $\Omega_F$ . This is equivalent to describing the dynamic pressure (i.e. overpressure associated with an acoustic wave) in  $\Omega_F$  as  $\partial_t^2 \chi = -P$ . The associated weak form in the fluid domain is then

$$\begin{aligned} \int_{\Omega_F} \kappa^{-1} w \partial_t^2 \chi d^3 \mathbf{r} + \int_{\Omega_F} \rho^{-1} \nabla w \cdot \nabla \chi d^3 \mathbf{r} \\ = \int_{\Sigma} w (\mathbf{u} \cdot \hat{\mathbf{n}}) d^2 \mathbf{r}. \end{aligned} \quad (2)$$

Note that in the acoustic (fluid) case,  $w$  is a scalar-valued test function. To keep consistency with Eqn. 1 we do not include a source term in the fluid on the right-hand side of Eqn. 2; however, one is implemented and available in AxiSEM3D and takes the form  $\int_{\Omega_F} w F_\chi d^3 \mathbf{r}$  for some scalar source  $F_\chi$  in  $\Omega_F$ .

In the generalised 3D case with undulating interfaces,  $\Omega_S$ ,  $\Omega_F$  and  $\Sigma$  become aspherical. AxiSEM3D makes use of particle relabelling (Al-Attar & Crawford 2016) to achieve the radial displacement of boundaries inward and outward to represent their different depths at different latitudes and longitudes.

## 2.2 Boundary conditions

In a global mesh, the only physically relevant boundary is the outermost surface. If this is a solid-surface boundary, the relevant boundary condition is a Neumann-type, stress-free one:  $\mathbf{C} : \nabla \mathbf{u} \cdot \hat{\mathbf{n}} = \mathbf{0}$ , which is automatically satisfied by Eqn. 1. If the outermost boundary is a fluid,  $P(\mathbf{x}, t) = -\partial_t^2 \chi(\mathbf{x}, t) = 0$ , and this is not automatically satisfied by Eqn. 2. This requirement, and the subsequent  $\partial_t \chi = 0$  and  $\chi = 0$ , must be imposed at each timestep.

AxiSEM3D is not restricted to global meshes: the computational domain may be truncated to a regional or local one, in either spherical or Cartesian geometry (Section 2.7.2), which introduces artificial boundaries that have no physical meaning. Energy incident on these boundaries must be absorbed to avoid it reflecting back into the simulation, wherein it would interfere with the rest of the wavefield. Full details of the absorbing boundary condition implementation in AxiSEM3D are given in Haindl et al. (2021), but in the simplest case, Eqns. 1 and 2 acquire an additional boundary term on the absorbing boundary  $\Gamma_{\text{abs}}$ . In the solid case the term  $B_{\text{abs}}^s$ , added to the right-hand side of Eqn. 1, is

$$B_{\text{abs}}^s = - \int_{\Gamma_{\text{abs}}^s} \mathbf{w} \cdot \mathbf{t}_{\text{abs}} d^2 \mathbf{r}, \quad (3)$$

where, crucially,  $\mathbf{t}_{\text{abs}}$  is not the elastic traction  $\mathbf{C} : \nabla \mathbf{u} \cdot \hat{\mathbf{n}}$  (which would merely restore the natural surface term dropped when the domain is truncated), but an absorbing (Clayton–Engquist) traction proportional to the boundary velocity,

$$\mathbf{t}_{\text{abs}} = \rho v_p (\hat{\mathbf{n}} \cdot \partial_t \mathbf{u}) \hat{\mathbf{n}} + \rho v_s [\partial_t \mathbf{u} - (\hat{\mathbf{n}} \cdot \partial_t \mathbf{u}) \hat{\mathbf{n}}], \quad (4)$$

which damps the normal and tangential components of the motion at the  $P$ - and  $S$ -wave impedances  $\rho v_p$  and  $\rho v_s$  respectively. The fluid case, Eqn. 2, acquires the analogous velocity-proportional term  $B_{\text{abs}}^f$  on its left-hand side,

$$B_{\text{abs}}^f = \int_{\Gamma_{\text{abs}}^f} (\rho c)^{-1} w \partial_t \chi d^2 \mathbf{r}, \quad (5)$$

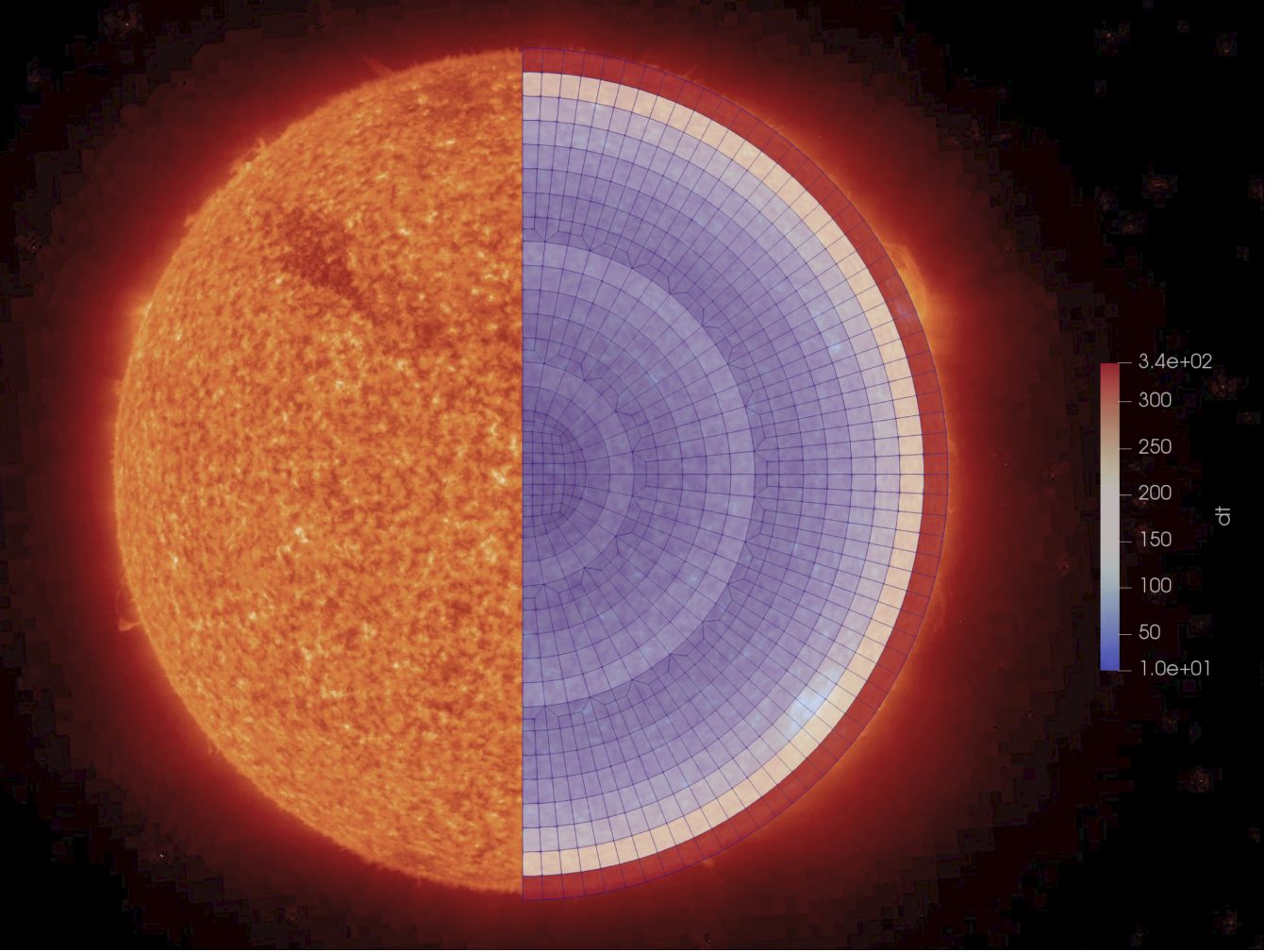
where  $c$  is the sound speed in the fluid.

### 2.3 Pseudospectral expansion and meshing

AxiSEM3D makes use of a pseudospectral (Fourier) expansion in the azimuthal direction to represent both the properties of the solid Earth (e.g. wavespeed, density, etc.) and the displacement wavefield. Practically, this means that the computational mesh is planar (‘D-shaped’ in the global case), and rotated by an angle of  $2\pi$  about the central axis.

An example of such a mesh is given in Fig. 1. This example is chosen to illustrate the flexibility of the *Salvus* meshing tool (which is used to generate AxiSEM3D’s meshes) and the AxiSEM3D solver itself. Both are able to stably accommodate many orders of magnitude of variation in sound speed and density. The most extreme use case tested successfully generates a mesh that spans the distance from the Sun’s centre to its photosphere, which involves changes in seismic properties orders of magnitude larger greater than those within terrestrial planets and Moons. We emphasise that the background model used in making AxiSEM3D meshes like that shown in Fig. 1 is radially symmetric (1D), and despite being 2D-planar in topology, the mesh itself is effectively radially symmetric as well. All 3D structure is instead added at runtime, as detailed below.

In the plane (i.e., the 2D space defined by the radial and meridional axes), the SEM is used to solve for the wavefield at defined quadrature points, specifically the Gauss-Lobatto-Legendre (GLL) points (Abramowitz & Stegun 1972, eq. 25.4.32). In the third direction (the azimuthal or out-of-plane direction), a pseudospectral expansion is used. The number of terms used in the pseudospectral representation may be adjusted depending on the complexity of the 3D models used in the simulation. Models with stronger lateral gradients (for example,



**Figure 1.** An example AxiSEM3D mesh for the Sun at 2,000 s minimum period. Key features to note include the ‘cubed sphere’ (Ronchi et al. 1996) to avoid a singularity at the mesh centre and refinement layers where the cell size increases with depth to avoid oversampling the wavefield. Each cell in the mesh is colour-coded by the minimum timestep (dt) required to ensure computational stability. This mesh is based on the Solar Model S seismic profile (Christensen-Dalsgaard et al. 1996) and the background image is from NASA’s Solar Dynamics Observatory (Pesnell et al. 2012).

models of seafloor bathymetry) require more terms to capture their complexity than those where the gradients are almost all radial (e.g. deep-mantle tomographic models).

The highest-order Fourier term included in the pseudospectral expansion is denoted  $n_u$ . A radially symmetric model with a monopolar source requires only  $n_u = 0$ ; increasing either the complexity of the model or the complexity of the source requires increasing  $n_u$ .

Working in a cylindrical basis in which  $(\hat{s}, \hat{\phi}, \hat{z} = \hat{g}_1, \hat{g}_2, \hat{g}_3)$ , we may represent the displacement,  $\mathbf{u}$ , and fluid potential,  $\chi$ , as

$$\mathbf{u} = \hat{\mathbf{g}}_i(\phi) u_i(s, \phi, z; t) \simeq \hat{\mathbf{g}}_i(\phi) \sum_{|\alpha| \leq n_u} u_i^\alpha(s, z; t) \Psi^\alpha(\phi), \quad (6)$$

and

$$\chi(s, \phi, z; t) \simeq \sum_{|\beta| \leq n_u} \chi^\beta(s, z; t) \Psi^\beta(\phi), \quad (7)$$

respectively, where  $\Psi^\alpha(\phi) = e^{\sqrt{-1}\alpha\phi}$  are the terms with order  $|\alpha| \leq n_u$ , and similarly for  $\Psi^\beta(\phi)$ . Following Leng et al. (2019), subscripts on field variables denote spatial indices and superscripts denote Fourier-series indices (not powers); the Einstein summation convention

applies to the spatial (subscript) indices only, and  $\simeq$  denotes truncation of the Fourier series at order  $n_u$ . Note that the number of azimuthal cardinal points  $N_r$  is given by  $N_r = 2n_u + 1$ .

In the simplest case, the user may set  $n_u$  to their desired value based on the expected complexity of the 3D model and the resultant wavefield.  $n_u$  need not be constant across the entire simulation mesh; for example, it may vary with depth or meridional position (latitude). However, for most realistic 3D models, the required  $n_u$  is difficult to estimate in advance, is generally frequency dependent, and geographically variable. AxiSEM3D therefore incorporates Azimuthal Complexity Adaptation (ACA), the procedure termed ‘wavefield scanning’ by Leng et al. (2019). ACA enables the code to ‘learn’ the maximum  $n_u$  required to accurately represent the wavefield at each depth and meridional position.

