This manual is a pre-print, non peer-reviewed copy of:

"AxiSEM3D - an introduction to using the code and its applications"

AxiSEM3D – an introduction to using the code and its applications

Benjamin Fernando[1,*], Jonathan Wolf[2], Kuangdai Leng[3], Tarje Nissen-Meyer[4], Will Eaton[5], Andrew Walker[7], Tim Craig[6], Jack Muir[7], Ceri Nunn[8], Maureen D. Long[2]

Abstract

Welcome to the wonderful world of AxiSEM3D, a flexible, high-performance computational method for solving the elastodynamic wave equation in three-dimensional, heterogeneous media. It has been used in seismology for the Earth, the Sun, the Moon, and many of other rocky planets and moons of the Solar System.

In this manual, we will explore the practicalities of using this code, touching on the mathematical aspects as relevant to the casual user, the input and output files, and pre- and post-processing.

This guide is not a replacement for any of the AxiSEM3D papers, which you will find listed in the next section. Nor does it go into any detail about how to install, build, configure, or make the code as these are dealt with in a separate installation guide. However, it does contain everything to do with the scientific aspects of the code and the user interface post-installation.

[*]Corresponding author

Email address: `bfernan9@jh.edu` (Benjamin Fernando)

[1]Department of Earth and Planetary Sciences, Johns Hopkins University, Baltimore, MD, USA

[2]Department of Earth and Planetary Sciences, Yale University, New Haven, CT, USA

[3]Rutherford Appleton Laboratories, UK

[4]Department of Mathematics and Statistics, University of Exeter, UK

[5]Department of Geosciences, Princeton University, NJ, USA

[6]School of Earth and Environment, University of Leeds, UK

[7]Department of Earth Sciences, University of Oxford, UK

[8]NASA Jet Propulsion Laboratory, California Institute of Technology, CA, USA

Version	Date	Comments
1.0	March 5, 2024	First online draft of manual
1.1	June 17, 2024	Edits to citation/document management

Table 1: Document history table

How to cite this manual:

Fernando, B., Wolf, J., Leng, K., Nissen-Meyer, T., Eaton, W., Walker, A., Craig, T.J., Muir, J., Nunn, C. and Long, M., 2024; EarthArXiv. AxiSEM3D-an introduction to using the code and its applications.

doi: `https://doi.org/10.31223/X5TH7P`

BibTeX:

```
@article{fernando2024axisem3d,
  title={AxiSEM3D-an introduction to using the code and its applications},
  author={Fernando, Benjamin and Wolf, Jonathan
  and Leng, Kuangdai and Nissen-Meyer, Tarje
  and Eaton, Will and Walker, Andrew
  and Craig, Timothy J and Muir, Jack and Nunn, Ceri},
  year={2024},
  url = {https://doi.org/10.31223/X5TH7P},
  doi = {10.31223/X5TH7P},
  publisher={EarthArXiv}}
```

1. First things first - should I be using AxiSEM3D?

The question of which modelling software you ought to be using probably has no definite or finite-length answer. However, the common pieces of software used for global wavefield simulations include SPECFEM (Komatitsch and Tromp, 2002a; Komatitsch and Tromp, 2002b), AxiSEM3D (Leng et al., 2016; 2019), and Salvus.

There are also normal-mode codes such as MINEOS which are very different in implementation and functionality to AxiSEM3D, SPECFEM, and Salvus (which are all spectral-element based codes), but nonetheless useful if you are looking at normal modes, gravity or ellipticity, and so on (Panning et al., 2017).

The advantage of AxiSEM3D over the other methods is its ability to undertake calculations at much higher frequencies, but this also comes with limitations on how complex a scenario you are able to simulate.

If you are interested in the global 5 s resolution wavefield in the presence of strong off-plane scattering, AxiSEM3D can do this where the other two could not, at least not with any reasonable resource usage. Likewise, if you want to look at how a planet's rotation or self-gravity from large seismic oscillations influence the normal-mode spectrum, AxiSEM3D is not for you.

Also, if you are planning to calculate global wavefields for simple 1D models at high frequencies such as PREM (Dziewonski and Anderson, 1981), AxiSEM3D is the most efficient way to do it.

If, on the other hand, you are interested in local-scale wavefields in coastal regions with mixed surface patches of ocean and land, AxiSEM3D is absolutely not the correct code to be using. Before undertaking any synthetic studies, it is worth deciding upon what functionality is important to you, and choosing accordingly.

Other factors worth bearing in mind is that in AxiSEM3D creating a mesh is trivially easy but creating a 3D model to superimpose on the mesh can be extremely challenging to do or indeed to debug. AxiSEM3D and SPECFEM also have the advantage that they are free and open-source, but therefore do not come with dedicated technical support. On the other hand, Salvus is proprietary and paid - so the technical support is commensurate with that.

2. A brief introduction into AxiSEM3D

AxiSEM3D *(Axisymmetric Spectral Element Method - 3D)* is a seismological modelling code which allows users to undertake simulations of wave propagation in complex, 3D environments.

It is based on AxiSEM (Nissen-Meyer et al., 2014), which could do '2.5D' propagation. Sometimes AxiSEM is referred to as 'old AxiSEM' to distinguish it from AxiSEM3D. AxiSEM is mostly deprecated/surpassed, except for a few relatively niche operations, we suggest new users start with AxiSEM3D instead.

2.1. Literature

It may be worth reviewing recent papers on AxiSEM3D theory and implementation before you begin using the code. In general, the level of detail presented in these papers is beyond what that the casual user needs to be familiar with, unless they plan on editing the source code or undertaking detailed comparison benchmarks to other methods.

- Nissen-Meyer et al. (2014): AxiSEM: broadband 3-D seismic wavefields in axisymmetric media (an introduction to the '2.5D' version of AxiSEM3D, known as AxiSEM).

- Leng et al. (2016): Efficient global wave propagation adapted to 3-D structural complexity: a pseudospectral/spectral-element approach (an introduction to the 3D version).

- Leng et al. (2019): AxiSEM3D: broad-band seismic wavefields in 3-D global earth models with undulating discontinuities (an extension to the 3D version from the 2016 paper including details of boundary undulations, etc).

- Fernando et al. (2020): Oceanic high-frequency global seismic wave propagation with realistic bathymetry (the 3D version extended to include a treatment of oceans).

- Nissen-Meyer et al. (2019): Extends Fernando et al. (2020) to propagation with sources in fluid layers and an absorbing rather than reflecting outermost boundary.

- Szenicer et al. (2020): A complexity-driven framework for waveform tomography with discrete adjoints.

- Haindl et al. (2021): A 3D complexity-adaptive approach to explore sparsity in elastic wave propagation (more on the local/regional scale methods of AxiSEM3D).

2.2. Physical and mathematical background

The mathematical background to the AxiSEM3D method is rather complex, but a brief summary might prove useful.

In short, AxiSEM3D solves the 3D equations of motion (which describe the propagation of seismic waves) using a spectral element-pseudospectral method. What this means is that the in-plane parts of the solution are found through one method (spectral methods), whilst the azimuthal (i.e., longitudinal) solutions are found through another (pseudospectral methods).

This may seem like an unusual way to do things, given that the azimuthal solution follows exactly the same physics as the radial and meridional parts. However, what it does let us do is simplify the problem considerably, and hence save on computational cost.

The reason for this is that seismic properties in the Earth vary much more slowly laterally (i.e., in latitude and longitude) than they do radially (i.e in and out toward and from the core). This means that the wavefield is much smoother (less complex) laterally, and is therefore simpler to compute. Of course, the lateral gradients in density and sound speed are not unimportant – so we need to account for them somehow – but equally they are unlikely to cause as much of a challenge from a computational perspective.

In mathematics, it is often common to represent complex functions by series – for example, the Taylor Series of $\sin(x)$ can be truncated and used as an approximation. In 3D seismology, we can do a Fourier expansion of the wavefield in the azimuthal direction, and choose how many terms we have in our Fourier series depending on how complex the azimuthal wavefield is. This is just like adjusting the approximation of $\sin(x)$ depending on how accurate we want the solution to be: sometimes $\sin(x) = x$ is appropriate, sometimes we need $\sin(x) = x - \frac{x}{3!}$ is fine, and sometimes we need more terms.

This is how AxiSEM3D works: it turns out a Fourier order of 0 is sufficient for a radially symmetric ('1D') seismic profile with an implosive/explosive source, 1 is sufficient for a dipole, and 2 for a quadrupole (second rank moment tensor). If we want to have a non-1D model, such as Crust 1.0,

we simply increase the Fourier order. How much to increase it by is a non-trivial question and depends on the simulation in question, but a few hundred to a few thousand is common in simulations we have run.

2.3. Meshes

- See here details of the mesher used by AxiSEM3D, called 'salvus mesher lite': https://gitlab.com/Salvus/SalvusMeshLite.

- The installation page for AxiSEM3D here also contains an excellent section on the mesher: https://github.com/AxiSEMunity/AxiSEM3D/wiki/mesher.

In general, you have a choice between cartesian (box-shaped) meshes, and D-shaped (semi-circular) meshes. These obviously solve for the same physics; and you can actually adapt the cartesian simulation to account for the curvature of the Earth's surface (to move from local to regional scales) or reduce the D-shaped mesh to a wedge-shaped mesh (to move from global to regional scales).

It is worth bearing in mind that unless you use a full D-shaped (i.e., 180°/full semi-circle) mesh, you need to think about the 'false' boundaries that you impose at the edges of your box or wedge. There is more on this in the mesher description in Haindl et al. (2021), but in short you can use an absorbing or reflecting boundary. In the former case you have a few options depending on what you need, the latter is far simpler and somewhat cheaper but will also contaminate your seismograms with reflections from the edge of the box if you let the simulation run on for too long.

2.4. Physical Constraints

When designing AxiSEM3D simulations, or running them, it is worth bearing in mind what the limitations of the code are and what they might mean for this project. We will briefly detail those relevant here:

2.4.1. Boundary conditions

These need to be consistent along the outer surface. What this means is that you cannot have arbitrarily alternating patches of solid and fluid boundaries (ocean/land), or alternating bits of absorbing and reflecting – at least at the moment. Instead, your boundary condition needs to be the same across the length of any azimuth.

Note that we have worded this rather carefully: it should, in theory, be possible to create a 'part-ocean' Earth, where the ocean occupies a 'trench' in a ring around the planet (imagine excavating everything between 10° N and 20° N to a depth of 3 km, and filling it with water). This might be useful if you are interested in things like quakes at subduction zones or mid ocean ridges – but you would have to edit the mesh file manually in python, and we have not tried this. It should not be too difficult though. If you try this, take care with the geometry: you will need to rotate your crustal models and source-receiver pair to represent the angles correctly.