During an initial simulation with ACA enabled, AxiSEM3D computes the spectral power contained within each Fourier component as a function of depth and latitude. The maximum value of  $n_u$  along any azimuth in subsequent simulations using similar sources and 3D models is then capped to those components which contained more spectral power than a given threshold (e.g.,  $> 0.1\%$ ) in the original simulation. This avoids wasting resources on calculations involving higher-order Fourier terms which are essentially irrelevant to the simulation at hand.

## 2.4 Sources

### 2.4.1 Point sources

AxiSEM3D is able to simulate a wide variety of sources in both solid and fluid media. In fluid media, where non-diagonal elements of the stress tensor vanish, an isotropic pressure source is implemented. This acoustic source is fully described by means of a location, a source-time function, and a single (monopolar) magnitude which is imposed upon the fluid potential (recalling that  $P = -\partial_t^2 \chi$ ).

In solid media, sources may take the form of a multipole of order 0, 1, or 2. The order-zero case is equivalent to the isotropic source in fluid media and is equivalent to a pure implosion or explosion. Such non-deviatoric sources are practically quite rare in solid media, but may occasionally be relevant in very specific nuclear monitoring and forensic seismology contexts (Patton & Taylor 2011). The order-one case represents a dipolar (vector) force, with directionality. Such forces have been used to represent more realistic impulsive sources, including underground nuclear explosions and meteoroid impacts (e.g. Daubar et al. 2018; Fernando et al. 2022), either in isolation or in combination with a monopolar source. The order-two term is sufficient to represent the entire seismic moment tensor, including both isotropic and deviatoric components. Such a source is the most appropriate representation of an earthquake radiation pattern when the fault is treated as a point source.

### 2.4.2 Distributed sources

AxiSEM, and the original version of AxiSEM3D, required that a single source be used. The code then internally rotated the simulation geography such that the source lay on the north pole. In this release of AxiSEM3D, that restriction no longer applies. Distributed sources (representing, for example, kinematic fault rupture or large-scale excitation from distributed atmospheric sources) are accepted as inputs.

Practically, distributed sources are treated as a cloud of point sources, each of which is defined by its own location, magnitude, and

source-time function. Thus, each component of the body force,  $\mathbf{f}$ , in Eqn. 1 may be expressed in solid media as

$$f_i(\mathbf{x}, t) = - \sum_{k=1}^N M_{ij}^k S^k(t - t^k) \partial_j \delta(\mathbf{x} - \mathbf{x}^k). \quad (8)$$

Here the superscript  $k$  is a label (not a Fourier index) that indexes the individual points (‘sub-faults’), of which there are  $N$  in total, each with its own moment tensor components  $M_{ij}^k$  and source-time function  $S^k$ .

The implementation of distributed sources introduces no new physics: because the discretised equations of motion are linear, for a given mesh and azimuthal expansion order, the wavefield excited by a distributed source is exactly the superposition of the wavefields of its constituent point sources. The implementation within AxiSEM3D simply assembles the corresponding discrete force terms in a single simulation, avoiding the need to undertake separate runs. The practical requirement is that the azimuthal expansion order  $n_u$  be large enough to resolve the azimuthal dependence of off-axis sub-sources; this is discussed in Section 2.3 and illustrated in Example 6 (Section 3.6).

This functionality significantly increases the realism with which AxiSEM3D simulates ground motion, with important implications for seismic hazard modelling (Haindl 2021). For example, faults may now be treated kinematically, with a finite length and a rupture propagation time, rather than as point sources. Similarly, acoustic phenomena such as sonic booms may be modelled (in a linearised sense) in a single run as a line source, without the need to undertake multiple simulations, each with a different source location and temporal offset.

## 2.5 Implementation, performance, and documentation

The original version of AxiSEM was written in Fortran, whilst AxiSEM3D is written in C++ and parallelised with MPI; it runs on architectures ranging from laptop computers to large high-performance computing clusters (Leng et al. 2016). Full details of AxiSEM3D’s performance relative to AxiSEM and SPECFEM are included in Leng et al. (2016), but it is useful to note that for a given 3D model, AxiSEM3D’s runtime scales with frequency  $\omega$  as  $\omega^3$ , whilst SPECFEM’s scales as  $\omega^4$ .

As such, doubling the resolution (e.g. going from 10 s dominant period to 5 s dominant period) increases the computational cost by a factor of 8 in AxiSEM3D versus 16 in SPECFEM. Because the ratio of computational costs (SPECFEM relative to AxiSEM3D) scales as order  $\omega$ , AxiSEM3D’s performance advantage is greater at higher frequencies. This naturally favours AxiSEM3D for the computation of high-frequency synthetics (e.g. at periods of 5 s and shorter on a global scale). This holds true even when realistic 3D models are implemented (Leng et al. 2019), though the advantage narrows as the azimuthal complexity of the model increases: in the limit  $n_u \rightarrow \infty$  (which is not physically meaningful in any realistic situation), the runtimes of AxiSEM3D approach those of SPECFEM.

These are algorithmic scalings on like-for-like hardware, derived from operational runs, rather than benchmarked wall-clock performance across varying architectures. SPECFEM (Peter et al. 2011) and Salvus (Afanasyev et al. 2019) in particular have highly optimised GPU implementations, whereas AxiSEM3D currently runs on CPUs only (Section 5.1); whether a CPU-based AxiSEM3D run is faster in practice than a GPU-based full-3D run therefore depends on the hardware available to the user as well as on frequency and model complexity.

Actual solution of the equations of motion forward in time uses either a Newmark scheme or a symplectic scheme, the latter being more accurate but also more computationally intensive (Leng et al. 2019). Currently, timestepping is global, such that the smallest timestep in the mesh determines overall runtime. To achieve its efficiency, AxiSEM3D makes use of a number of external dependencies including Eigen (Guennebaud et al. 2010), FFTW (Frigo & Johnson 2005) and Boost (<https://www.boost.org>) for linear algebra and numerical

computation; MPI (Message Passing Interface Forum 2023) for parallelisation; METIS (Karypis & Kumar 1998) for domain decomposition; and Parallel NetCDF (Li et al. 2003) for I/O. If desired, these can all be installed and used in the configuration and build of the AxiSEM3D source code using a provided Conda script.

The details of this and other installation- and usage-related matters are included in the AxiSEM3D Manual (hosted on [Read the Docs](https://axisem3d.readthedocs.io/en/latest/); <https://axisem3d.readthedocs.io/en/latest/>) and in the accompanying introduction to using the code by Fernando et al. (2024), so we do not repeat them here. The open-source code, its licence and contributor code of conduct, community resources, and a permanent archive are detailed in the Data Availability statement.

## 2.6 Verification and benchmarking heritage

Whilst different functionality has been added to AxiSEM3D by different groups, each new capability (e.g. the addition of fluid oceans) was at the very least benchmarked against an independent modelling method and validated against observed data. In releasing version 2.1 of AxiSEM3D we do not replicate these benchmarking exercises, as we have verified that version 1.0 of AxiSEM3D produces the same outputs for these examples as version 2.1.

Nonetheless, we briefly summarise the verification and benchmarking heritage of the code for the purposes of reproducibility (Table 1). Other users attempting to replicate these benchmarks should note that some of them can only be undertaken ‘piecewise’, that is, testing individual components such one-by-one against other methods rather than all at once. This is largely due to AxiSEM3D including capabilities that we are unaware of any other open-source method being able to replicate end-to-end in 3D on a global scale. As an example, benchmarking global-scale simulations of solid-fluid coupling from the oceans into the atmosphere is a relatively complex exercise involving multiple steps. This is because no other methods that we are aware of can simultaneously include an atmosphere, add a reflecting boundary condition at the top of the atmosphere, and do this in full 3D on a global scale. Therefore, past AxiSEM3D publications stepwise benchmarked (1) the solid-ocean and solid-atmosphere couplings against YSpec (Al-Attar & Woodhouse 2008) on a global scale (Fernando et al. 2020), (2) the absorbing boundaries in fluid media against SPECSEM3D on a local scale (Haindl et al. 2021), and (3) the local and regional-scale implementations of AxiSEM3D against each other (Leng et al. 2020; Haindl 2021). As such, this functionality is fully benchmarked, but ‘piecewise’.

## 2.7 Inputs

Having described the mathematical framework behind AxiSEM3D, we now briefly describe the structure of the inputs and outputs needed, introducing concepts rather than duplicating the step-by-step instructions in the online AxiSEM3D Manual.

### 2.7.1 Simulation parameters

All simulation parameters are passed to the AxiSEM3D solver by means of five input files (termed ‘inparam’ files), dealing respectively with the model, the source, the output, the Fourier expansion, and advanced parameters. These are plain-text, human-readable YAML files that may also be generated via provided Python scripts for convenience during ensemble runs. Additional files needed in the input folder include

**Table 1.** Summary of code capabilities described in this paper, indicating previous benchmarks and verifications. Each capability has at the very least been benchmarked against independent numerical solvers or semi-analytical reference solutions, and been verified against real data. The validation given is for the event described in the corresponding citation; comparison to other earthquakes with new simulations is of course possible.

| Capability                                      | Benchmark                                                | Validation                         | Reference(s)                               |
|-------------------------------------------------|----------------------------------------------------------|------------------------------------|--------------------------------------------|
| Global wavefields                               | AxiSEM; SPECFEM3D_GLOBE; YSpec                           | 2011 Virginia earthquake           | Leng et al. (2016); Fernando et al. (2020) |
| 3D heterogeneity/discontinuities                | SPECFEM3D_GLOBE                                          | 2011 Virginia earthquake           | Leng et al. (2016, 2019)                   |
| Global surface fluid oceans                     | YSpec                                                    | 2015 New Britain earthquake        | Fernando et al. (2020)                     |
| Global planetary atmospheres                    | HOPT                                                     | <i>No published comparison</i>     | Saade et al. (2019)                        |
| Full anisotropy                                 | Semi-analytical shear-wave splitting;<br>SPECFEM3D_GLOBE | 2011 Virginia earthquake           | Tesoniero et al. (2020)                    |
| Local/regional domains and absorbing boundaries | SPECFEM3D                                                | 2018 Berkeley Earthquake           | Haindl et al. (2021)                       |
| Discrete adjoint sensitivity kernels            | Born-predicted versus forward-modelled traveltime shifts | 2011 Virginia Earthquake           | Szenicer et al. (2020)                     |
| Finite distributed sources                      | Exact axial-source reference solution                    | 2018 Berkeley Earthquake           | Szenicer et al. (2020); Haindl (2021)      |
| Small-scale volumetric scattering               | Scattering theory                                        | 1970-76 Apollo impact observations | Leng et al. (2020); Nunn et al. (2024)     |

a list of stations (or station groups) and the details of the source. For the latter, the user may provide either a standard CMTSolution file or a ‘point cloud’ of sources to represent a distributed source.

### 2.7.2 Meshes and meshing

Meshes used by AxiSEM3D are generated by the stand-alone `salvus_mesh_lite` package, a Python tool that can be driven from the command line (Afanasiev et al. 2019). `salvus_mesh_lite` is the freely available, GPLv3-licensed ‘lite’ version of the `SalvusMesh` mesher and is distributed from the AxiSEM3D community GitHub ([https://github.com/AxiSEMunity/salvus\\_mesh\\_lite](https://github.com/AxiSEMunity/salvus_mesh_lite)); it should not be confused with the full `SalvusMesh` package, which is part of the proprietary `Salvus` seismic modelling suite. We retain this independent package due to its robustness and stability for generating suitable meshes.

`salvus_mesh_lite` accepts inputs in the form of 1D seismic profiles termed ‘.bm’ files for *background medium*. These may be as simple as an isotropic, elastic medium (requiring only  $v_p$ ,  $v_s$ , and  $\rho$  to be specified against radius or depth); or as complex as a fully anisotropic, anelastic medium (including  $v_s^v$ ,  $v_s^h$ ,  $\eta$ , etc.). The resultant mesh is saved as an Exodus file for ease of portability and viewing and must be copied into the AxiSEM3D input directory. Global meshes (such as that shown in Fig. 1) and local/regional-scale meshes (such as that used for the Cartesian domain of Fig. 3) are both supported by `salvus_mesh_lite` and AxiSEM3D.

Global meshes must necessarily use cylindrical geometry (i.e. with a curved outermost edge), whilst regional and local meshes may use either cylindrical geometry or Cartesian geometry. In general, Cartesian geometry is appropriate up until the point at which the curvature of the planet becomes relevant to the simulation, which will generally depend on frequency and the required accuracy of the synthetics. We note that global-scale meshes do not need to include the entire depth of the planet. For example, a surface wave simulation may feature an absorbing boundary at 1,000 km depth to reduce computation time spent on mesh elements in the lower mantle and core which are not meaningfully contributing to the surface wave properties. Similarly, a global mesh could feature an absorbing boundary at  $100^\circ$  distance from the source. An alternate approach is to define a spatially varying  $n_u$  profile that concentrates azimuthal resolution where the 3D structure demands it (Sec. 2.3; a worked example is given in Example 2).

## 2.7.3 3D models

3D structures are added at runtime as perturbations to the radially-symmetric mesh properties, and may take the form of either geometric perturbations (moving interfaces or the surface inward or outward) or volumetric perturbations (changing material parameters such as  $v_p$ ,  $\mathbf{C}$ ,  $\rho$ , etc). Both geometric and volumetric perturbations are supplied to the solver as a structured grid. For example, a geometric perturbation corresponding to a Moho undulation would simply specify the absolute change in the Moho depth (or radius) with latitude and longitude as compared to that set in the background model (.bm) file. Conversely, the volumetric perturbation corresponding to a sediment layer could specify the absolute or relative changes in any seismic properties as a function of latitude, longitude, and depth/radius. The advantage of this approach is that changing the 3D model does not necessitate re-making the mesh, and for similar 3D models a user may take advantage of the previously described Azimuthal Complexity Adaptation (ACA) to optimise the simulation cost. The corresponding disadvantage applies to volumetric perturbations: a sharp material contrast specified only on the structured grid need not fall on an element boundary, and because the material properties within each element are sampled at its GLL points and represented by a single polynomial, such an interface is smoothed across the element rather than honoured exactly, as it would be in custom-built mesh honouring it exactly.

## 2.8 Outputs

Whilst Eqns. 1 and 2 were formulated in terms of displacement  $\mathbf{u}$ , AxiSEM3D is also able to directly output ground velocity and acceleration, or other derived quantities including strain, curl, and stress. Users may define the discrete locations at which the wavefield is outputted via a plain-text list of stations, or may opt to write the entire wavefield (for the purposes of wavefield visualisation).

In the case where seismograms are recorded at specific locations only, the linear nature of Eqns. 1 and 2 means that a delta function may be used as the source term, and the source-time function convolved after the fact with the synthetic Green's function. This has the advantage that only one simulation needs to be undertaken even if a variety of different source-time functions need to be tested. In the case in which the entire wavefield is being used, it is generally recommended to specify the source-time function prior to undertaking the simulations to simplify post-processing. The former approach is the principle underlying precomputed Green's-function databases such as *Instaseis* (Section 3.1).

Outputs may take the form of plain-text, human-readable files, but NetCDF files are recommended for efficiency. If parallel NetCDF is used when building the code, a single assembled file containing all stations may be generated as an output, else each process may produce a separate output file.

## 3 RESULTS (I): READY-TO-RUN TEMPLATES FOR EARTH

Having described the mathematical and computational approaches behind AxiSEM3D, we now showcase the range of problems in seismology and seismoacoustics that it can address, from local to global scales. We present a total of eleven examples of various scales and complexities, with applications for Earth, for other planetary bodies, and for the Sun. A template for each of these examples, including documentation, exists in the GitHub repository along with the AxiSEM3D source code. Each of these templates is designed to be readily adaptable, minimising the time taken for a user to find and modify a given template to fit the problem they are attempting to model.



**Table 2.** AxiSEM3D example simulations. Row labels give the example number used in the text and GitHub repository; Example 2 is listed twice (2a: mantle structure only on the global mesh, Fig. 2b; 2b: crust plus mantle on a regional mesh, Fig. 2c, the configuration described in Section 3.2).  $N_{\text{el}}$  is the number of spectral elements and  $\sum N_r$  the total number of azimuthal degrees of freedom ( $N_r = 2n_u + 1$ , summed over all mesh points); the product of  $\sum N_r$  with the number of time steps controls the cost. “CPU-h” is wall-clock core-hours on the Yale HPC cluster *Bouchet*, computed as elapsed time  $\times$  number of allocated CPUs. Example 7 (sensitivity kernels; Section 3.7) is run at a 50 s dominant period on a desktop and is not included here.

| Example                   | Period | $N_{\text{el}}$ | Model used                             | Record  | CPU-h | $\sum N_r$ ( $10^6$ ) |
|---------------------------|--------|-----------------|----------------------------------------|---------|-------|-----------------------|
| 1. Global 1D (PREM)       | 2 s    | 2,911,386       | PREM                                   | 1800 s  | 2,220 | 14.6                  |
| 2a. S362ANI global        | 5 s    | 478,222         | S362ANI (global mesh)                  | 1800 s  | 1,305 | 23.9                  |
| 2b. 3D crust + S362ANI    | 5 s    | 194,994         | S362ANI + CRUST1.0 (regional mesh)     | 1800 s  | 860   | 19.5                  |
| 3. Local salt body        | 0.2 s  | 2,000           | SEG/EAGE 3-D salt                      | 10 s    | 1.1   | 0.10                  |
| 4. Simple 3D shapes       | 0.08 s | 281,250         | Homogeneous box + 1,000 random spheres | 50 s    | 5,585 | 100.6                 |
| 5. Anisotropy (US32)      | 5 s    | 475,710         | Isotropic PREM + US32 anisotropy       | 2000 s  | 2,850 | 47.5                  |
| 6. Finite source (SFBA)   | 2 s    | 33,900          | USGS SF Bay Area 3-D                   | 30 s    | 1,643 | 270.3                 |
| 8. Mars’ atmosphere       | 20 s   | 204,456         | TAYAK + 60 km atmosphere               | 1800 s  | 20.5  | 0.21                  |
| 9. Enceladus’ ice sheet   | 2 s    | 9,856           | Enceladus ice shell + ocean            | 1000 s  | 4.6   | 0.05                  |
| 10. Sun (helioseismology) | 500 s  | 1,080,586       | 1-D solar model (fully fluid)          | 12000 s | 1,363 | 7.6                   |
| 11. Impacts on the Moon   | 2 s    | 1,001,664       | ISSI_MOON_M1 + scattering              | 1000 s  | 6,456 | 254.6                 |

The first seven of the eleven examples focus on increasingly complex Earth models. These are designed to be cross-compatible with each other, such that a user can create a new example with features from multiple existing examples with relative ease. The four final examples are from planetary science and helioseismology. These too are designed to be cross-compatible, and are chosen also to showcase the range of physical scales (length, density, and sound speed) that AxiSEM3D can handle. Where an example contains a self-contained quantitative test, that is, a result that can be checked directly against an independently known answer, we say so in the text describing that example.

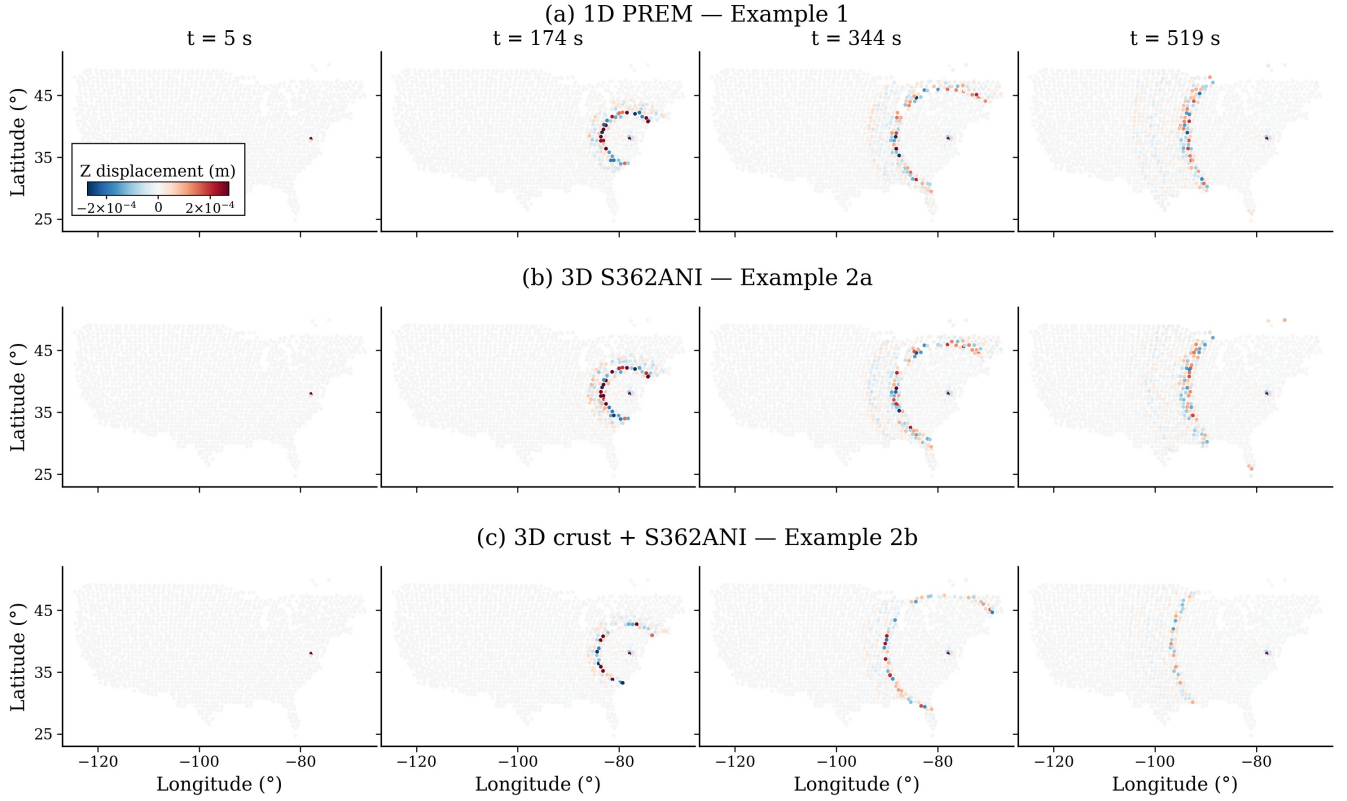
Two versions of each example exist. Those downloaded along with the source code from GitHub are low-resolution runs to keep file sizes manageable, with most global examples at 50 s resolution. Higher-resolution runs also exist for all examples and are available from the GitHub repository but are not downloaded by default; these runs are used to generate figures for each example. Figures for the global Earth examples are created from higher-resolution runs (typically 2–5 s period; the exception is the sensitivity-kernel example, Example 7, illustrated at 50 s), with the remaining examples illustrated using the periods stated in their figure captions and in Table 2. The templates for these runs are not downloaded by default with the rest of the source code, but are contained within the `AxiSEM3D_example_gallery` repository on the AxiSEM3D community GitHub (see Data Availability).

### 3.1 Example 1: Global wavefields in a 1D model

Example 1 is designed as a ‘first introduction’ to AxiSEM3D that will run quickly on a laptop or a single compute node (2.4 minutes on 4 cores of an Intel Xeon Platinum 8268 node for 1800 s of simulation time). It produces low-resolution (50 s dominant period) seismograms which are easily visualised. This configuration has been benchmarked against AxiSEM, SPECfEM, and YSpec (Section 2.6). The background model in this case is PREM (Dziewonski & Anderson 1981).

For users seeking 1D, high-frequency synthetics, this example is an ideal starting point, with few changes required to the input files other than a new mesh and a narrower source-time function. On a laptop with 4 cores, a 10 s set of global synthetics half an hour long can be generated in around 10 hours. For users with access to high-performance computing resources, even 5 s synthetics become trivially accessible.

Unlike most global-scale seismic modelling codes, which represent the ocean only as an equivalent surface mass load (e.g., Komatitsch & Tromp 2002b), AxiSEM3D can include an actual fluid ocean layer at the surface of this model and so simulate acoustic propagation within



**Figure 2.** Snapshots of the vertical (Z) displacement wavefield sampled at the USArray Transportable Array stations following the 2011  $M_w$  5.8 Virginia earthquake, computed with AxiSEM3D at a 5 s dominant period. Rows show three Earth models of increasing structural complexity: (a) 1D anisotropic PREM (Dziewonski & Anderson 1981) (Example 1); (b) the 3D whole-mantle model S362ANI (Kustowski et al. 2008) (Example 2a, mantle structure only); and (c) S362ANI plus the 3D CRUST1.0 crustal model (Laske et al. 2013) (Example 2b). Columns show four successive times ( $t = 5, 174, 344$  and  $519$  s) as the wavefront sweeps across the continental United States; the added 3D structure progressively scatters and reshapes the wavefield. Red and blue denote upward and downward ground motion, respectively.

it. This requires only editing the .bm file to produce a mesh with a surface fluid layer; the code will automatically detect the fluid surface and impose the pressure-free boundary condition described by Fernando et al. (2020).