If the previous paragraph seems unnecessarily complicated, you can (and probably might want to?) stick to using an all-solid or all-fluid boundary condition. If you need to, you can account for the weight of the water column in a non-uniform way across the whole surface using the 'ocean load approximation' or by deforming the physical water layer as described in the particle relabelling section below.

2.4.2. Discontinuities

AxiSEM3D allows you to insert any discontinuity you might want into your 'base' (1D) structural model: the Moho, the CMB, 410/660 km, the seafloor, etc. You can also undulate these boundaries (see manual/Leng et al., 2019/Fernando et al., 2020) to represent the variation in depth of a particular boundary with location.

However, this undulation remains subject to a very important constraint - the undulated configuration must remain homeomorphic to the original, non-undulated one. This is a fancy way of saying that all boundaries must remain smooth and well-defined – the Moho cannot jump from 8 km depth to 15 km depth at a plate boundary (for example), unless you smooth this transition out across some number of elements. Similarly, you cannot have two Mohos at different depths beneath a particular point on the surface.

This is not normally important on a global scale, as you would not resolve a subduction zone finely enough for these details to be important. In the case of some projects (e.g., simulating a subducting slab), it might be important – and you may have to think carefully about how to incorporate the correct Moho (or seafloor) configuration.

2.5. More on undulation

In regard to the above point, it is also worth briefly touching upon some challenges associated with undulating boundaries in the cases where they are strongly varying, such as those we will consider here.

Particle relabelling (the process through which boundaries are undulated) always increases the computational cost of simulations – the main reason for this is the extra floating-point computations which need to be undertaken.

Another potential reason for the added cost is a decrease in the minimum element size. For example, if you have a uniform 8 km depth Moho, and deform it such that in places it is only 5 km beneath the surface, remember that elements cannot be added or removed, only stretched or shrunk. As the elements get smaller, the minimum timestep required for stability will also decrease.

The timestep in AxiSEM3D is globally set by the lowest timestep in the whole model. This means that if the element with the smallest global timestep shrinks, the global timestep also goes down - and the overall cost of the whole simulation increases by at least the same fraction.

Adding in multiple undulating boundaries (e.g., a seafloor and a Moho) normally further increases the computational cost – but not always. If the smallest timestep is set in a particular single element (which will be the case if you also have a 3D structural model overlaid, like crust 1.0), and that element ends up being stretched because the Moho moves down and the seafloor goes up, this will actually decrease the cost. Whether or not this will happen in your particular case is impossible to determine – it very much depends on the models, undulations, and periods you are using – but it is worth thinking about!

One potential problem that you should bear in mind is that discontinuities can never cross. If you do not get any unexpected errors related to the undulations you can ignore this point, but if you do, it is worth a check. This issue may be most prominent in trenches, where the seafloor dips steeply toward the Moho's position. In reality the two never cross, but when the code interpolates crustal and bathymetry model they may artificially do so – especially if you have rescaled the bathymetry to ensure that all land areas are underwater for the purposes of an AxiSEM3D simulation. If this is an

issue, you can either just change the bathymetry rescaling, or possibly go to a higher frequency (more elements means a finer sampling of the models and ought solve the issue).

We will come back to some of the challenges associated with debugging the implementation of undulating interfaces later, but for now it is sufficient to remember that the deformation of each element from the spherical configuration to the 3D one can be described using the transformation's Jacobian. Things get unstable when the Jacobian becomes negative or otherwise badly behaved; physically this corresponds to elements doing things that they should not be doing (becoming overly stretched, crossing into other elements, etc).

2.6. Cost and resolution

In any seismic simulation, the resolution (seismic period) that you choose is obviously crucial. Higher frequencies are more computationally intensive, though if you choose a smaller domain you can of course go to a higher frequency for the same cost.

In general, simulation cost in AxiSEM3D scales with roughly the third power of the frequency: i.e., increasing to 5 s period from 10 s will increase the cost by a factor of 2^3, or 8.

One positive is that AxiSEM3D's efficiency over other codes grows as you get to higher frequencies, as most comparable method (e.g., SPECFEM3D) scale roughly with the fourth power of the frequency. The extra computational burden of slow velocity layers (including an ocean) is also less as a fraction of total run time at higher frequencies – in short, although the overall cost is higher, so is the efficiency.

3. Code Capabilities

The capabilities of AxiSEM3D have been detailed extensively in the papers published about it. We briefly re-iterate them here (so that they are all in one place), but also emphasise the things that the code **cannot** do especially things that we have thought about implementing at some point or another. Largely, we do this so that others can build upon this work if they so fancy.

3.1. Things the code can do

These include:

- Solve the elastodynamic equations of motion via the weak form of the wave equation for arbitrarily complex 3D media (subject to some boundary condition constraints),

- Do this for both solid-fluid coupled bodies, fully solid worlds, and fully fluid ones (e.g. stars),

- Account for the oblateness of objects, either directly through mesh deformation or through post-simulation corrections,

- Implement a variety of relevant physical processes, including but not limited to seismic attenuation, scattering, arbitrary seismic anisotropy

- Represent a variety of relevant physical processes, including but not limited to wave reflection, refraction, diffraction, and dispersion,

- Simulate source processes of both infinitesimal and finite size, and

- Generate full-waveform sensitivity kernels.

3.2. Things the code cannot do

These include the following physical features:

- **Patched surface boundary conditions** – These would allow you to simulate a planet where the surface boundary condition is not the same everywhere, without having to implement fudges like having a thin layer of water over the continents. To do this, you would need to re-write the code with localised rather than global basis functions.

- **Local timestepping** - potentially a big time saver!

The code also does not currently include the following physical effects:

- **Rotation** is not currently implemented in AxiSEM3D, however this is not expected to be particularly difficult. A simple Coriolis term should allow for accurate inclusion of rotational effects, though this is not a particular priority as the effects of rotation on high-frequency waves is expected to be small.

- **Magnetic fields** - their influence upon the solar mode spectrum is not well constrained. It may be possible, though certainly very challenging, to build some treatment of the linearised MHD equations into our model.

- **Gravity** - see note below.

3.2.1. Self-gravitation

We thought about gravity in AxiSEM3D quite a bit more, specifically self-gravity. We eventually decided not to implement it, but a potential cost-saving approach is described in this section.

The "Cowling approximation" Cowling (1941) proposes that the changes in gravitational potential induced in a body by the passage of a seismic wave through it are negligible, and hence can be ignored in forward modelling. Although this assumption holds for most terrestrial seismology applications, it is inappropriate for the Sun, where changes in potential can be quite significant, in addition to long-period seismology ($\geq \sim 10^2$ s).

However, most models continue to ignore the effects of this "self-gravitation" (or indeed all gravitational terms generally) due to how computationally expensive considering it can be. This comes about because the perturbations to the Poisson equation, which describes the Newtonian gravitational potential ϕ in terms of the mass density ρ:

$$\nabla^2 \phi = 4\pi G \rho \tag{1}$$

are felt everywhere instantaneously. Furthermore, there exists a coupling such that feedback from wave propagation affects the local gravitational potential, which in turn further changes the wave propagation, and so on. This means that the Poisson equation must be solved on every element at every timestep, which on similar spectral element codes (such as SPECFEM) reduces the efficiency of the code substantially. A second major challenge occurs due to meshing, since the gravitational potential is defined in all of space and has a Dirichlet boundary condition defined at an infinite distance from the model. The reader is referred to publications such as Chaljub and Valette (2004), van Driel et al. (2021), and Gharti et al. (2023) for current methods to overcome this on spectral-element meshes. However, it has recently been proposed a formulation of the Poisson equation derived from the Einstein

Field Equations Hirai et al. (2016) may be significantly faster to implement, as the solutions are wave-like and hence inherently local. The potential ϕ is here expressed as the sum of propagating and static terms:

$$-\frac{1}{c_g^2}\frac{\partial^2 \phi}{\partial t^2} + \nabla^2 \phi = 4\pi G\rho \qquad (2)$$

where c_g is the propagation speed. Physically, this speed is the speed of light (c), as this is the velocity at which gravitational effects propagate. However, it has been suggested that using a speed that is significantly slower than c but still faster than other relevant timescales (in our case, seismic) is appropriate. This has the advantage of localising the effects of self-gravity, such that the Poisson equation does not have to be solved at every timestep on every element.

The question is of course what minimum propagation speed c_g needs to be used in order to yield physically meaningful results, as a slower propagation speed permits longer computational timesteps to be used, hence speeding up the simulation. One proposal is that the arrival of the propagating potential at any element only needs to occur a minimum of one seismic period before the arrival of the first acoustic waves. If successfully implemented, this would to our knowledge be the first use of propagating gravity in seismology.

4. Credits

This manual is a community effort which has been compiled by AxiSEM3D code users in their own time.

We welcome contributions from the community, especially if you think there is content which could be clearer or needs adding to this manual. Please also note that the community-orientated status of this manual means that we cannot claim that it is complete, comprehensive, or free of all errors.

If you wish to cite AxiSEM3D, you should cite the relevant papers as detailed in the 'Literature' section. **If you have found this manual useful, please feel free to cite it too, to increase awareness that it exists.** The citation is:

AxiSEM3D - an introduction to the code and its applications Fernando, B., Wolf, J., Leng, K., Nissen-Meyer, T., Eaton, W., Styczinski, M., Walker, A., Craig, T., Muir, J., Nunn, C., and Long, M. D. *(2024)*.

5. Installing the code

This is dealt with in a separate manual, called "II. Installation Guide" which you can find on the GitHub under "install" on the Master branch.

We suggest that you read through this manual as well before you start the install process to make sure that you are aware of what the code can do, what it cannot do, and the relative challenges of doing different kinds of simulations.

There are also configuration scripts in the "Install" folder which we have prepared for the most commonly used machines. We will try and keep these up to date, but you will probably need to adjust the package versions in these files from time to time.

Note that it is not our aim to merge the installation guide into this manual. This manual is focussed on science usage, and should not be regularly updated except when newe functionality is added to the code. Conversely, we hope to keep the configuration scripts up to date when we are aware that packages are being superceded on HPC systems.

6. Changing the input files (1D, global models)

In order to explore problems of geophysical interest, you are going to need to change the input files. There are many options available to you and most of them do not need to be edited. We will cover some of the main ones. If you open the input folder, you will see the following files/folders:

```
inparam.advanced.yaml
inparam.model.yaml
inparam.nr.yaml
inparam.output.yaml
inparam.source.yaml
GSN.txt (also USArray.txt, but you can delete the latter)
```

Note that the .yaml suffix just denotes the file type – the files are human-readable.