The original AxiSEM (2.5D) code used this 1D case to produce a precomputed database called *Instaseis* of high-frequency seismograms at up to 2 s period, which could be retrieved near-instantaneously (van Driel et al. 2015). Comparable databases have not yet been generated from AxiSEM3D; recomputing them, potentially including the effects of an ocean, is among the development priorities tracked on the AxiSEM3D GitHub (Section 5.2).

### 3.2 Example 2: Global wavefields in a 3D model with crust and mantle structure

For many users undertaking global-scale FWI, Example 2 likely achieves a good balance between realistic model complexity and computational cost. The fundamental model setup is the same as Example 1, but three-dimensional structure is included, with the crust represented via the 3D CRUST1.0 (Laske et al. 2013) model and the mantle via the S362ANI model (Kustowski et al. 2008). The difference between these models is shown in Fig. 2, which shows synthetic vertical-displacement wavefields for the 2011  $M_w$  5.8 Virginia earthquake for a sequence of increasingly complex Earth models, from 1D PREM only, through to 1D PREM with full 3D crust and mantle models superimposed on top.

Whilst S362ANI is read in as an external model (as a structured grid contained within a NetCDF file), CRUST1.0 is hard-coded in

AxiSEM3D as an option which can be enabled with a single flag in the input files. This inclusion of CRUST1.0 is a convenience to the user given how widely it is used, and it is entirely possible to use a different crustal model by reading it in as an external structured grid as well.

Example 2 can be combined with the optional fluid ocean described above in Sec. 3.1, wherein topography on the global solid surface as specified by CRUST1.0 becomes bathymetry. As discussed by Fernando et al. (2020), the ocean must cover the entire surface, but can be made arbitrarily thin over areas that are not actually covered by water.

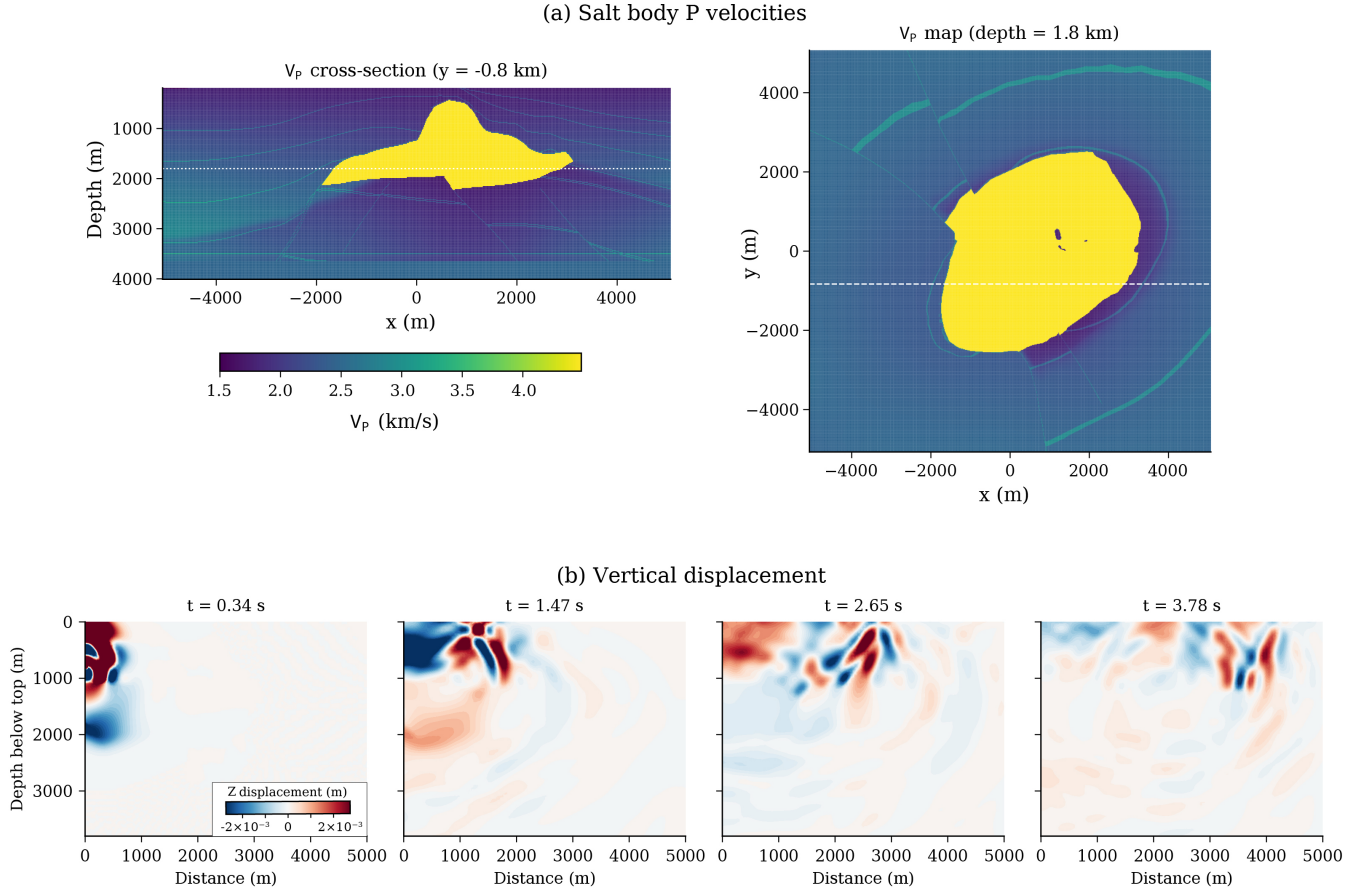
$n_u$  in this example is set to a constant value of 100 across the entire mesh. This is sufficient to resolve the long-wavelength, smooth S362ANI model fully, but insufficient to fully resolve the CRUST1.0 model, which is sampled at  $1^\circ \times 1^\circ$  (corresponding to an order of  $\sim 180$ ). Practically, this means that the mantle model is fully resolved, and further increase of  $n_u$  would increase computational cost whilst having no effect on the realism with which wave propagation in the mantle is simulated (that is, full convergence has already occurred). However, with a value of  $n_u = 100$  the crustal model is being under-sampled and hence represented as a smoothed version of itself. Increasing  $n_u$  would hence better resolve fine-scale crustal structure, up to a point where the azimuthal Fourier order in the simulation is approximately equivalent to the azimuthal Fourier order in the model. Beyond this point, further increases of  $n_u$  would serve to increase computational cost for no return.

It is up to the user to decide how to balance the higher cost of increasing  $n_u$  against increased simulation realism. The choice generally depends on the goal of the simulation. AxiSEM3D does, however, offer options to help reduce costs and balance the cost-realism tradeoff appropriately. Firstly, a depth-defined  $n_u$  profile may be used. A user investigating deep-mantle structure might, for example, use  $n_u = 100$  in the top 50 km of the lithosphere, but reduce this to  $n_u = 50$  below 100 km depth, with a linear transition in between, thus keeping S362ANI fully resolved but minimizing the use of resources on unnecessary higher-order terms. The input parameters needed to implement this are included in the input files for this example, and can be implemented by changing the  $n_u$  argument from *Constant* to *Analytical*. Alternatively, ACA can derive such a spatially varying  $n_u$  field automatically (Sec. 2.3); this is likely the better approach for users undertaking multiple simulations with similar 3D models, making the initial, more expensive scanning run more (relatively) affordable.

### 3.3 Example 3: Local-scale simulation of 3D, highly heterogeneous models

Having demonstrated how multiple 3D models can be combined at global-scale in AxiSEM3D, we now illustrate how the same can be achieved on a regional or local scale in Example 3. Here, we make use of Cartesian geometry, with absorbing boundaries (Section 2.2) damping the unphysical edges of the domain.

The model is the SEG/EAGE C3 salt body (Aminzadeh et al. 1997), a canonical 3D benchmark for exploration imaging. This model (in a purely elastic configuration, with the overlying water replaced by a solid overburden) was used by Haindl et al. (2021) and Haindl (2021) to benchmark the complexity-adaptive AxiSEM3D approach against the full-3D spectral-element solver SPECFEM3D. The salt body is a stringent test of the azimuthal-smoothness assumption that AxiSEM3D exploits. Its steep, high-impedance flanks scatter energy strongly out of the source–receiver plane, raising the local azimuthal complexity so that  $n_u$  must be increased markedly in the vicinity of the salt relative to its smoothly layered surroundings; even so, ACA recovers substantial savings by concentrating azimuthal resolution only where the wavefield requires it. Example 3 additionally includes an overlying ocean (not resolvable in Fig. 3, coupling the solid salt-and-sediment section to a thin fluid layer with an undulating sea floor. This example is therefore directly relevant to both exploration geophysics and carbon



**Figure 3.** Here at a local scale, the SEG/EAGE C3 salt body (Aminzadeh et al. 1997) is simulated in Cartesian geometry at a 0.2 s dominant period (5 Hz). (a) Input P-wave velocity model shown as a vertical cross-section (left) and a horizontal depth slice at 1.8 km (right); the high-velocity salt body ( $v_p \approx 4.5 \text{ km s}^{-1}$ ) is embedded within slower, layered sediment beneath a thin water layer (not visible at this scale), with the dashed and dotted white lines marking the locations of the complementary slices. (b) Snapshots of the vertical displacement wavefield on an in-plane cross-section at four successive times, illustrating the strong scattering and reverberations generated by the salt body.

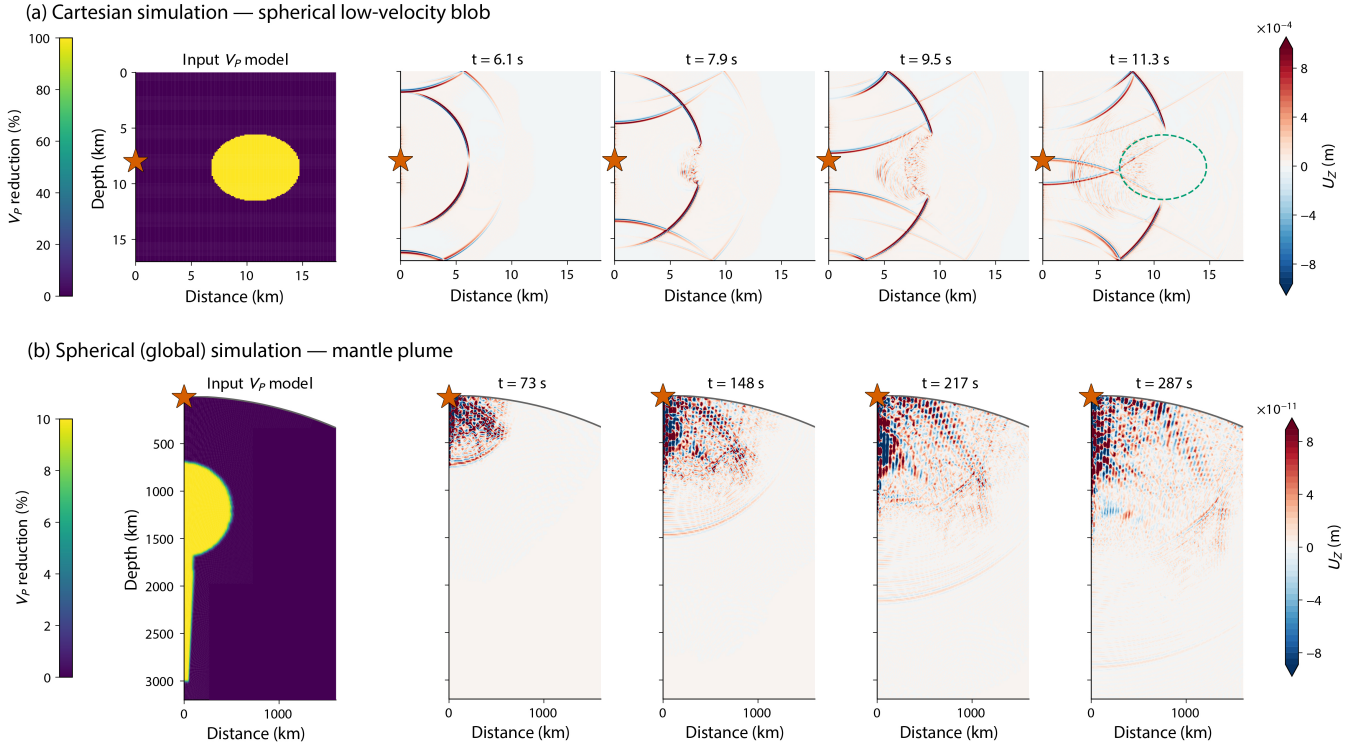
capture and storage (CCS) settings, and the off-plane scattering from the salt together with the solid–fluid coupling leaves a clear imprint on the recorded wavefield.

### 3.4 Example 4: Mantle plumes and other geodynamic problems

Whilst Example 3 involved reading in an existing complex 3D model, there are many settings, especially relevant to conceptual problems in geodynamics, in which a user may need to create their own 3D model from scratch. Example 4 therefore contains scripts needed to both generate geodynamically-relevant 3D shapes (e.g., mantle plumes or arrays of scattering bodies) and simulate wave propagation through them.

Fig. 4 shows two such cases: a low-velocity sphere in a small Cartesian box (Fig. 4a) and a synthetic mantle plume consisting of a low-velocity head and conduit, placed within a spherical planet (Fig. 4b). These low-velocity regions may be used to represent, for example, hotter or more melt-rich inclusions. Whilst in this case only perturbations to the wavespeeds and density are included, perturbations to other properties (e.g., anisotropy) are also easily implemented.

It is important to note that AxiSEM3D cannot handle ‘detached’ fluid inclusions. In other words, to ensure the continuity of boundary



**Figure 4.** Analytically defined 3D bodies injected into otherwise laterally homogeneous meshes (Example 4). (a) A low-velocity sphere in a Cartesian box (0.2 s dominant period): the input  $v_p$  model (leftmost) followed by snapshots of the vertical displacement  $u_z$  at  $t = 6.1, 7.9, 9.5$  and  $11.3$  s, as the wavefront from the source (orange star) scatters off the inclusion (scattered coda in the green dashed ellipse). (b) A synthetic mantle plume (10%  $v_p$  reduction) on the symmetry axis of a homogeneous spherical planet (radius 4000 km;  $v_p = 10 \text{ km s}^{-1}$ ,  $v_s = 6 \text{ km s}^{-1}$ ,  $\rho = 6 \text{ g cm}^{-3}$ ): the input  $v_p$  model (leftmost) and  $u_z$  at  $t = 73, 148, 217$  and  $287$  s. Red/blue denote upward/downward vertical motion and the percentage change in  $v_p$  is relative to the homogeneous background.

conditions, the deformed mesh must be homeomorphic to the original. As such, a fluid layer must span the entire mesh, meaning that in a Cartesian grid it stretches from one edge to the other and in cylindrical geometry it exists at all angles along a constant radius. Nonetheless, because  $v_p$  and  $v_s$  may be perturbed separately within the 3D structured grid, so variations in the  $v_p/v_s$  ratio may be incorporated to represent areas of, for example, high melt fraction.

Of course, decreasing wavespeeds locally still has a global effect on the minimum timestep required to ensure computational stability, and hence modelling such inclusions, especially if they are small, can be computationally expensive. Similarly, realistic modelling of out-of-plane wave propagation or scatter requires increasing  $n_u$  as the size of such inclusions decreases, so simulation geometry should be carefully considered; as before, the threshold beyond which higher  $n_u$  no longer changes the wavefield is best found automatically using ACA (Sec. 2.3).

### 3.5 Example 5: Full anisotropy

AxiSEM3D is also able to support anisotropy, either simple (radial) anisotropy or full anisotropy implemented via arbitrary modification of the elastic tensor  $\mathbf{C}$ . In the simplest case of radial anisotropy, the user may specify this either in the .bm file used to create the mesh or via a 3D structured grid that is read in at runtime and used to modify any or all elements of  $\mathbf{C}$ . This dual functionality also enables users to verify their procedure for implementing anisotropy via a radial anisotropy test case. More complex anisotropies can only be implemented via 3D models, which have been benchmarked and fully validated by Tesoniero et al. (2020).

Because AxiSEM3D is designed for high-frequency runs, it remains efficient down to the short periods ( $\sim 5$  s and below) useful for shear-wave splitting observations. AxiSEM3D has been applied to study anisotropy throughout the Earth’s interior, from the upper mantle (Wolf & Long 2023) to the transition zone and uppermost lower mantle (Wolf et al. 2024b) to the lowermost mantle (Wolf et al. 2026a,b). It has also been applied to the development of new splitting-measurement strategies for the high-frequency global S-wavefield (Wolf et al. 2024a,b).

To illustrate these capabilities, in Example 5 (Fig. 5) we model SKS splitting for a deep (239 km) earthquake beneath Cook Strait, New Zealand, recorded across the High Lava Plains of the western United States (Long et al. 2009). Following Wolf & Long (2022), anisotropy is confined to the upper mantle as an olivine E-type elastic tensor (Karato 2008), oriented to follow the local orientations found in the US32 azimuthal-anisotropy model (Zhu et al. 2020), embedded in an isotropic PREM background.

Because SKS is radially polarised for a spherically symmetric, isotropic Earth, any transverse energy in these synthetics is a direct signature of the anisotropy we impose; in the real Earth, shorter-wavelength isotropic 3D heterogeneity can also scatter energy onto the transverse component (e.g., Wolf et al. 2022a, 2024b). Shear-wave splitting parameters measured by transverse-energy minimisation (Silver & Chan 1991) implemented in SplitRacer (Reiss & Rumpker 2017) reproduce the observed fast polarisation directions well, whereas the delay times are underpredicted. AxiSEM3D-based forward models thus suggest that US32 underestimates the strength of upper-mantle anisotropy (as reflected in SKS splitting delay times) in this region by a factor of perhaps 2, which is not unusual for surface-wave derived models (e.g., Wagner & Long 2013).

### 3.6 Example 6: Kinematic fault rupture for seismic hazard

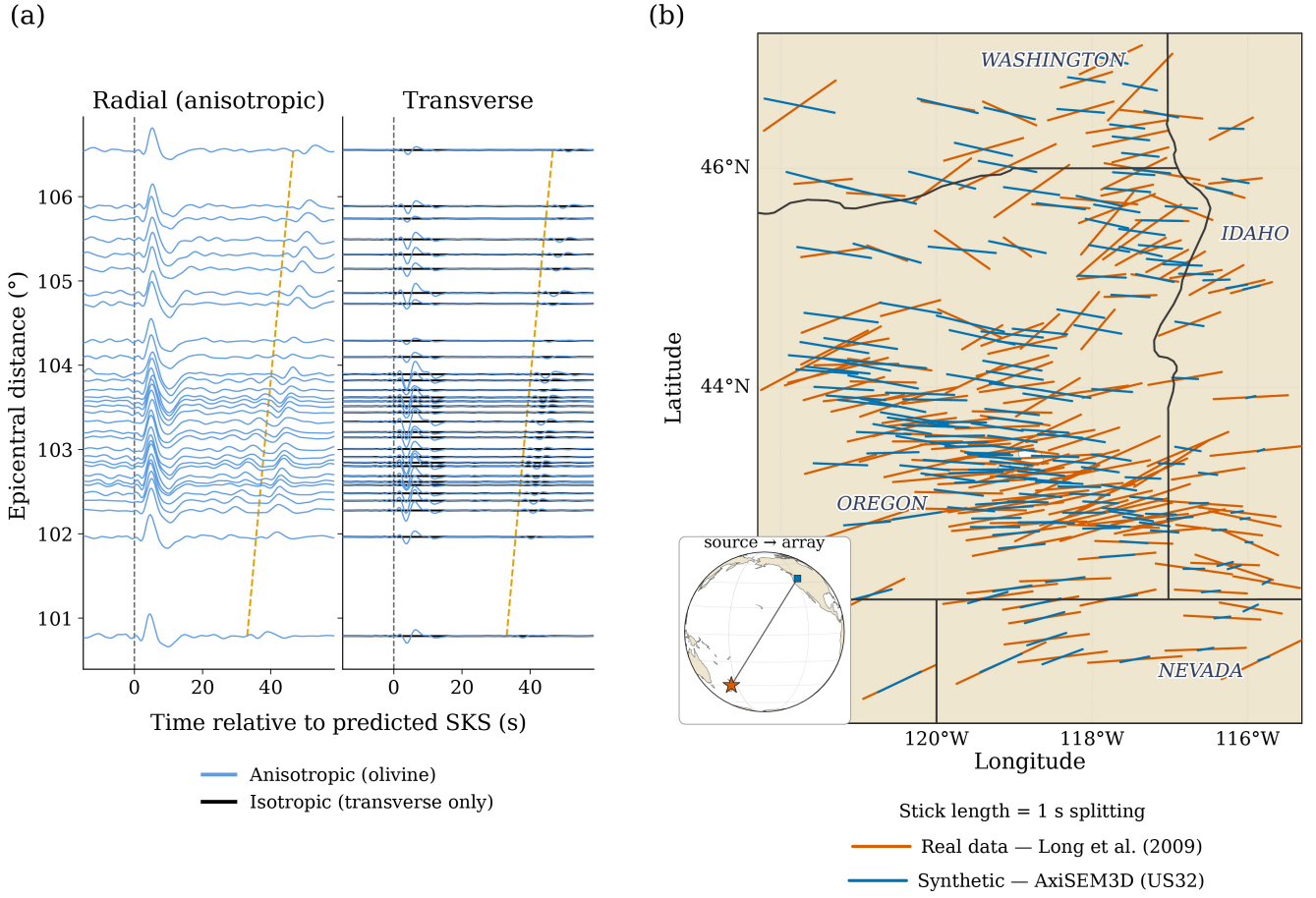
For many of the previous examples, using a point-source representation of the earthquake source was sufficient. However, this approach is not realistic enough for seismic hazard modelling on a local-to-regional scale. Using the distributed-source capability described in Section 2.4.2, the code is now able to simulate finite-fault rupture kinematically (Szenicer et al. 2020; Haindl 2021).

In Example 6, we model the Hayward Fault within the San Francisco Bay Area (SFBA). This fault occurs within a densely populated region, forecast to have a high probability of a magnitude 6–7 earthquake in the coming decades (Field et al. 2017). The SFBA is also a notoriously demanding target for ground-motion simulations. Low-velocity sediments infilling basins reach shear-wave velocities as low as  $\sim 80 \text{ m s}^{-1}$ , and the very small elements and time steps these velocities demand have historically forced modellers to impose an artificial (and unphysically large) floor on the minimum shear-wave velocity. This compromise is now known to underestimate peak ground velocities (PGVs) in exactly the basins where shaking is most damaging (Rodgers et al. 2019).

AxiSEM3D is able to relax this requirement, as demonstrated in Example 6. The kinematic rupture is represented as a dense cloud of tightly spaced sub-faults spanning the fault plane, each associated with its own moment tensor and rupture-time offset (Eqn. 8). This style of finite-rupture modelling in AxiSEM3D was established by Haindl (2021), who generated the rupture with the Southern California Earthquake Center Broadband Platform (Maechling et al. 2015) and projected it onto the mapped Hayward Fault geometry.