6.1. inparam.advanced.yaml

It is unlikely that you will need to change anything in this file, as the options are quite technical and likely of limited interest to the casual user. The one possible exception is *max_num_time_steps* which you can set to 1 or 10 or something similar if you want to make sure that the code will at least run through a small number of timesteps without becoming unstable.

6.2. inparam.model.yaml

This is probably the folder that you will spend the most time editing. exodus_mesh: should be the path to the mesh that you want to use, ending in ".e".

For the purposes of this project you are unlikely to need to change the geodesy inputs, nor the absorbing boundary inputs (unless you start using mesh 'chunks', more on these later).

Attenuation does what it says on the tin: setting it to CG4 or Full will enable a simple linear attenuation model.

6.3. inparam.nr.yaml

This file is only really relevant for when you start including 3D models. In 1D, in a limited set of cases, and if you are really pushed for computational resources, you can make a tiny saving by setting *type_Nr* as *CONSTANT* and equal to *3* (if you're only using a point force/dipole source) or *1* if you're using a monopolar (isotropic pressure) source instead of the standard *5*.

6.4. inparam.output.yaml

Here, you need to set the station(s) that you want the displacement or velocity recorded at. *list_of_station_groups* can take as many networks (groups of stations) as you want.

We tend to keep *global_seismic_network_GSN* as it is a useful set of stations all around the world with good data, for testing purposes. If you are doing something specific though, like array beamforming, you will want to add your own networks too.

station_file is the name of the text file within the /input folder that contains the station coordinates. Subsequent options like *horizontal_x1_x2* and *vertical_x3* set what the columns in the *station_file* text file correspond to. For the GSN, these are *LATITUDE_LONGITUDE* and *DEPTH* (so in your file GSN.txt, the columns are *name, network, latitude, longitude, elevation, depth* – note that elevation is not used in AxiSEM3D but it is there so that you can swap files with SPECFEM).

You also need to set the output coordinates using *coordinate_frame* and *channels*. We suggest that you leave these as *RTZ* and [U] (where [U] = [U1, U2, U3]) for our purposes.

The big choice that you need to make is whether to save your outputs as text files (*ASCII_STATION* or *ASCII_CHANNEL* depending on what you're doing), or netcdf files (netcdf). netcdf is a lot more efficient, but a little harder to use, especially if you are not used to the file type before. ASCII has the advantage that you can just open the output and look at whether it makes sense (if the ground velocity is 10e10 m/s after 10 seconds, it is probably wrong. . .) but it is a lot less space-efficient.

In the processing examples we will stick to ASCII for ease of use but if you are doing more complex runs or lots of them we would suggest using netcdf.

6.5. inparam.source.yaml

This file does not change whether you are working in 1D or 3D, so it is important to get to grips with it.

time_axis does pretty much what it says on the tin. The default *courant_number* of *1.0* is very unlikely to be stable: start with something like *0.6* and increase once you know it is working.

list_of_sources is also important. The key that you use is arbitrary – name it what you like, we normally use the CMT Catalogue designator for the earthquake in question.

For these sorts of computations, it is worth sticking to *latitude_longitude*, remembering that the north and east is positive. *depth* is in metres – this is important!

The *ellipticity* correction is easy to change and makes little difference unless you need very exact arrival times.

We will come back to *depth_below_solid_surface* and *undulated_geometry* in the 3D models section.

You are most likely to use the *mechanism: type: MOMENT_TENSOR*, in which case you should input the *data* as the components of the moment tensor in the order given by CMTSOLUTION. Remember that CMT uses the non-SI unit of dyne-cm, so you need to add a correction factor by setting *unit* to *1e-7* to turn this into N-m.

For most purposes (seismogram generation) you can do everything involving the source-time function after the simulation is complete in post-processing. In this case, set *half_duration* to *0.0* and the code will make the width of the STF something like 5x the timestep (much less than the mesh period, i.e. a delta function). Note that in a model like this this is as good as you are going to get – the half-duration cannot be exactly 0.00000, but the difference is miniscule and irrelevant. Leave *class_name* as *GaussianSTF* and *use_derivative_integral* as either *ERF* or *GAUSSIAN* depending on whether you want displacement or velocity output. We will come back to how to process the output in a later section.

If you are doing something like wavefield visualisation, then you need to set the STF before you do the simulation. In that case, you can set the half-duration and decay factor as you want, or use *netcdf_STF* or *STREAM_STF* (netcdf vs. ASCII - more on this later) to read in a particular source-time function that you want to use, for example one downloaded from SCARDEC.

A general note of caution: although you can use any STF you want for seismogram generation, and then deconvolve it out before reconvolving with a new STF, we find that this is rarely a sensible option as it ends up producing numerical artefacts. If you are not sure what STF to use, use a delta function (as described above) and deal with it later.

7. 3D models part I – creating and understanding models

There are two parts to using the full 3D functionality in the code: the input files and the model files themselves. There are two kinds of model files in AxiSEM3D: geometric and volumetric.

7.1. Geometric models

Geometric models are those that take a specific boundary (discontinuity), and deform/undulate it is no longer spherically symmetric with respect to the planet's centre. The discontinuities you are most likely to undulate are probably the surface or seafloor, the Moho, and the CMB; though in principle you can create a boundary wherever you like and undulate it.

If you like, you can think of a geometric model as taking a 2D surface embedded within the Earth and moving it inward out outward radially, with the degree of stretching or shrinking depending on where on the globe you are.

As such, the geometric model files are not too complicated, as they consist of three coordinates: a series of latitude and longitude points (together forming a geometric grid), and a third variable defining the position of the boundary at each point on the grid. The third variable is either a depth or a radius (which you use depends on the boundary: radius may make more sense for the surface and depth for the Moho.

Crucially (and in both cases), the depth and radius are given with respect to the boundary's depth or radius in the 1D case. Note that the undulations on a particular boundary are given as depth/radii with respect to the boundary in question itself. This means that an undulation of 1 km on either the Moho or the surface is given in your model file as +1000 at that particular point, not 6372000, 6372, or anything else. In the input files you set which interface this is in reference to, e.g., 6371 km km radius (or 0 km depth) for the surface. So if you are using PREM and have a Moho undulation dataset where the Moho's point at each point on the sphere is expressed as a depth below the surface, you probably need to subtract 24.4 km from it, because that is the PREM Moho depth.

As an illustrative but pointless example, if you created a 3D geometric model file for the Earth's surface but wanted the surface to be totally flat, you would have a series of latitude and longitude points ($-90°$ to $90°$ and $-180°$ to $180°$) respectively, and the third variable would be an array of zeros (meaning no change in either direction from the surface position in the 1D case). If you were doing the same for the Moho, the array would be completely identical (all zeroes in the third variable) – it would be in the input file that you specify which boundary you are deforming.

Obviously the number of depth/radius points in your 3D model must match the number of latitude/longitude gridpoints you have. If you sample latitude and longitude each at a spacing of 1°, that gives you 180×360 gridpoints, each of which must have a value for the surface elevation or depth. You can choose the spacing that you want: 1° is probably fine for most things.

7.1.1. Creating new geometric models

The base structure for global scale, 3D geometric models is included in Ben's AxiSEM3D GitHub repository (we should move it to the main one at some point, but you can find it here: `https://github.com/benjaminfernando/axisem3d-3dmodels/tree/main`). In short we have created two python files ("etop01.py" and "moho.py") which can be used to create and edit topographic surface and moho geometric models.

Crust 1.0 Moho:

- The Crust 1.0 Moho is sampled at 1° intervals (Figure 1), and generally you will not need to resample this as the frequency changes. Certainly you cannot get to anything less than 1° resolution, as this is as good as the data gets!

- Some of the strongest gradients in Crust 1.0's Moho are at the western edge of South America. Obviously this is not simply a coincidence - there is a good physical reason for it! Unfortunately, it does mean that the Moho and the seafloor/Earth's surface end up being quite close to each other. This both shrinks elements (making timesteps small, and cost expensive), and risks the boundaries interpolating into each other (which stops the interfaces being conformal, and breaks the code).

ETOP01:

- ETOP01 is a global topographic/bathymetric model (Figure 2) that is sampled at 1-arcminute resolution.

- 1 minute sampling is very much overkill for most projects, and is not feasible due to the amount of memory to store a model of this size. It should be downsampled to something more like 1 degree. If you want a more accurate determinant of how to downsample it, you can calculate the minimum resolved seismic wavelength at a particular period, and use a sampling which is at least as fine as this. Remember that as the period of the simulations you are running decreases (i.e., as the

frequency increases), the waves become sensitive to smaller and smaller spatial structures, so you can get away with less downsampling.

- The strongest gradients in ETOP01 (by quite some margin) are also off the west coast of South America, where the Andes meet the coast and the subduction trench. We'll come back to the errors that this can cause later, but you can get around some of it by applying some smoothing.

The python scripts available in the GitHub repository are able to write your Moho and topographic models to a format that will be read by AxiSEM3D. We assume some familiarity with python and that you are able to run the functions given and are aware of how they pass outputs to one another using return.

You are not obliged to use these scripts by any means, but they are designed such that the file structures, variable names, and sampling all match the template input files provided. If you have your own model which is in a similar gridded format and you want to convert it into something you can use, you should just be able to read in the filenames and use the same functions in the python scripts to write the output. It is always worth re-reading in a new model that you have created and then plotting it to make sure that it is doing what you think it is doing.

Crust 1.0 Moho: Let us start with the Crust 1.0 Moho (Figure 1) script because it is somewhat simpler to understand. The script is called "moho.py" and takes as input a grid file (.xyz) called "depthtomoho.xyz" which is a list of latitudes, longitudes, and moho depths at each pair therein.

The first function, load_moho_data, takes the input file and uses a series of numpy functions to split it, for simplicity we have only actually kept the 3rd column ([2] in python) which is the depths, and re-created the latitude and longitude from scratch. Make sure that the coordinates are sorted in ascending order (-90° to 90°, -180° to 180°) or else the code will not like it.

The second function, write_data_to_netcdf_file, writes the inputs of the above function to a netcdf file. If you have not come across netcdf files before it is worth looking them up, they are basically a highly efficient way of storing data. Unlike ASCII files you don't need to worry about pairing up the points correctly, within each file is a header called 'latitude' (similarly for the other

variables) which contains the points you have created.

There are a few stages to writing your new model file into netcdf format. First you need to create the file using Dataset (a method in the python netcdf4 module), and then create the three dimensions. You can specify the length of each dimension (latitude being 180 points, longitude being 360), or set this to 0 to allow them to grow as needed.

Then, you need to create the variable spaces to go with the dimensions you have created, and specify that the values will be floating point numbers ('d'). Finally, you add the actual points into the variable fields. Make sure that the units match, add corrections for metres to kilometres or vice versa if needed.