The simulation runs on a local Cartesian mesh carrying realistic surface topography and a 24 km deep Moho (both imposed by particle relabelling) over a multi-layer 3D crustal velocity model, with Kosloff–Kosloff sponge and Clayton–Engquist absorbing boundaries damping the truncated edges (Haindl et al. 2021). At a 2 s dominant period with a highly-complex and variable-velocity 3D model, this is the most

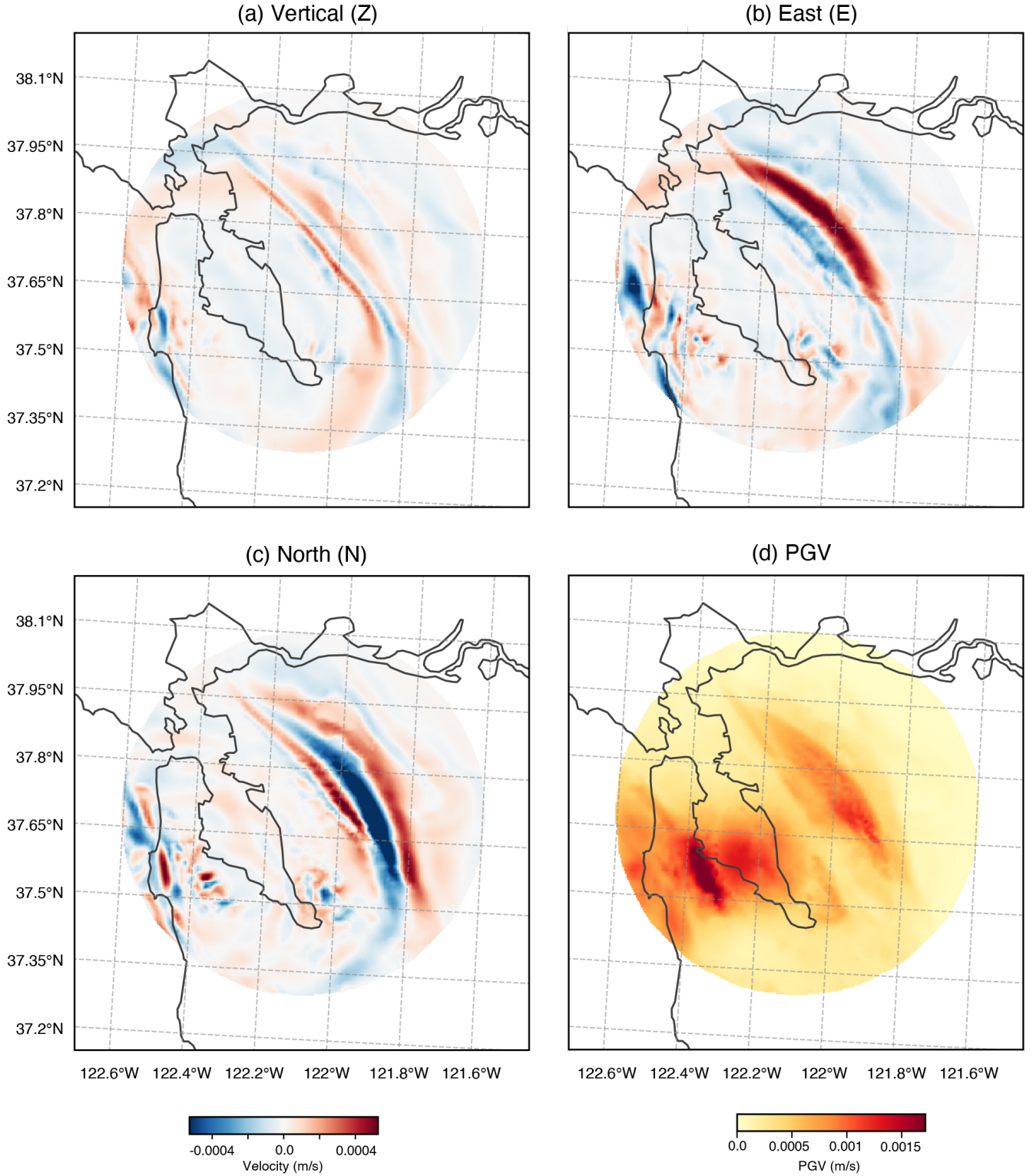




**Figure 5.** AxiSEM3D applied to global seismic anisotropy and SKS shear-wave splitting (Example 5). We use a 5 s isotropic PREM mesh (Dziewonski & Anderson 1981) with anisotropy confined to the upper mantle, represented as an olivine E-type tensor (Karato 2008) oriented according to the US32 model (Zhu et al. 2020). Synthetics are for a deep (239 km) earthquake beneath Cook Strait, New Zealand (3 July 2012), recorded in the High Lava Plains region (source–array path in the inset of b). (a) Radial (left) and transverse (right) SKS record sections versus epicentral distance, aligned on the predicted SKS arrival ( $t = 0$ , grey dashed; predicted SKKS, orange dashed). The transverse component is identically zero in the spherically symmetric, isotropic reference simulation (black) but carries energy in the anisotropic model (blue), the direct splitting signature; the two panels are jointly normalised per station. (b) Resulting splitting measured with SplitRacer (Reiss & Rumpker 2017): each ‘stick’ gives the fast-polarisation azimuth and delay time (1 s reference, lower right). Red, observations of Long et al. (2009); blue, AxiSEM3D synthetics. Fast directions agree, but delay times are underpredicted, implying that US32 may underestimate the anisotropy strength here.

computationally demanding example described in this paper. Although the rupture is centred on the axis, the off-axis sub-sources that compose it demand very high azimuthal resolution in their immediate vicinity to accurately represent near-source wavefield complexity.

The example produces a dense regional ground-motion field: three-component velocity maps across thousands of points in the SFBA. Fig. 6 shows this output part-way through the simulation, with snapshots of the three velocity components as the wavefield sweeps across the region (Fig. 6a–c) alongside the peak ground velocity accumulated up to the same instant (Fig. 6d), in which the imprint of the fault geometry and of the low-velocity basins is clearly visible. In the equivalent 1 s study on which it is based, Haindl (2021) showed that such a finite rupture captures features a point-source idealisation cannot. Specifically, spreading the moment release over the rupture duration lowers and redistributes the near-field PGVs and removes the spurious four-lobed radiation pattern centred on a single hypocentre, the dip of the Hayward Fault concentrates motion on the hanging wall, and the low-velocity bay muds both amplify and prolong shaking, trapping energy that reverberates within the basins. Example 6 thus shows that finite-fault, basin-resolving ground-motion simulation is feasible in AxiSEM3D, and likely necessary for meaningful hazard assessment.





### 3.7 Example 7: 3D, high-frequency sensitivity kernels

As a final terrestrial example, we demonstrate that AxiSEM3D can be used to compute finite-frequency sensitivity kernels (Fréchet derivatives) (Marquering et al. 1998; Dahlen et al. 2000). Such sensitivity kernels form the basis of adjoint FWI and hence are a crucial part of quantitative exploration of the Earth’s interior structure (Tarantola 1984; Tromp et al. 2005). Because AxiSEM3D is itself a forward solver, the companion `axikernels` method constructs the adjoint source from a chosen measurement, runs the backward simulation, and evaluates the kernels (Szenicer et al. 2020). `axikernels` is a set of Python processing scripts supplied with this example on the AxiSEM3D GitHub. A single framework yields both volumetric kernels (e.g. for  $v_p$ ) and interface (geometric) kernels, in 1D and fully 3D Earth models alike. Because spherically-symmetric forward and backward runs are inexpensive, and 3D runs can be optimised through ACA, kernels of this kind can be computed on a desktop computer rather than HPC architectures.

Example 7 illustrates these concepts for a P400P (a P-wave reflecting off the 400 km discontinuity in PREM) cross-correlation traveltime measurement (50 s dominant period) at a single source-receiver pair  $40^\circ$  apart. The volumetric  $v_p$  kernel displays the characteristic ‘banana–doughnut’ geometry, with sensitivity concentrated in the first Fresnel zone and vanishing along the geometric ray; while the Moho interface kernel  $K_{SS}$  localises sensitivity to the discontinuity beneath the source and receiver. Recomputing the same kernels through a 3D model, in this case S362ANI (Kustowski et al. 2008) with a deliberately-imposed Gaussian Moho undulation on an isotropic PREM background (Dziewonski & Anderson 1981), modulates both kernels (Fig. 7). The resulting interface kernel can then be compared directly against the topography that produced it, providing a built-in check of the 3D computation.

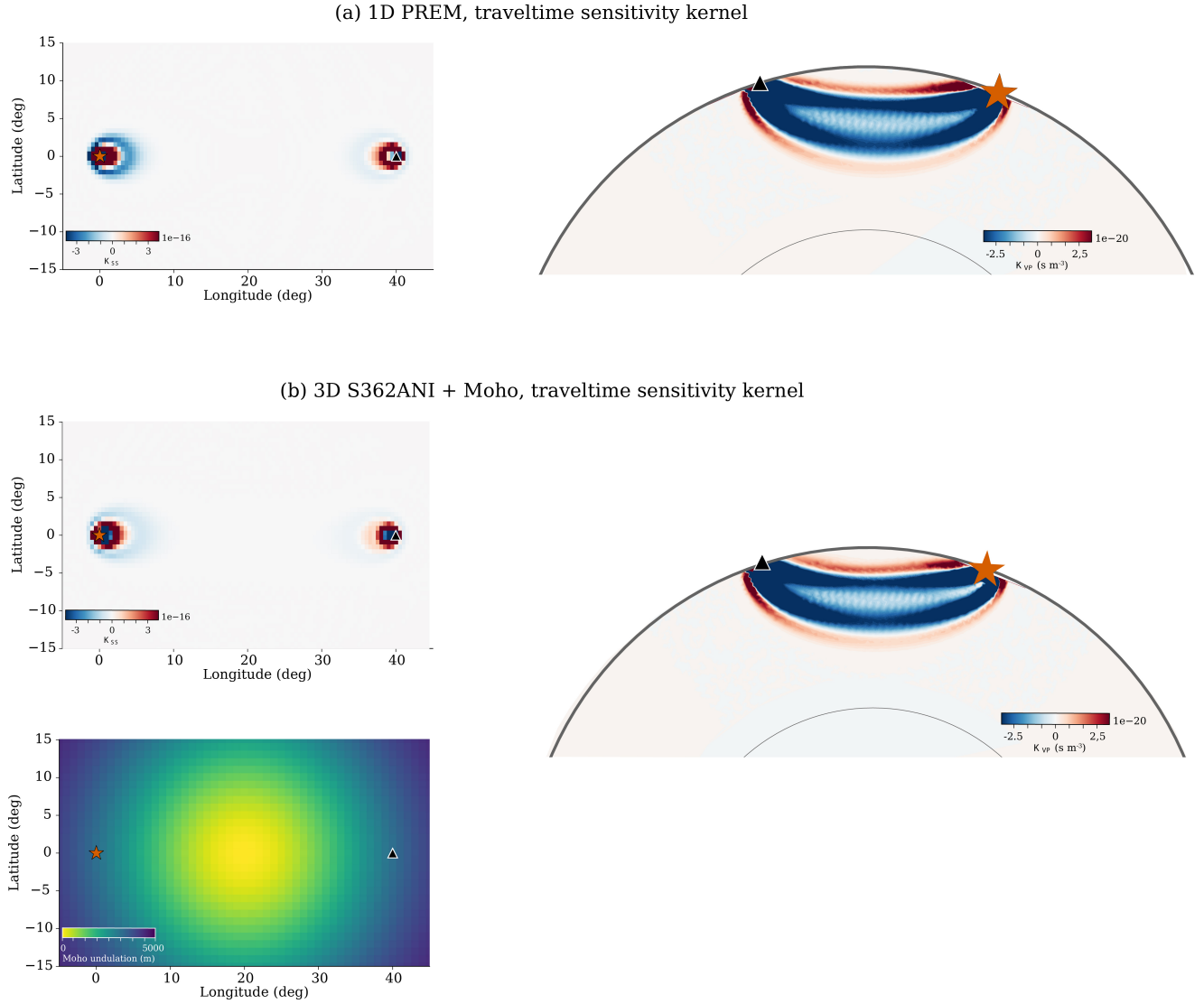
## 4 RESULTS (II): READY-TO-RUN TEMPLATES FOR PLANETARY SCIENCE AND HELIOSEISMOLOGY

We now present four examples from planetary science and helioseismology. It should be emphasised that the main point here is not that the underlying background model has changed from one world to another: changing from an Earth model to a Mars model in AxiSEM3D is no more complicated than changing between two Earth models, and simply requires updating the `.bm` file with a new seismic profile (e.g. replacing PREM with TAYAK). Likewise, for worlds with an atmosphere (e.g. Mars, Venus, and Titan), an atmosphere can just be added within the `.bm` file with few changes required other than activating an absorbing boundary at the top of the mesh.

Instead, we use these examples to focus on different regimes of physics that may be of interest to users: coupled seismoacoustic propagation, complex multi-media propagation in water and ice, fully acoustic propagation, and strong scattering to the point that wavefields are fully diffusive and non-ballistic. For compactness, we showcase the first three of these (Examples 8–10) within a single figure (Fig. 8). This also has the advantage that the differences between the wavefields in each case can be easily seen.

### 4.1 Example 8: Mars: global-scale seismoacoustics from atmospheric explosions

Our first planetary science example concerns the simulation of acoustic waves from explosions in the Martian atmosphere. With its thin atmosphere and position closer to the asteroid belt than the Earth, Mars’ surface is less well shielded from incoming meteoroids than the Earth’s (Daubar et al. 2018). Combined with its lower seismic activity compared to Earth’s (given the absence of plate tectonics), a far higher proportion of Mars’ seismic budget arrives from off-planet in the form of meteoroids (Lognonné & Johnson 2007). These meteoroids



**Figure 7.** Finite-frequency sensitivity kernels for a P400P cross-correlation traveltime measurement, computed from AxiSEM3D output with the companion `axikernels` package (Example 7). The dominant period is 50 s, and one source-receiver pair is used with the source at the orange star and the receiver  $40^\circ$  away at the triangle. Kernels shown are (a) 1D PREM (Dziewonski & Anderson 1981): the volumetric  $v_p$  kernel  $K_{vp}$  on the source-receiver cross-section (right), showing the finite-frequency ‘banana-doughnut’ with vanishing sensitivity along the geometric ray, and the Moho interface kernel  $K_{SS}$  (left). (b) The same kernels in a 3D Earth (S362ANI (Kustowski et al. 2008) plus an imposed Gaussian Moho bump): the interface kernel  $K_{SS}$  (top left), the imposed Moho topography (peak  $\approx 5$  km) that produced it (bottom left), and the  $v_p$  kernel (right).

463 generate sonic booms as they enter the atmosphere, and occasionally explode (Garcia et al. 2022; Fernando et al. 2022). Such events act  
 464 as localisable seismic sources, and the InSight mission demonstrated their value as probes of interior seismic structure (Kim et al. 2022;  
 465 Posiolova et al. 2022; Charalambous et al. 2025a).

466 Simulating the coupling of acoustic-elastic waves at a global scale on Mars is challenging (Martire et al. 2018): sound speeds in the  
 467 atmosphere are slow (necessitating small spectral elements and timesteps as compared to solid media), and a reliable absorbing boundary  
 468 must be implemented at the top of the atmosphere. Additionally, different acoustic profiles in the atmosphere must be used for different times  
 469 of day, as the diurnal cycle has a substantial effect on Mars’ thin atmosphere (Fernando et al. 2021).

470 Fig. 8(a) shows seismograms from an explosion at a height of 10 km, in a model containing a 30 km realistic atmosphere layer and a  
 471 30 km constant-density ‘sponge’ layer on top of that to absorb upgoing waves. As a base model for the Martian interior, we use TAYAK,

which combines geochemical and geodetic models to produce a profile of the Martian interior (Clinton et al. 2017; Khan et al. 2018). The solid–fluid coupling machinery is the same as that benchmarked for global surface oceans (Section 2.6).

Stations are located on the surface to mimic the position of the InSight lander. The significant change to the waveform behaviour from the addition of even a thin atmosphere above the surface can clearly be seen, with long-lasting codas produced by energy propagating slowly through the atmosphere along various paths and then coupling into the ground. Similar behaviour was observed by Fernando et al. (2020) when even a thin fluid ocean was added to a PREM model. It should be noted that this coda can be substantially suppressed when realistic surface topography is added (not present in this 1D model).

#### 4.2 Example 9: Icy worlds: complex, multi-media propagation in water and ice

In the outer Solar System, there are entire planetary bodies covered in water ice. The icy moons of Jupiter, Saturn are of particular interest as several are thought to be home to sub-surface liquid water oceans, kept above the solidus by tidal heating and protected from the vacuum of space above by the ice layers. Many, especially Jupiter’s Europa, Saturn’s Enceladus, and Neptune’s Triton, are geologically active. All of these features combine to make the icy moons a promising target for explorations of past, present, or even future habitability (Cockell et al. 2016). Seismology is likely to be a key method for constraining the internal properties, and hence habitability, of icy worlds (Vance et al. 2018). Hence, Dragonfly will carry a seismic payload (Lorenz et al. 2019) and most concepts for potential upcoming missions advocate the same (Marusiak et al. 2021; MacKenzie et al. 2022).

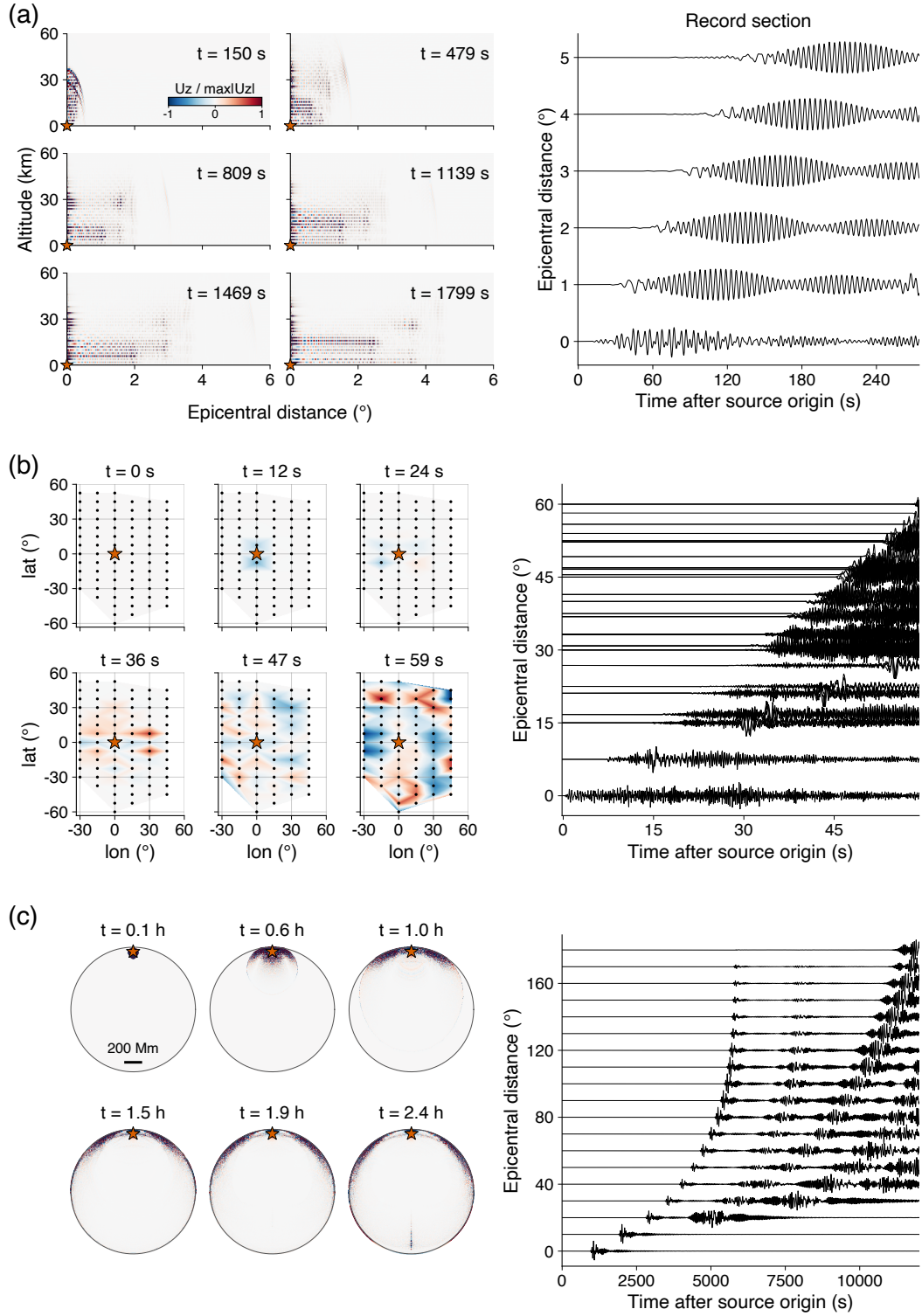
On the one hand, seismic modelling for icy ocean worlds is made easier by their small size necessitating fewer mesh elements. On the other hand, unusual geological configurations (such as sub-surface oceans) and exotic sources (e.g., possible seafloor volcanism) and seismic phases (such as flexural waves in the icy crust) need to be accurately represented (Stähler et al. 2018). Fig. 8(b) shows regional-scale simulations of wave propagation on Saturn’s moon Enceladus using the structural model of Dapré & Irving (2025), and the topographic model from Čadež et al. (2016), with a volumetric model based upon the topography and other data.

As can be seen in the record section, these 3D models introduce strong scattering into the seismic data, obscuring many phases though some higher-amplitude ones can still be seen. Whilst previous investigations such as those of Stähler et al. (2018) were unable to simulate sources in the sub-surface ocean, this functionality is now included in AxiSEM3D (as per Example 8) and could be used to represent acoustic energy release from hydrothermal activity, fluid motion, or sub-surface volcanism.

For Titan, the only icy ocean world with an appreciable atmosphere, the features described in this Example and Example 8 can easily be combined to simulate acoustic and coupled seismoacoustic wave propagation in the ocean, atmosphere, ice shell, and deep interior together.

#### 4.3 Example 10: The Sun: fully acoustic simulations with extreme gradients

The Sun is, in fact, one of the most seismically active places in the Solar System (Christensen-Dalsgaard 2002). Convective turbulence in its outer layers continuously excites and damps pressure-restored standing modes (p-modes) with a dominant period of around 300 s. In addition to the excitation of solar normal modes, various discrete events (such as flares, reconnection-driven shocks, and infalling material) excite a whole host of wave families, from acoustic to magnetohydrodynamic and many in between. Measurements of p-mode propagation in the Sun have been used to map many properties of the solar interior (Deubner & Gough 1984), in many cases to a degree of precision exceeding that



**Figure 8.** AxiSEM3D across planetary and solar bodies, run with the same solver for solid, fluid and atmospheric domains. Each row pairs wavefield snapshots (individually normalised) with a record section. (a) Mars: a pressure source coupling into the 60 km fluid atmosphere overlying the solid planet (TAYAK model; 20 s), shown as altitude–distance cross-sections of the atmospheric wavefield and the vertical-component record section out to  $\sim 6^\circ$ . (b) Enceladus: a shallow moment-tensor source in a regional model of the ice shell and subsurface ocean (2 s), with interpolated surface snapshots (receiver locations as dots) and the vertical-component record section. (c) The Sun: helioseismology in a fully fluid (acoustic) solar model, with interior cross-sections (note the 200 Mm scale bar and times in hours) and a vertical-displacement record section to  $180^\circ$ . Stars mark the source; red and blue denote opposite signs of (normalised) vertical motion.

which is possible for Earth. Although AxiSEM3D includes neither gravity nor magnetic fields, much of the fluid-domain functionality was originally developed for simulating acoustic wave propagation in the solar interior.

Terrestrial seismologists rarely consider or map perturbations within the Earth’s fluid layers but these do exist and can be quite reasonably simulated in the Sun. Local changes in temperature, which could be associated with any manner of phenomena from cool sunspots to topography on the tachocline, may manifest as changes in sound speed that leave an imprint on ballistic wave propagation.

Simulating such phenomena is entirely possible in AxiSEM3D, at least in the high-frequency limit where gravity is not an appreciable restoring force. The computational difficulty in doing this should not be underestimated, not least because of the enormous length scales involved (the Sun is more than half a million kilometres in radius), but also because of the huge variations in density ( $150 \text{ g cm}^{-3}$  in the core to  $10^{-7} \text{ g cm}^{-3}$  at the photosphere) and sound speed ( $\sim 500 \text{ km/s}$  to  $\sim 5 \text{ km/s}$ ) that need to be accurately represented.

To stably mesh such strong gradients (and to avoid unfeasibly small timesteps set at the photosphere that render simulations intractable), we implement two strategies not required elsewhere. Firstly, the polynomial order used to interpolate the seismic profile and the wavefield is increased from its default value of 4 (used in all other simulations) to 8. This ensures that even within the elements with the strongest density contrasts (near the surface), the interpolated density is never allowed to be negative, which would otherwise destabilise the simulation. Secondly, we force the mesher to add additional refinement layers near the surface. This procedure is described extensively in the AxiSEM3D Manual.

Fig. 8(c) shows a cross-section of the wavefield for a near-surface pressure source (e.g., representing convective turbulence) within the Sun. As this simulation is undertaken at 500 s resolution, a reflecting boundary is actually most appropriate, as acoustic waves are reflected from the photosphere at this period. For local-scale simulations using higher frequencies than the acoustic cutoff (around 5.3 mHz), however, an absorbing boundary is likely more suitable (Gizon & Birch 2005).