Note that if at any point you get errors about not being able to open a file, that is probably because it is already open. You just need to close it before opening it again.

Finally, read_data_from_netcdf_file allows you to just reload, and if you want to, plot (*set plot=True*) the saved netcdf file to check that it looks like what you think it should look like.

Using the ETOP01 script is slightly more complicated than using the Moho one, because you need to downsample (and possibly also average or smooth) the topography from the raw file that you download for the reasons that we already discussed.

The functions in "etop01.py" are similar to those in "moho.py" but with a few of additions. When you read in the raw model, there are two things that you can do to it:

- Average: average across n datapoints to produce a new topographic model.

- Filter: smooth the gradients in the new topographic model out using a gaussian filter.

If this seems confusing, consider that **average** basically means that you take a set of n by n points in the original 1-arcminute resolution model and represent their average as a single point in your new topographic model that AxiSEM3D is going to use. Choosing how big n is allows you to choose how fine your new model is (larger n = coarser model because a larger area is
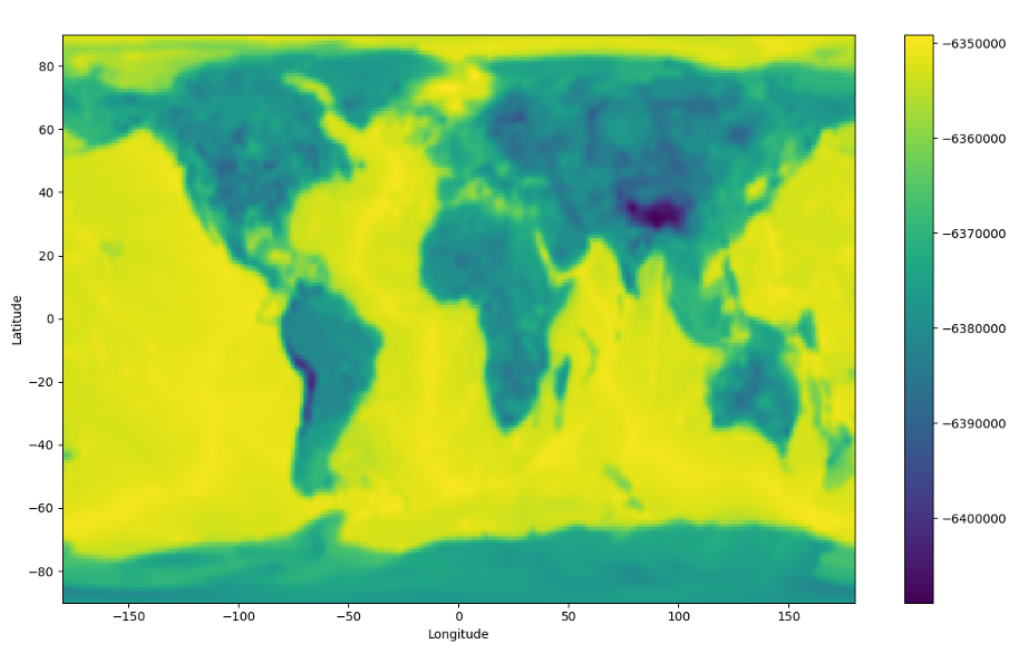
Figure 1: Crust 1.0 Moho undulation as a function of latitude and longitude. This plot shows the model with 1° smoothing, sampled at 1°. For more details on the radial coordinates used, see below. Note that even with 1° smoothing, there are still strong gradients in Moho depth off the west coast of South America. We suspect that this area (or somewhere like it elsewhere in the world) is the cause of many issues.

being represented by a single new elevation point). Once you have your new model you can further smooth the gradients in it by applying a 2D filter (like a blurring filter on Instagram).

The default sampling that we have chosen for the new 3D model is 1°, to match what is used for the Moho. If you want to change this it is relatively straightforward, just edit the relevant functions in "etop01.py".

Rather than just simply choosing the midpoint of every 1×1° cell you instead take the arithmetic mean of each 1×1 arcminute cell within it to create your new elevation point, as per method 1). This naturally averages out extremes in your new model, and makes it less likely that the Jacobian will be badly behaved. We can get this to work for around 10 s period global runs, but not 5 s. This is probably because some of the gradients are still too large to be stably interpolated by AxiSEM3D. The issue is likely off the coast of South

America, where a trench and an altiplano are found in close proximity. If you are doing regional-scale runs away from this area that might solve the issue, but in the more general case, you need to use 2): a **filter**.

Starting with 1) – an average across each $1 \times 1°$ degree cell – the copy of ETOP01 provided in these files is then filtered using 2): a 2D 1° degree standard deviation Gaussian (Figure 2). In effect, this treats the output array from the averaging as an image and applies a slight blurring filter; or technically a 2D convolution with a Gaussian kernel.
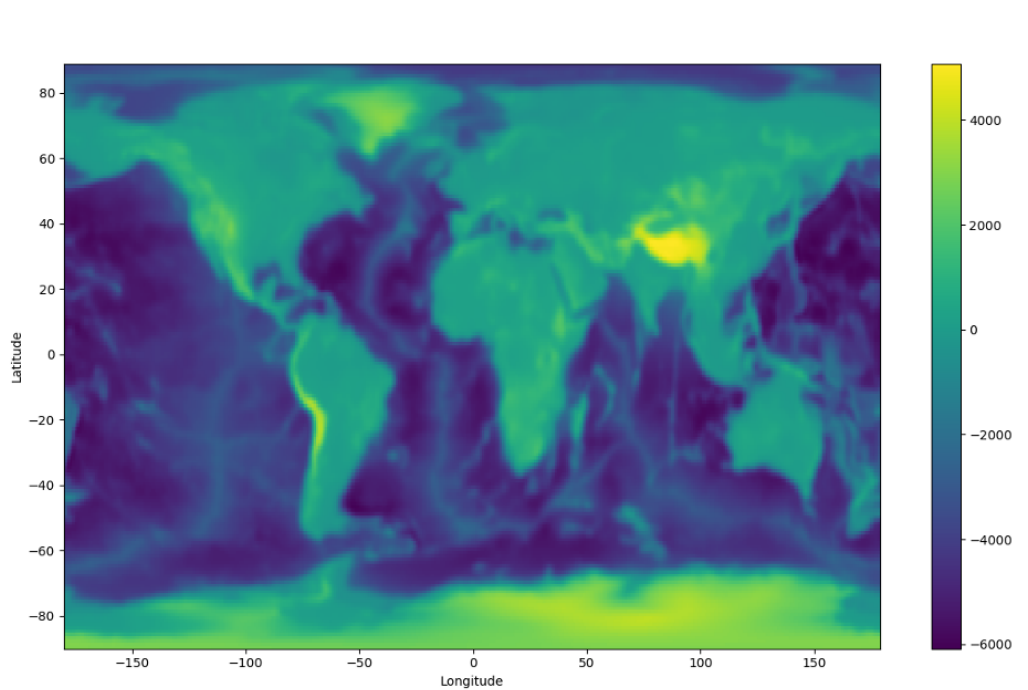

Figure 2: ETOP01, sampled at 1° and smoothed using a 1° sigma Gaussian. Again, note that the strongest gradients in topography are at the same locations as the strongest gradients in Moho undulation, i.e. at the western edge of South America.

This simply smooths out some of the largest gradients in averaged array. You can choose how much smoothing happens by changing the value of *sigma* in filter_data. The default is 1°, reducing this toward zero makes the Gaussian kernel steeper and narrower and reduces the degree of blurring (in the limit of a zero standard deviation, the original image is returned). Similarly if you still get an error, you can increase the standard deviation which smooths out

even more of the gradients. Note that you do not need to pass the units of *sigma* to the code, it does this in terms of sampling points (i.e., *1* ends up being 1° because there are 180 × 360 points, i.e. one per degree). If you do edit the python script to change the sampling, make sure the units of sigma are also changed to match.

Note that there are potentially some issues associated with switching from grid-centred to cell-centred systems at the poles – see the "moho.py" file for some comments on this topic.

7.2. Volumetric models

Volumetric models are those which change the seismic properties of mesh elements not at interfaces: for example, decreasing Vs in a particular region to represent a region of partial melt.

In AxiSEM3D, you can alter multiple parameters at any point in the mesh, for example Vp, Vs, density, or the elastic tensor C_{ij}. The volumetric models are like the geometric ones in structure, but rather than there being two spatial dimensions there are three (latitude, longitude, and radius/depth).

Volumetric models require the production of a netcdf dataset file (.nc) which can be done using your favourite coding language such as MATLAB or Python. It is important to remember that these two languages save multidimensional arrays in column-major and row-major formats respectively, by default, but more on that later. If you are unfamiliar with netcdf files we would recommend reading: `https://towardsdatascience.com/create-netcdf-files-with-python-1d86829127dd`.

AxiSEM3D incorporates 3D models by rotating the 1D mesh around its axis, forming a cylinder (or sphere if using a D-shaped mesh). Any parts of the 3D model that are within that cylinder will then be incorporated into the overall 3D model that AxiSEM3D uses (Figure 3). Figure 3 shows a mesh rotating around a source-centred axis. The 3D input model is shown by a blue cuboid. Any part of this input model that is within the teal cylinder is sampled. So, how do we create this 3D model shown in the blue box?

The netcdf file holding the 3D model needs to contain multiple variables, which can contain information about, for example, x, y, z (or equivalently, depth); Vp, Vs, density, or the elastic tensor C_{ij} – though you do not need to change all of these from the 1D values if you do not want to.
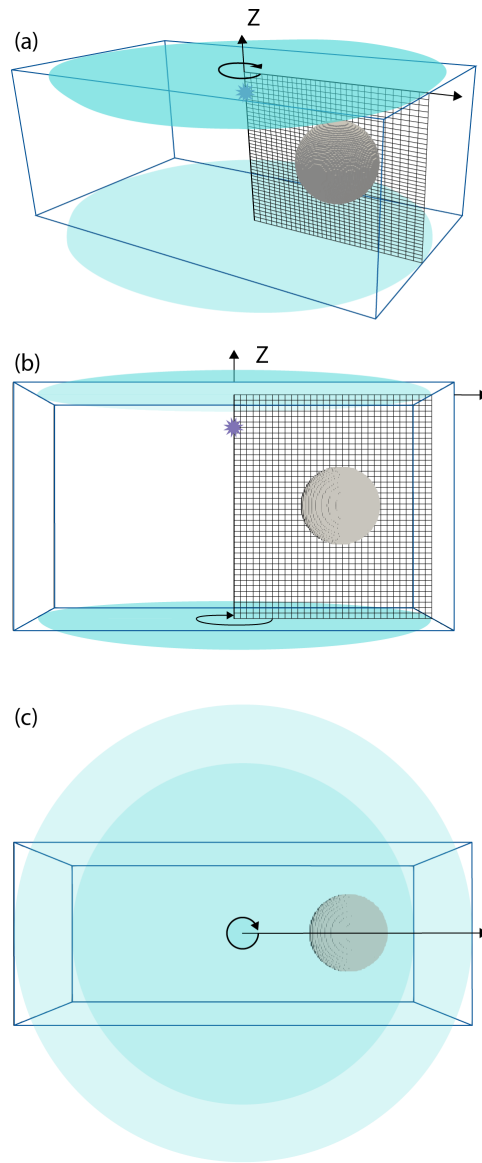
Figure 3: Mesh rotating (green arrow) around a source-centred (source: violet star) axis to incorporate 3D perturbation. Side (a, b) and top (c) views are shown. The 3D input model is the cuboid marked by blue lines. This model a 0 valued perturbation except in the sphere region which is displayed. The mesh is rotated about its source-centred axis to produce a cylinder. Any part of this 3D input model that is within the cylinder (teal) is sampled and incorporated into the mesh values used by the solver.

Note that the names of these variables within the .nc file do not matter. This is because you will specify what you have named them using the variables *nc_variables* (for x, y, z) and the variable factor for each of the properties, for example *VP*, *VS*, and *RHO*. As long as the names are consistent, then all is good!

The .nc file will also need to have three dimensions. These need to be the dimension of the x, y and z array variables, i.e. the variable has a defined and specific value at each point in the grid. Each of the location variables x, y, and z (or depth) have a single dimension. Each of the parameter variables, for example *VP*, *VS*, and *RHO*, will have three dimensions (corresponding to the dimensions x, y, z). To see this in action, you can load the .nc file provided in Example 3 (see template folders in main AxiSEM3D GitHub), and load it into python using:

```
import netcdf4 as nc
data = nc.Dataset("path/to/file/SEG_C3_SOLID.nc")
print(data)
```

In doing this, you will see the 6 variables in which x, y, and depth are 1D; while *VP*, *VS*, and *RHO* are 3D. The x, y, z variables are simply an array of coordinates for the limits of your model, e.g with x going from -5062.5 km to $+5062.5$ km with 676 elements. You can make these using a normal linspace function. To print the actual data values of a variable "x" held in the dataset called "data" you can use:

```
print(data["x"][:])
```

Equivalently, the *VP*, *VS*, and *RHO* variables hold a 3D array (e.g., a numpy array) with corresponding values at each of those coordinate points in x, y, z space.

7.2.1. Creating new volumetric models
The example directory "*04_simple_3d_shapes*" contains a number of python files for producing 3D models. You can inject shapes such as spheres (technically known as blobs), cylinders, ellipsoids and cuboids at certain points, so that your 3D model may look like Figure 4. In addition to the relevant python source code to generate such 3D models, an interactive python notebook ("*Example_4_README.ipynb*") can guide you through two examples: one for a cartesian mesh, and one for a spherical (D-shaped) mesh. Even

if such simple shapes are of no interest/use it may be worth checking out the "writeNetCDF" function within "*model.py*", which demonstrates how to generate a netCDF file in python from NumPy arrays.
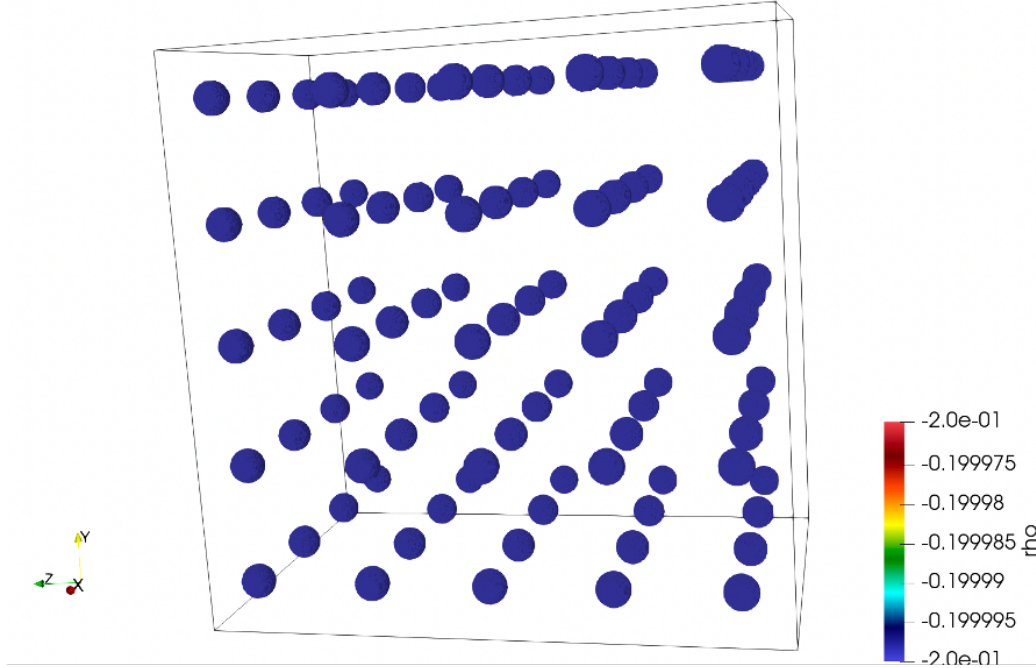

Figure 4: Example volumetric model containing spheres.

Additionally, to create volumetric models that include seismic anisotropy, scripts exist in the "05_anisotropy_global" example folder in the AxiSEM3D GitHub page. AxiSEM3D is capable of calculating synthetics for input models that include arbitrary anisotropy, described by the the full elastic tensor C_{ij}. Example papers that do this are Tesoniero et al. (2020) and Wolf et al. (2022b,a, 2023a).

To start using seismically anisotropic volumetric models, we suggest repeating the exercise from Tesoniero et al. (2020) (Figure 5), who calculated seismograms for anisotropic PREM in two different ways:

- For a "prem_ani" mesh. (Approach 1)

- For a "prem_iso" mesh, plus a volumetric 3D model specifying radial

27

anisotropy between 220 and 24.4 km depth using the full elastic tensor to describe the seismic anisotropy. (Approach 2)

Examples for this exercise are provided in the "05_anisotropy_global" folder, including scripts to create the volumetric input model.
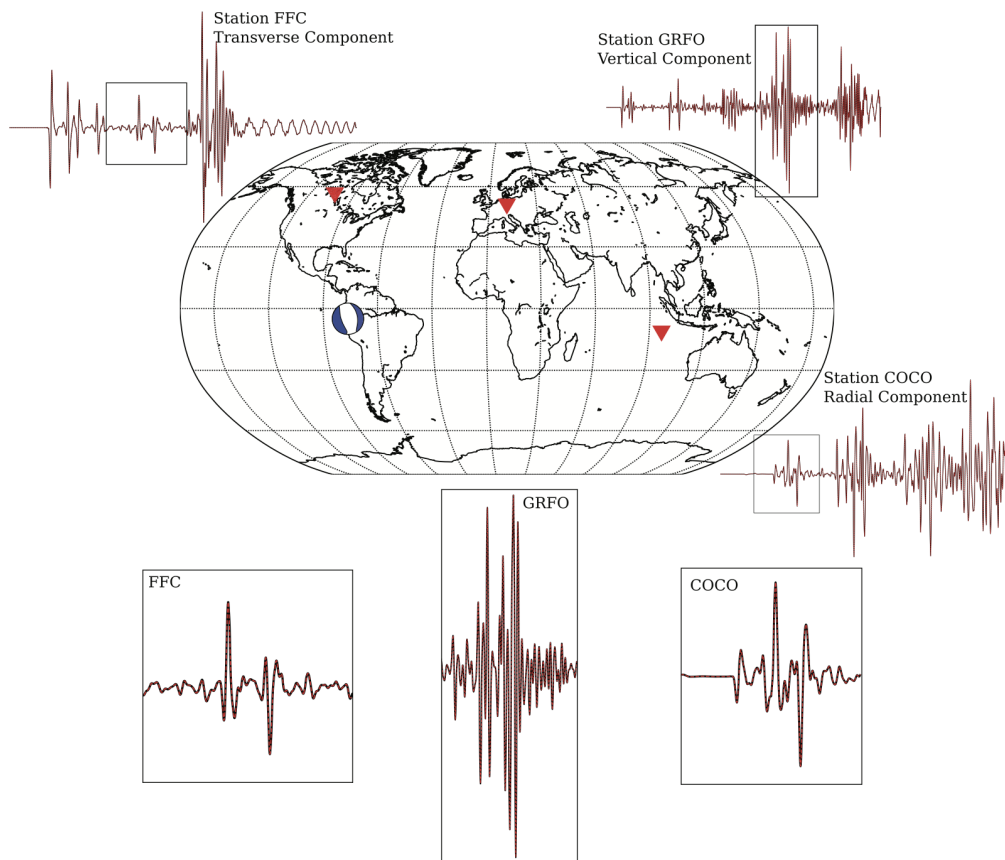

Figure 5: Results for the test from Tesoniero et al. (2020). The identical red and black seismograms are calculated using two different approaches (see text)

Approach 2 requires the calculation of the full elastic tensor from the vertical transverse isotropy of PREM in a depth range between 220 and 24.4 km. This is possible via the so-called Love parameters A, C, L, N and F (see "prem_ani_Cijkl.m" file in "PREM_anisotropy_w_and_wo_full_Cij_50s/processing").

The PREM-test mentioned above is simple because the vertically isotropic

geometry of the anisotropy implies that the rotation of the elastic tensor around the vertical (or radius) axis does not matter. In general though, if more complicated seismic anisotropy is implemented into the input model, this orientation will be crucial. In AxiSEM3D seismic anisotropy is implemented such that the one of the horizontal axes of the elastic tensor (specifically, x-axis in MSAT, Walker and Wookey, 2012) is aligned with the north direction. To explore this, it is useful to implement a horizontally transversely isotropic elastic tensor into an input model, for example by rotating the PREM-anisotropy by 90°. For this case the effects of the rotation of the elastic tensor around the vertical (radius, z) axis can be investigated. Please note that the way that elastic tensor is implemented in AxiSEM3D means that, if you are close to the pole, you have to be careful about whether you would like your seismic anisotropy to change as a function of longitude (which it does by construction) or not. If you would like to have your anisotropy not change, you can just rotate by the longitude value.