As can be seen in Fig. 8(c), acoustic propagation is slow, with a sound-crossing timescale within the solar interior that is on the order of hours. Much of the energy remains trapped close to the surface, and propagates substantially slower than the deep-going energy. With a sufficiently long simulation, the frequency spectrum of the seismograms may be used to recover the solar (pressure) normal modes, which is how these data are normally described.

Whilst this example used a single source, and hence propagation is ballistic rather than diffusive, both excitation and damping in the Sun are generally stochastic and continuous. Such solar simulations are possible using AxiSEM3D’s new ability to simulate distributed sources, but are also very relevant to terrestrial seismologists as a route to simulating ambient noise excitation and propagation; for example, as a distributed pressure field on the seafloor overlain by a fluid ocean. This is perhaps unsurprising, given the origin of ambient noise interferometry in time-distance helioseismic studies (Duvall Jr et al. 1993).

We note that the seismic profiles of other stars could quite easily be implemented, for example using models derived from stellar evolution simulations. Such efforts are unlikely to be of great relevance in the present time, given that most stellar disks are unresolved and hence asteroseismology observations are only sensitive to low-degree normal modes rather than ballistic wave propagation (Aerts et al. 2010). However, AxiSEM3D could in theory be used to compute changes to normal-mode spectra in the presence of strong 2D or 3D features such as rapid rotation or starspots. More practically, this ‘fluid sphere’ template may be of use in future planetary science explorations of acoustic

wave propagation in the atmospheres of giant planets, for example simulating pure acoustic waves from cometary or asteroid impacts similar to Shoemaker-Levy 9 on Jupiter in 1994 (Lognonné et al. 1994).

#### 4.4 Example 11: The Moon: diffusive wave propagation from strong scattering

Whilst there are some locations on Earth where seismic waves are strongly scattered, none comes close to the Moon in terms of global wavefield diffusivity (Dainty et al. 1974; Sato 2019). In fact, strong scattering is expected to occur on most planetary bodies, either from scattering within thick layers of regolith generated by meteoroid impacts or from inhomogeneities that are not well-mixed into background material in the absence of plate tectonics (Lognonné et al. 2020; Marusiak et al. 2022; Charalambous et al. 2025b).

Simulating geophysical scattering processes is challenging, especially in a planetary science context. They occur across a range of spatial scales, and the wavefields produced lie somewhere on a spectrum between fully ballistic and fully diffuse, whilst not uniquely constraining the geological scattering conditions which produced them (Eaton et al. 2024; Charalambous et al. 2025b). Previous work by Nissen-Meyer et al. (2019), Leng et al. (2020), Eaton et al. (2024), and Nunn et al. (2024) has demonstrated AxiSEM3D’s capability to simulate seismic scattering across a range of spatial and temporal scales, in both terrestrial and planetary contexts. The effects of volumetric scatter (from inhomogeneities) can be investigated either separately from, or in parallel with, the effects of purely geometric scattering (e.g. from strong topography on the surface or external interfaces).

AxiSEM3D is ideally suited to undertaking such suites of simulations, in which geometric and volumetric effects can be enabled and disabled at will without any requirement to re-mesh the computational domain (Leng et al. 2019). With careful choices of model geometry, multiple scattering regimes can even be investigated in a single simulation without the wavefields interfering with each other (Nissen-Meyer et al. 2019).

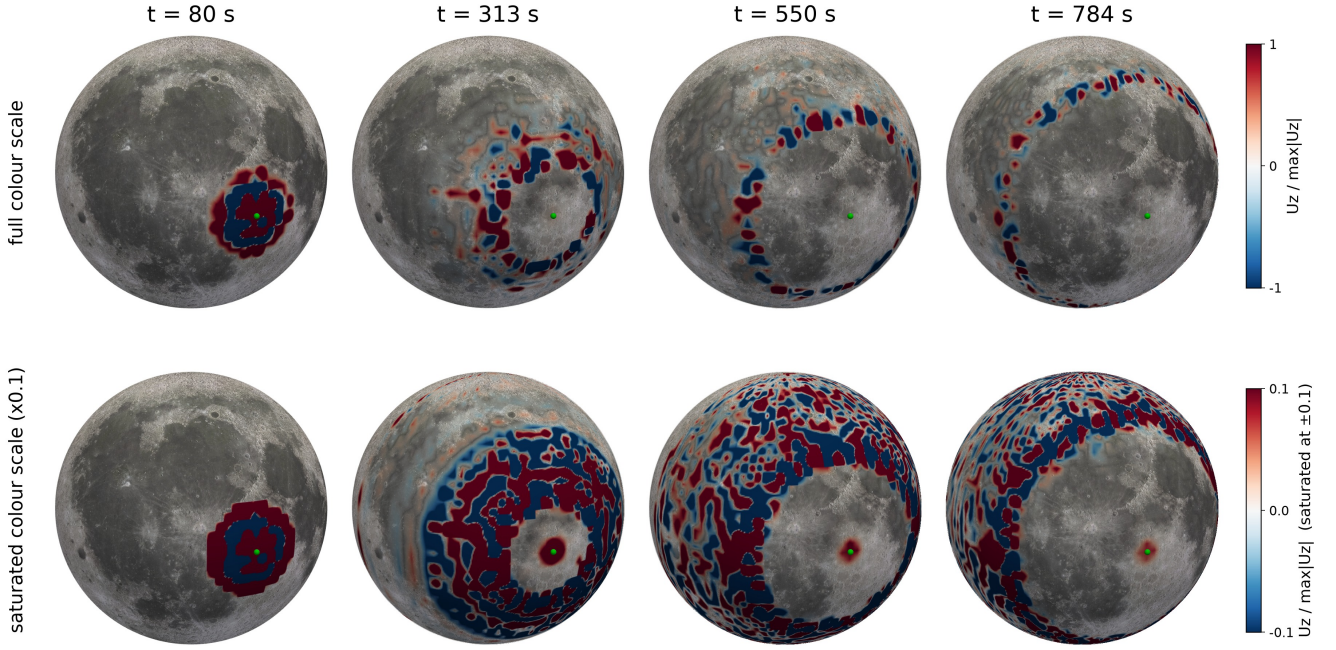
Fig. 9 shows a visualisation of the wavefield for an impact source on the Moon, using the ISSI\_MOON\_M1 background model of Garcia et al. (2019) and a scattering model derived from Nunn et al. (2024). This wavefield is less diffuse than would actually be expected on the Moon (retaining some surface wave character, as can be seen in the bright expanding ring in the lower row), but is chosen for visualisation purposes. The strong scattering traps some energy near the source location, where it reverberates for hundreds of seconds (as is actually seen on the Moon; Dainty et al. 1974).

A set of scripts to produce wavefield visualisations is also included with this example; the rendering requires a background image to be used, which here is from the Lunar Orbiter Laser Altimeter onboard NASA’s Lunar Reconnaissance Orbiter (Smith et al. 2010).

## 5 DISCUSSION

### 5.1 Performance

As with all methods designed for high-performance computing architectures, computational efficiency must be a goal. Detailed performance analyses of AxiSEM3D, including comparisons with other codes, are given by Leng et al. (2016) and Leng et al. (2019). As this release does not alter the numerical core, those analyses remain the appropriate reference for the code’s computational behaviour; indicative computational costs for the examples presented in this paper are given in Table 2.



**Figure 9.** Vertical surface displacement  $u_z$  on the Moon following a shallow impact (modelled here as an isotropic source at the green marker), from a high-resolution global simulation at a 2 s dominant period. Orthographic snapshots for four successive time steps ( $t = 80, 313, 550$  and  $784$  s, overlaid on lunar topography) show the wavefront expanding from the impact and sweeping across the surface, developing the complex, long-lived reverberating coda characteristic of lunar seismograms. Each snapshot is individually normalised ( $u_z / \max |u_z|$ ). Top: full colour scale; bottom row: same snapshots with a colour scale saturated at  $\pm 0.1 \max |u_z|$  to highlight the long-duration coda. Red and blue denote opposite signs of vertical motion.

Two developments would further improve efficiency but are not yet implemented: GPU acceleration, which would remove the main practical advantage currently held by GPU-enabled full-3D codes (Section 2.5); and localised time stepping, which would address the cost penalty imposed by thin, slow fluid layers such as oceans and atmospheres (Section 3.1). Both require re-writing substantial parts of the domain-decomposition and load-balancing routines and remain future work.

## 5.2 The AxiSEM3D community

AxiSEM3D is now part of the NSF-funded Computational Infrastructure for Geodynamics (CIG) code community, and its codebase remains entirely open source. Contributions from users and developers are welcome and encouraged, and the AxiSEM3D Manual is now hosted on Read the Docs rather than distributed as a PDF, so that new contributions are more straightforward to make and review. Development priorities and open issues are tracked on GitHub (<https://github.com/AxiSEMunity/AxiSEM3D/issues>), where flags demarcate longer-term development priorities from high-priority issues and indicate good starting projects for a new user wishing to contribute. Future open science workshops conducive to ‘hackathon’ style code development are also being planned.

## 5.3 Long-term outlook

At present, AxiSEM3D is a community-maintained code without any funded or dedicated developer effort. Our ongoing partnership with CIG offers stability and greater permanence; however, it is not a substitute for dedicated development and maintenance. AxiSEM3D, and its user community, would strongly benefit from dedicated funding to support code development, maintenance, and user training. Whilst the

authors intend to continue maintaining this code pro bono in the absence of longer-term funding, we encourage the wider computational seismology community to consider contributing to it, either directly or through the inclusion of developer time in grant applications.

## 6 CONCLUSIONS

We have presented a new version (`version 2.1`) of the AxiSEM3D spectral element-pseudospectral modelling method. A set of eleven examples and templates, with available code downloads, help to illustrate significant aspects of the code’s functionality. In its present implementation, AxiSEM3D is able to simulate seismic, acoustic, and seismoacoustic data at global, regional, and local scales in either cylindrical or Cartesian geometries. The physical effects included (a non-exhaustive list) are:

- Reflection, refraction, and diffraction (i.e., full-waveform effects that are not accurately captured by ray-tracing models),
- Heterogeneity, including undulation of surface or internal interfaces and localised alteration of seismic properties including wavespeeds and density,
- Attenuation, both intrinsic and scattering,
- Anisotropy, ranging from simple radial anisotropy to arbitrarily complex modification of the stiffness tensor,
- Ellipticity, which may be implemented either as a post-simulation coordinate transform (adjusting arrival times only) or a deformation of the spherical surface to an ellipsoidal one (adjusting arrival times and waveforms),
- Solid-fluid coupling at arbitrary interfaces, including the inner and outer core boundaries, the upper and lower edges of internal or surface oceans, and the atmosphere,
- Point- or finite-source energy injection, from simple multipolar injection of order 0-2 through to a kinematic description of a finite fault.

Those effects not presently built in include:

- Gravitation in any form,
- Rotation, though the indirect effects of rotation (ellipticity) are included, and
- Fluid inclusions or patched solid-fluid oceans, i.e. any feature requiring discontinuous internal interfaces.

In summary, AxiSEM3D `version 2.1` presents a unified, community-maintained release that consolidates a decade of individually benchmarked capabilities into a single, cross-compatible codebase. AxiSEM3D now supports fast and efficient computation of synthetic data for the Earth, Moon, and other worlds, including some functionality that cannot be replicated by other open-source methods on a 3D global scale.



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## DATA AVAILABILITY

AxiSEM3D is, and always will be, free and open source, released under an MIT licence with the developers as the copyright holders. The source code is available on GitHub (<https://github.com/AxiSEMunity>), alongside a stand-alone copy of the `salvus_mesh_lite` package and the `AxiSEM3D_example_gallery` repository ([https://github.com/AxiSEMunity/AxiSEM3D\\_example\\_gallery](https://github.com/AxiSEMunity/AxiSEM3D_example_gallery)) containing the higher-resolution templates used to produce the figures in this paper. The Computational Infrastructure for Geodynamics website (<https://geodynamics.org/resources/axisem3d>) hosts further useful resources, including a users’ discussion forum (<https://community.geodynamics.org/c/axisem/75>). A permanent archive (serving as a version of record) for this release is available on Zenodo at <https://doi.org/10.5281/zenodo.20142088>. A citation file for AxiSEM3D is available on GitHub; please cite the code as Leng et al. (2026).

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