7.2.2. Values used in 3D arrays

The actual values that you use in your 3D arrays can be used by axis in a number of ways:

- Absolute values - the value in .nc is what is used by axis;

- Ref 1D – a perturbation relative to the 1D model (e.g., 0.2 is 20 %)

- Ref 3D – perturbation relative to the 3D model;

- Ref_perturb - perturbation relative to the current perturbation at that point.

Most of the variables in the inparam.model.yaml file are quite self explanatory for the 3D case. The ones to draw attention to are: *data_rank* – this is where you need to be careful in respect to python vs Matlab, and tell AxiSEM3D what order your coordinates are in; *nc_variables* – tells AxiSEM3D the name of x, y and z variables that you used in the .nc file – e.g. this could be 'X', or 'x', or 'x_arr' etc...

8. 3D models part II – usage

Once you have created a new 3D model and saved it as a netcdf file, you need to upload it to the *input* folder. Then, there are two input files that

you need to alter in order to get the model to be read in and represented properly: *inparam.model.yaml* and i*nparam.nr.yaml*.

8.1. inparam.model.yaml

The portion of the *inparam.model.yaml* file that needs to change from the 1D case is the *3D Models* section. Under the header *list_of_3D models*, you can add as many as you want. Let us start with *etopo1*, which you can put as the *key* in the first indented line. If you are doing checks and want to run the code without the model being read in, but don't want to rewrite the whole input file, just toggle *activated* to *false*.

class_name for all 3D geometric models will be *StructuredGrid3D*.

class_name for a 3D volumetric model on a structured grid will be *StructuredGridV3D*.

nc_data_file is also just the name of the 3D model file that you have created and saved in the /input folder.

For coordinates, this project will probably use *LATITUDE_LONGITUDE* and either *DEPTH* or *RADIUS*. Just make sure you get the latter correct: *etopo1* is defined as an elevation with respect to some mean sea level whereas the Moho file we are using is defined as a depth with respect to sea level.

Again, you can use the *ellipticity* correction if you want to but it is unlikely to make an enormous difference.

If you've used the provided python scripts, you should not need to change the *data_rank*, *length_unit*, *angle_unit*, or *factor* flags from those we have given (*[0,1]*, *m*, *degree* and *1.0* respectively).

The things that you will need to change are as follows. Close and careful attention is needed when changing these, as mistakes can be very challenging to debug. The order that we go through these is not the order that they appear in the input file, but we think it is more logical.

- *nc_variables* and *nc_var*: these are the variable names used in the netcdf file. If you have kept the defaults, the first one should be *[latitude, longitude]* and the second one should be *depth*, moho and elevation for etop01 and C_{11}, C_{12}... for seismic anisotropy. Note that these are just the labels that we used in our netcdf file, they can be called anything

and just because you set 'depth' or 'radius' as the name does not mean that the code will treat it as such unless you also set the flags below.

- *vertical* should be *DEPTH* for the Moho and seismic anisotropy, and RADIUS for topography. Make doubly sure this is consistent, if you have files which you think are the wrong way round and do not want to remake them, you can always swap *factor* from *1.0* to *-1.0*.

- *undulation_range: interface* should be the depth or radius of the interface you are undulating, as defined in the background 1D model. If you are using depth as your variable (as we used for the Moho), then this should be, for example, *-24400.0*, as the Moho is 24.4 km below the surface in PREM. If you are using radius as your variable, as we do for the surface topography, this should be *6371000.0*. Remember that you will define the undulations as elevations above the boundary in consideration. So, at a subduction trench where the Moho is at 7 km below the surface, you would define the gridpoint for the Moho's depth as +17400 (-7000 + 24400 = 17 400 m). Similarly, in Tibet where the Moho is at 80 km depth, the gridpoint would be -55600 (-80000 + 24400 = -55 600 m).

- *depth_below_solid_surface* is an important flag. Lots of models in seismology (e.g., PREM) do not include the ocean, so if you add one on top, you need to either add one right on top (making the total radius 6371 km), or remove 3km of rock first (to keep the radius as 6368 km). This flag allows you to define whether your interface coordinates are with respect to the seafloor (*true*) or the ocean surface (*false*). You might also want to think about whether, when you read in a 3D model for subsurface features, the depths should be defined with respect to the solid surface in the 1D case, or the 3D case – as the position of the surface may have moved considerably in between these.

- *undulation_range: min_max* is the final variable to think about here. This is hard to visualise, but in effect it tells the code in which range it is permissible to stretch or shrink elements to accommodate your deformed boundary. For example, if you set the Moho to be at 24 km and then undulate it, elements on either side need to deform to accommodate the undulated boundary. *min* and *max* define the lower and upper edges of the deformation zone, which should be at least twice as large as the undulation range. For example, in Crust 1.0 the Moho

depth varies between 75 km and 7 km, so doubling the deepest depth and halving the shallowest one in this range would give you *min_max = [3500.0, 150000.0]*. Again, just make sure that the signs are consistent and correct: 3500 m is actually a shallower depth (i.e., the minimum deformed depth), rather than the maximum! Either way the interface needs to be contained within the bounds you have set, else the undulation will not work!

For volumetric models, *nc_variables* should be set in the order *[lat, lon, depth]* or *[lat, lon, radius]*. The names should match the names in the netcdf file.

Data rank should map to the order of the variables in the netcdf file. For example, if the netcdf file is in the order radius, longitude, latitude, then the data rank would be set as follows: *data_rank: [2, 1, 0]*.

8.2. inparam.nr.yaml

8.2.1. Fourier series introduction

This input file, which we did not touch upon earlier, is used to set the azimuthal (i.e. variation in longitude) parameters of the simulation. You will recall that AxiSEM3D works by taking a 2D mesh and representing the third dimension through a pseudospectral (Fourier) expansion. The order of this expansion determines the complexity of the entire simulation in the azimuthal direction. Note that this does not just affect the degree to which 3D models are accurately represented, lower Fourier order expansions also reduce the azimuthal complexity of the seismic wavefield that you are going to record.

To understand this another way, the Fourier expansion in AxiSEM3D is akin to the representation of any normal mathematical function in terms of sines and cosines. The more terms you include, the more accurate the function's approximation is. For an arbitrary function, an infinite number of terms is needed for an exact solution - but we can make do with a smaller (finite) number of terms Nu, Nr if we are happy for the solution to only be accurate to within a given degree. *what is the conversion between these two? Not sure it is consistently defined...*

How much smaller than infinity the number of terms/Fourier order Nr can be depends on a number of different factors:

1. The complexity of the 3D model that you add to AxiSEM3D. If you have a very long-wavelength model with relatively smooth variations, like SEMUCB, you need far fewer terms than if you have something that is strongly varying and densely sampled, like ETOP01. For a 1D model, you never need more than $Nr = 5$.
2. The complexity of the wavefield that you want to represent: in general, you will only add in complex 3D models if you want to see what impact they have on synthetic seismograms. However, if you wanted for some reason to use a complex 3D model but were not interested in the fine detail of the wavefield, you could get away with a lower Fourier order.
3. The complexity of the source: as noted before, if you are only using a 1D model you can save a small amount of time by reducing the Fourier order needed to represent the source term. A second rank moment tensor (i.e. something from CMT) requires $Nr = 5$, a point force requires $Nr = 3$, an isotropic/monopolar pressure term requires $Nr = 1$. For most 3D models the value of Nr needed to capture their variations will be far larger than 5, so there is no saving to be made even if you only use a point force or pressure term.

Remember that the overall resolution of the simulation (i.e., the smallest scale that you can resolve meaningfully) is still limited by the mesh resolution, so increasing the Fourier order too much becomes pointless as you are not sensitive to these small spatial scales anyway. For this reason you should leave *bound_Nr_by_inplane = true*.

8.2.2. Choosing input parameters
You will probably be wondering by now, 'how small a Fourier order can I get away with?' - the answer is of course that this depends on how accurate a simulation you want, and what much computational resources you have available - a higher Fourier order increases both runtime and memory demands. There are four options that you can choose in AxiSEM3D for how the Fourier order is calculated, which may help with this question. These are, *type_Nr* = :

- *CONSTANT*: here, the same Nr is used throughout the mesh. As mentioned previously, for a 1D model with a moment tensor 5 is both necessary and sufficient.

- *ANALYTICAL*: this is like constant, but with slightly finer user-control,

in that you can choose how Nr varies through the interior of the planet. As an example, if you wish to investigate the effects of crustal structure on surface waves, you might want a high expansion in the mantle, but not in the core. This is thus a finer level of control than in *CONSTANT*, which can save you both time and memory.

- *STRUCTURED* allows you to specify even finer degrees of control, by setting the fourier order on individual elements. You can thus save even more time and resource with respect to *ANALYTICAL*, but a more detailed knowledge of how to create the appropriate grid of points is needed.

- *POINTWISE* allows you to go even further by having the code try and optimise the variation of *Nr* through the mesh. See below for more details.

Within *ANALYTICAL*, you can specify the variation of *Nr* with depth that you wish to use within the *depth_dependent_AxiSEM3D_default* option. Using the options *control_depths* and *Nr_at_control_depths* you can make a point-wise specification of how Nr varies, remembering to give your depths in metres.

For example, *control_depths: [0., 6371.]* and *Nr_at_control_depths: [100, 100]* would set *Nr = 100* across the whole of the Earth's radius. Changing *Nr_at_control_depths* to *[100, 1000]* would set *Nr* to *100* at the surface, and *1000* at the planet's centre, with linear interpolation in between. You can add as many control points as you want into these arrays. For example, if you wanted to look at high-resolution crustal structure, you might do something like:

control_depths: [0, 50e3, 200e3, 6371e3] and *Nr_at_control_depths: [1000, 1000, 100, 10]* which would give you *Nr = 1000* in the top *50* km, decreasing to *100* in a linear fashion by *200* km depth, and then linearly again from 100 at *200* km to 10 the centre.

8.2.3. Wavefield scanning
Wavefield scanning is an advanced feature of AxiSEM3D. It involves the code trying to 'learn' the most optimal *Nr* profile it can, using past runs as a guide. In a way, this lets the code do all the optimisation described in the steps above itself, such that the runtime and memory requirements are

minimised.

This method works by analysing the frequency spectrum at all the interpolation points in the mesh. For a given point, if the energy above a given frequency is below some threshold value (which you can set), the code determines that frequencies above this point are not contributing to the overall solution, and the Fourier series can thus be truncated. In subsequent runs, the value of Nr at these points can therefore be reduced as they are determined to have a reduced azimuthal wavefield complexity.

If you want to try this, you can set *enable_scanning* to *true* and *type_Nr = POINTWISE*. Follow the instructions in the input file to make sure that you match the filenames and copy the relevant files across.

9. Common Errors

It is probably worth covering some of the common errors that may occur in your simulations. In general, errors will be one of three types: preloop, runtime, or result. Preloop errors occur because the code has been unable to initialise properly, for example because something has gone wrong with one of the inputs. Runtime errors occur within the time loop, and will generally cause the code to crash. Result errors are where the result you get out does not make any physical sense. Some errors are also common to preloop and runtime and may occur during either.

You can sometimes diagnose errors by checking either the .e or the .o files that appear in your code directory. For example, if the script you use to submit the batch job is called "run_script.sh", you should get two files that form in the same directory as the submission script called "run_script.sh.eX" and "run_script.sh.oX" where "X" is the job ID of that particular job. The ".o" file contains code-specific information, i.e. what would have been printed to the terminal. You can check that the output matches what you were expecting, and see where the code stops working. The ".e" file contains system information and may highlight what sort of error it was.

If you are using the *-m be* flag in your submission script, the 'complete' email might also tell you whether it was a qsub related issue (out of time, out of memory) or something else.

9.1. Either preloop or runtime errors

- *Out of time:* Probably the most common error will be an out-of-time error, where the AxiSEM3D simulation does not finish within the time window that you specified in the scheduler using h_rt (on ARC4). There are two ways to address this without changing the simulation: increase the runtime, or increase the number of cores being used. If you cannot do this, you can: reduce the record length, increase the mesh period, or decrease the Fourier order.

- *Out-of-memory:* Sometimes it can be hard to diagnose out of memory errors, as the code may just crash, but the complete email might tell you that the scheduler killed the job as it exceeded the memory requirements (or words to that effect). The simplest option is to increase the memory allocated per node (change h_vmem). Note that it is not quite clear on the ARC4 pages, but the *-pe smp* flag confines you to a single node, whereas *-pe ib* allows you to split across multiple nodes, so use the latter. The h_vmem is per core so the total memory you are requesting is the *-pe ib* value multiplied by the h_vmem value. The total memory per node is 192GB (or 768GB on a large memory node), so you can probably ask for 10GB for a 40 core job (400GB total), or 1GB for a 400 core job (400GB total also), but not 10GB for a 400 (4TB total) core job. Alternatively, you can switch to the larger memory nodes, increase the number of cores that the load is split across, or change the simulation itself (lower Fourier order, lower mesh resolution, etc). Note that decreasing the simulation length is unlikely to change the memory requirements of a particular run. Other systems will have different parameters.

9.2. Preloop errors

- *Jacobian distorted:* This is a very common error which is due to the way that the 3D model is being applied. As discussed previously, it basically means that there is an error in the interpolation somewhere. There are a few options: 1) decrease the degree of undulation (which you are unlikely to want to do much of in reality) using some sort of filtering as done in the supplied python scripts, 2) or increase the min_max bounds in "inparam.nr.yaml" (allowing the deformation to be accommodated across more elements), or 3) change the mesh resolution (this could go

either way, as more elements resolves more gradients but also allows more elements to accommodate the deformation). Changing the *GLL order* in the *SOLVER/CMakeLists.txt* might also work (from say 4 to 6), but no guarantees here as we have not actually tried it. To do a test and make sure that it is an issue with the file itself.

9.3. Runtime errors

- *Code blew up:* The code should recalculate the necessary timestep dt to ensure stability regardless of how many 3D models you add onto the 1D base model. However, this does not always work, and sometimes the code will become unstable. The simplest option here is to adjust the *courant_number* in "inparam.source.yaml", from its default of *1.0* to something more conservative (e.g. *0.6*). Note that a decrease in the courant number gives you a roughly linear increase in the runtime, so avoid being over-zealous in reducing it. If you have reduced this below around *0.3* and the simulation is still unstable, it may be an issue with how the 3D model is being read in, and you should try checking that instead. If you need to diagnose an instability that you cannot get around, go to "inparam.advanced.yaml" and make sure that *stability_interval* is set to *1.0* (meaning that instabilities are checked at every timestep). If that does not work, go further down the file and set *max_num_time_steps=1* (or *10*). This will limit your runs to a single (or a few) timestep(s), and you can make sure that things are working properly without having to ask for longer runtimes; thus reducing the waiting time in the HPC queue.

9.4. Result errors

By result errors we mean things that when you plot them up, look wrong - obviously it is something that has gone wrong in the simulation, but you may have got to the end of the time loop without it being obvious what the issue is.

- *No signal present in seismograms:* The simplest explanation would be that you have not run the simulations for long enough for any of the energy to arrive at the stations you are looking at, but it could also be an issue with the source. Check "inparam.source.yaml", if nothing looks obviously wrong you can put a station at the exact position of the source and check that the source's shape is what you expect. If you

have used a delta function source, it should be something with a very steep peak.

- *Amplitudes are excessive:* It is possible for the runs to be unstable without triggering the instability checker. First, check that the units of your source term are what you expect – though this is a linear scaling so it will just give you amplitudes that are too high, but seismogram-like wiggles. If you are getting exponential growth or exponentially growing oscillations, try reducing the *courant_number* in "inparam.source.yaml".

- *Seismograms do not match benchmarks:* If for some reason you end up benchmarking AxiSEM3D against another code, like SPECFEM or YSpec, you need to be even more careful to get exact agreement between them. Bear in mind that the choice of *decay_factor* in "inparam.source.yaml" makes a big difference, and is not the same in all codes. Also, AxiSEM3D has no gravity and does not implement effects from the Coriolis force, whereas other codes do. Similarly, AxiSEM3D's ellipticity correction may be written slightly differently to other codes, so check that. Finally, the attenuation bands that you are using need to match, see "inparam.model.yaml" for a few more details and links to the relevant papers.

10. Plotting and processing data

Perhaps the most important part of the entire simulation process is actually plotting and processing the data that you have generated!

In this section we will assume that you have a series of ASCII (text) files containing the displacements recorded at the stations that you're interested in. As noted previously, netcdf files are much more efficient and we would recommend them if you are doing much more than generating basic seismograms. Also, if you are doing wavefield visualisation, definitely do not try to do this using ASCII!

10.1. Ascii file contents

The inparam.source.yaml and inparam.output.yaml define the contents of the ASCII files that we are going to plot. We assume that you have a file for each station containing three components of displacement; as set using the *format* and *channels* options in "inparam.source.yaml".

Rather than saving the time series (i.e. the list of timesteps) within each file, this is stored separately in a file called *data_time.ascii*. This should be a single column of floating point numbers, each of which is a different point in the time series. The first one is probably slightly negative, as AxiSEM3D ramps up the source time function before the zero time index on the simulation. The final entry should be roughly what you set the record length to be in "inparam.output.yaml".

If you have not changed the station list, you should have a series of other files. For example, in the folder *global_seismic_network_GSN*, you should have a series of stations, for example "IU.TEIG.ascii". These are your station files, and the number of columns in each (and the order) will depend on the *channels* options you set in "inparam.output.yaml". If you used *[U]*, you should end up with three components, in the order R, T, Z if you used *coordinate_frame = RTZ*.

10.2. Software for working with output files

There are obviously no fundamental limitations on how you can manipulate and use output files, you could even print them out and plot the points by hand if you want! Our strong recommendation would be to use Python, however – even if you think you are more comfortable with MATLAB, the open-source seismogram processing functionality exists only in Python.

Within Python, you can probably get by with ObsPy, NumPy, and SciPy. we presume that you already have NumPy and SciPy installed, you can find all the documentation needed to work with ObsPy here: `https://docs.obspy.org` which includes tutorials, documentation, and worked examples.

It is worth running through some of the first few tutorials, to get you used to the language used: streams, channels, Stats, UTCDateTime objects, and the like.

10.3. Reading in seismograms

As per the included Python scripts, we think the simplest way to read in the seismograms is:

- Use *numpy.loadtxt* to read them in.

- Use *numpy.hsplit* to split the columns into separate arrays, and then *concatenate* into a single array.

- Create an ObsPy *Stats* object which describes the sampling rate (note that you can make things work without this last step, but then you do not have a proper time axis to do temporal calculations like timestepping, filtering, etc and things are much more likely to go wrong).

- Finally, use an ObsPy *Trace* to combine the temporal data with the spatial data.

If you then just type the name of the trace, e.g. *axisem3d_trace*, it should return a *Trace* object which includes both the seismogram and the relevant displacements. You can combine multiple *Traces* into a single *Stream* if you so wish.

10.4. Plotting seismograms

Once you have created a *Trace* object, plotting the seismogram is trivial. You can either use the built-in method that *Trace* objects have, but we prefer to use *matplotlib.pyplot* as you get much more functionality and user-control.

To do this, inside the *plt.plot* command you just reference the Trace's time points and data points separately, using *trace.times()* and *trace.data*. Note that the data points are not called (i.e., no parentheses) but the time points are.

You can edit the figures using the same functionality you would for any other matplotlib plot, for example by setting labels, axes, linestyles, etc. You can also write relatively simple routines for doing things like plotting record sections (codes not included for simplicity – email us if you want them).

10.5. Filtering and convolution

If you used a delta function source, you need to either filter or convolve the Green's function to return a result that is free of 'noise' at above the mesh frequency. It is worth thinking about the subtle differences between *ObsPy's filter* routines and *SciPy's convolve* ones.

In the broadest sense, these are of course identical, as filtering is equivalent to a multiplication with a kernel in the frequency domain, as is convolution. However, the way in which these are implemented can vary, and you also
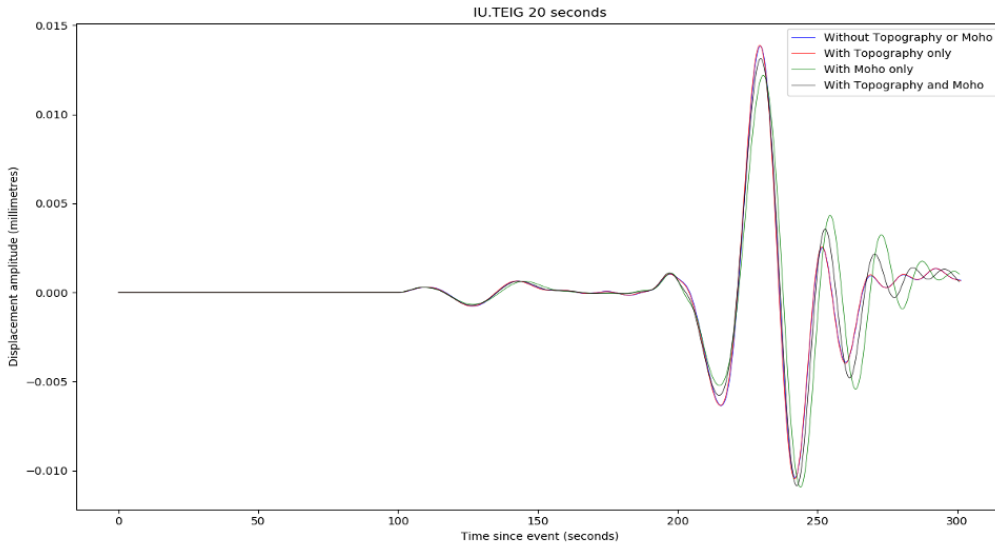
Figure 6: Example seismograms. Note that the Moho undulations had to be smoothed to 10% of their original amplitude to make this run work, but some differences are still appreciable.

need to think about how convolution ends up being more complex in a numerical sense (with finite windows) than it is in the simplest, infinite-domain analytical sense.

10.5.1. Butterworth bandpass filters

The simplest kind of filter that you might want to use is a Butterworth-bandpass filter, whose functionality is included in ObsPy at *obspy.signal.filter.bandpass*. This is as close to a 'rectangular' filter as you will want to get, for technical reasons simply removing all frequencies not between your two limits tends to give you numerical artefacts. A Butterworth-bandpass filter has steep, but not vertical sides. You can also choose the filter order (*corners*), and need to specify (default four) corner frequencies. In certain cases we have also found that running the filter both ways across the data (*zerophase=True*) can help.

For synthetic data, which effectively contain no noise other than that above the mesh period, the Butterworth-bandpass filter is a good choice. You can cut out the high-frequency noise by simply setting *freqmax* to the inverse of the mesh period, and you can remove low-frequency energy below 100 s by

41

setting *freqmin* to *0.01.* This is worth doing because, strictly speaking, frequencies below $100\,\text{s}$ (i.e. $0.01\,\text{Hz}$) are not simulated properly in AxiSEM3D because we have no ellipticity, rotation, or gravity.

If you were using actual data, with a non-white noise content, another filter might be more appropriate: for example a *log-gabor* filter, which does not come installed in ObsPy (We can also send it to you though).

10.5.2. Convolution with a Gaussian function

Convolution with a Gaussian using SciPy ends up being a bit more challenging than you might think – on a qualitative level, it is just equivalent to swapping the frequency-domain representation of the Butterworth-bandpass filter for the frequency-domain representation of a Gaussian, which is also conveniently another Gaussian.

However, if you use *scipy.signal.convolve*, you need to make sure that the convolution parameters of the Gaussian (or indeed whatever other source-time function with appropriate frequency content you might wish to use) are set correctly. This includes matching the *sampling rates* (you can use ObsPy's *Lanczos interpolation* to do this), and ensuring that the convolution mode is set to *valid* – to avoid padding out the seismogram with fake data points at either end.

10.5.3. Other operations and commutativity

In an analytical sense, all these operations should commute and it should not matter which order you do them in. In a numerical sense, this does not always appear to be the case (though this may just be due to poor processing on our part). So if something does not look right, try playing around with the order of operations.

We have also found that applying a *taper* to the seismograms can help, as if the end of a Green's function trace includes a large non-zero displacement when the simulation ends, sometimes the convolution can produce a seismogram with an overall non-zero slope (i.e., trending to negative values over time), which is of course nonsensical.

11. Glossary

Some terms that are used in this document, and relevant papers, might not be commonplace or otherwise clearly defined. Here they are, if useful:

- 2.5D: see 'axisymmetric'.

- Axisymmetric: Here, a model or method which does not have any longitudinal variation; i.e., where any variation in parameters or physics is confined to within a single plane ('2D slice') of the planet. What this means is that any 2D slice through the Earth is identical to all the others. Note that in a 2.5D method, any structure must wrap all the way around the axis: e.g., a high-velocity circular province in the 2D plane will become a torus in the 2.5D version.

- AxiSEM: The AxiSymmetric Spectral Element Method: the 2.5D version of the code we are using here.

- AxiSEM3D: The AxiSymmetric Spectral Element Method 3D: the 3D version of the above.

- Geometric model: A 3D model which involves the radial deformation of some interface to change its depth/radius at different latitudes and longitudes. An example is the Moho in Crust 1.0.

- Green's Function: In this case, the response of the simulation domain to a near-impulsive (quasi-delta-function) source. Note that we say near-impulsive because in a computational method of this type the source must have some width (here, a few timesteps). In general this is so much less than the seismic period that it is close enough to a delta function for most purposes.

- Jacobian: Computations on individual elements in AxiSEM3D are mapped back to a reference square element, which increases computational speed. As most elements are not square to begin with, the Jacobian (and its inverse) associated with each coordinate transform must be calculated.

- Pseudospectral Method: A method of solving the wave equation which uses basis functions to represent key quantities in the equations of motion. See Igel (2016) for more detail.

- Spectral Element Method: A fast and efficient way of solving the wave equation, see Igel (2016) for more detail.

- Volumetric model: A 3D model which represents a change (with respect to the 1D case) in seismic properties (e.g., Vp or Vs), such that they

vary with latitude and/or longitude and/or depth/radius.

References

Chaljub, E., Valette, B., 2004. Spectral element modelling of three-dimensional wave propagation in a self-gravitating Earth with an arbitrarily stratified outer core. Geophysical Journal International 158, 131–141.

Cowling, T., 1941. The non-radial oscillations of polytropic stars. MNRAS 101.

van Driel, M., Kemper, J., Boehm, C., 2021. On the modelling of self-gravitation for full 3-D global seismic wave propagation. Geophysical Journal International 227, 632–643.

Dziewonski, A.M., Anderson, D.L., 1981. Preliminary reference Earth model. Physics of the Earth and Planetary Interiors 25, 297–356. URL: `https://doi.org/10.1016/0031-9201(81)90046-7`.

Fernando, B., Leng, K., Nissen-Meyer, T., 2020. Oceanic high-frequency global seismic wave propagation with realistic bathymetry. Geophysical Journal International 222, 1178–1194. URL: `https://doi.org/10.1093/gji/ggaa248`.

Gharti, H.N., Eaton, W., Tromp, J., 2023. Spectral-infinite-element simulations of seismic wave propagation in self-gravitating, rotating 3D Earth models. Geophysical Journal International , ggad382doi:`10.1093/gji/ggad382`.

Haindl, C., Leng, K., Nissen-Meyer, T., 2021. A 3D Complexity-Adaptive Approach to Exploit Sparsity in Elastic Wave Propagation. GEOPHYSICS , 1–64URL: `https://doi.org/10.1190/geo2020-0490.1`.

Hirai, R., Nagakura, H., Okawa, H., Fujisawa, K., 2016. Hyperbolic self-gravity solver for large scale hydrodynamical simulations. Physical Review D 93. doi:`10.1103/PhysRevD.93.083006`, `arXiv:1602.05700`.

Igel, H., 2016. Computational Seismology: A Practical Introduction. URL: `https://doi.org/10.1093/acprof:oso/9780198717409.001.0001`.

Komatitsch, D., Tromp, J., 2002a. Spectral-element simulations of global seismic wave propagation—I. Validation. Geophysical Journal International 149, 390–412. URL: `https://doi.org/10.1046/j.1365-246X.2002.01653.x`.

Komatitsch, D., Tromp, J., 2002b. Spectral-element simulations of global seismic wave propagation—II. Three-dimensional models, oceans, rotation and self-gravitation. Geophysical Journal International 150, 303–318. URL: `https://doi.org/10.1046/j.1365-246X.2002.01716.x`.

Leng, K., Nissen-Meyer, T., van Driel, M., 2016. Efficient global wave propagation adapted to 3-D structural complexity: a pseudospectral/spectral-element approach. Geophysical Journal International 207, 1700–1721. URL: `https://doi.org/10.1093/gji/ggw363`.

Leng, K., Nissen-Meyer, T., van Driel, M., Hosseini, K., Al-Attar, D., 2019. AxiSEM3D: broad-band seismic wavefields in 3-D global earth models with undulating discontinuities. Geophysical Journal International 217, 2125–2146. URL: `https://doi.org/10.1093/gji/ggz092`.

Nissen-Meyer, T., van Driel, M., Stähler, S.C., Hosseini, K., Hempel, S., Auer, L., Colombi, A., Fournier, A., 2014. AxiSEM: broadband 3-D seismic wavefields in axisymmetric media. Solid Earth 5, 425–445. URL: `https://doi.org/10.5194/se-5-425-2014`.

Nissen-Meyer, T., Fernando, B., Leng, K., Schmerr, N.C., Panning, M.P., Stutzmann, E., Margerin, L., Fuji, N., Weber, R.C., Banerdt, W.B., et al., 2019. Modelling the effects of 3d shallow scatterers and atmospheric sources on martian seismic signals at high frequencies, in: AGU Fall Meeting Abstracts, pp. DI51A–0012.

Panning, M.P., Lognonné, P., Bruce Banerdt, W., Garcia, R., Golombek, M., Kedar, S., Knapmeyer-Endrun, B., Mocquet, A., Teanby, N.A., Tromp, J., et al., 2017. Planned products of the mars structure service for the insight mission to mars. Space Science Reviews 211, 611–650.

Szenicer, A., Leng, K., Nissen-Meyer, T., 2020. A complexity-driven framework for waveform tomography with discrete adjoints. Geophysical Journal International 223, 1247–1264. URL: `https://doi.org/10.1093/gji/ggaa349`.

Tesoniero, A., Leng, K., Long, M.D., Nissen-Meyer, T., 2020. Full wave sensitivity of SK(K)S phases to arbitrary anisotropy in the upper and lower mantle. Geophysical Journal International 222, 412 – 435. URL: `https://doi.org/10.1093/gji/ggaa171`.

Walker, A., Wookey, J., 2012. MSAT - a new toolkit for the analysis of elastic and seismic anisotropy. Computers and Geosciences 49, 81–90. URL: `https://doi.org/10.1016/j.cageo.2012.05.031`.

Wolf, J., Long, M.D., Creasy, N., Garnero, E., 2023a. On the measurement of Sdiff splitting caused by lowermost mantle anisotropy. Geophysical Journal International URL: `https://doi.org/10.1093/gji/ggac490`.

Wolf, J., Long, M.D., Leng, K., Nissen-Meyer, T., 2022a. Constraining deep mantle anisotropy with shear wave splitting measurements: Challenges and new measurement strategies. Geophysical Journal International , 507 – 527URL: `https://doi.org/10.1093/gji/ggac055`.

Wolf, J., Long, M.D., Leng, K., Nissen-Meyer, T., 2022b. Sensitivity of SK(K)S and ScS phases to heterogeneous anisotropy in the lowermost mantle from global wavefield simulations. Geophysical Journal International 228, 366–386. URL: `https://doi.org/10.1093/gji/ggab347`.