SphGLLTools

User Manual - Version: 1.0

Caio Ciardelli

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Northwestern
University

Contents

1 Author

This package was developed by Caio Ciardelli at the Colorado School of Mines, under the supervision of Prof. Ebru Bozdağ, the Northwestern University, under the supervision of Prof. Suzan van der Lee and the University of São Paulo, under the supervision of Prof. Marcelo Assumpção, from 2018 to 2020. The post-processing tools of SPECFEM3D_GLOBE written by Prof. Daniel Peter served as the basis for many routines of SphGLLTools.

2 Citation

If you use SphGLLTools, please, cite the following paper:

Ciardelli, C., Bozdağ, E. and Peter, D., 2020. SphGLLTools: A set of routines for visualization, processing, sharing, and spherical harmonics analysis of tomographic models defined on GLL meshes. *Computer & Geosciences*, submitted.

3 Introduction

SphGLLTools is a set of C, Python, Shell Script, and GMT6 (Wessel et al., 2019) routines for visualization, processing, conversion, spherical harmonics analysis, and sharing of tomographic models defined on Gauss-Lobatto-Legendre (GLL) meshes. It was designed to work with SPECFEM3D_GLOBE (Komatitsch et al., 2016) but, in theory, should work with other solvers with little modification.

4 Getting started

4.1 Dependencies

SphGLLTools requires:

- GCC 5.5.0 or greater
- OpenMPI 1.10.2 or greater
- Python 2.7.12 or greater
- GMT 6.0.0 or greater

4.2 Download

The easiest way of downloading the last stable version of SphGLLTools is using Git:

```
1 $ git clone https://github.com/caiociardelli/sphglltools.git
```

4.3 Installation

SphGLLTools requires no installation. The code is designed to run on clusters alongside SPECFEM3D_GLOBE. But it can also run on a personal computer, provided that you have enough computational power or are using low-resolution meshes. Just like SPECFEM3D_GLOBE, the routines allocate

memory on the stack, for performance reasons. However, the default stack size is too small (usually, around 65 MB).

On Linux systems, you can remove that limit by adding **ulimit -S -s unlimited** to your *.bash_profile* file or **limit stacksize unlimited** to your *.cshrc* file, to suppress any potential limit to the size of the stack.

Some Mac OS have hard stack limits that cannot be removed. In those cases, the code can crash due to a *stack overflow*. In general, wherever you can run SPECFEM3D_GLOBE, you should also be able to run SphGLLTools.

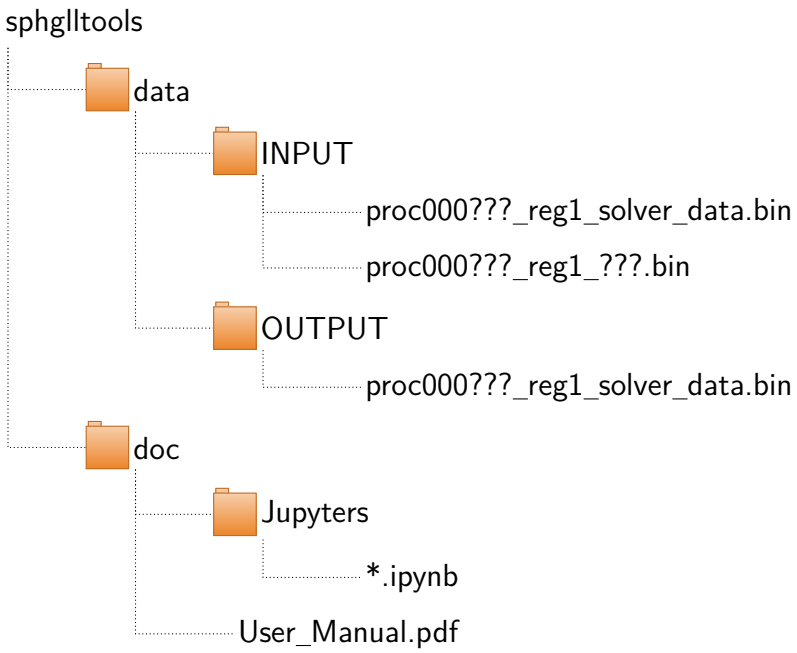
4.4 Compiling

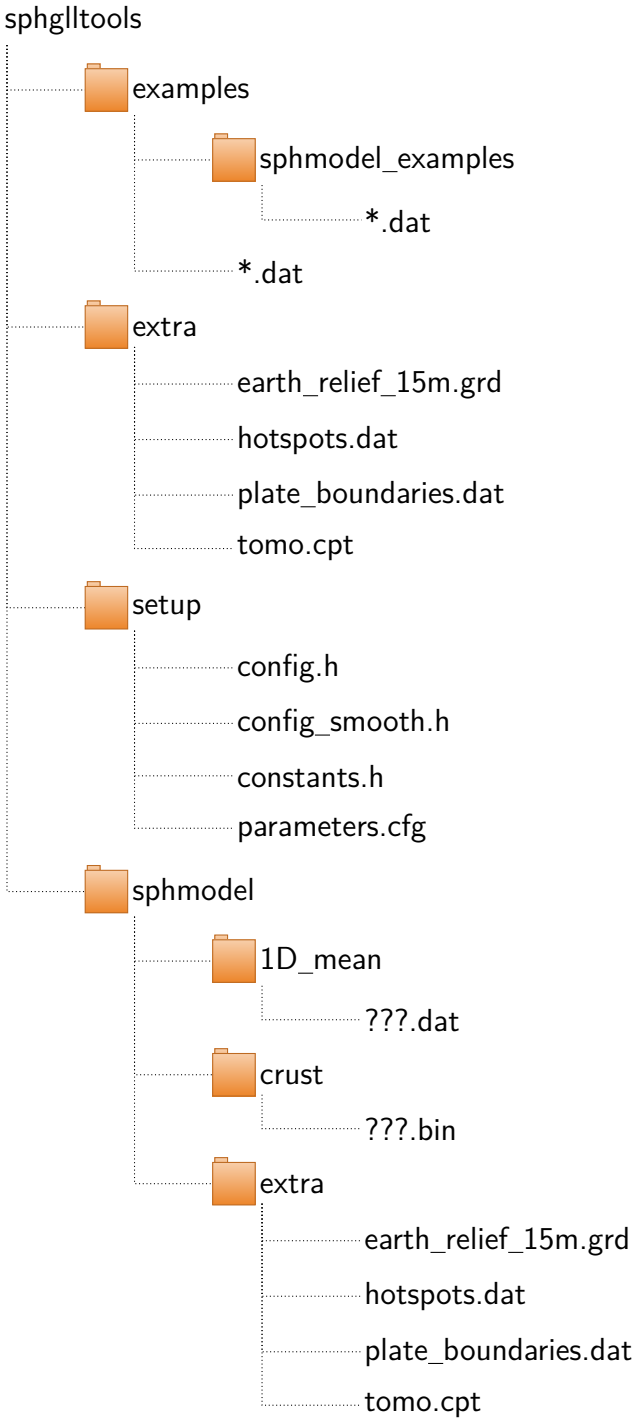
All you need to compile the routines is to run the Makefile inside the parent directory:

```
1 $ make -j4 all
```

5 Overview

The structure of the package looks like this:




sphglltools
examples
sphmodel_examples
*.dat
*.dat
extra
earth_relief_15m.grd
hotspots.dat
plate_boundaries.dat
tomo.cpt
setup
config.h
config_smooth.h
constants.h
parameters.cfg
sphmodel
1D_mean
???.dat
crust
???.bin
extra
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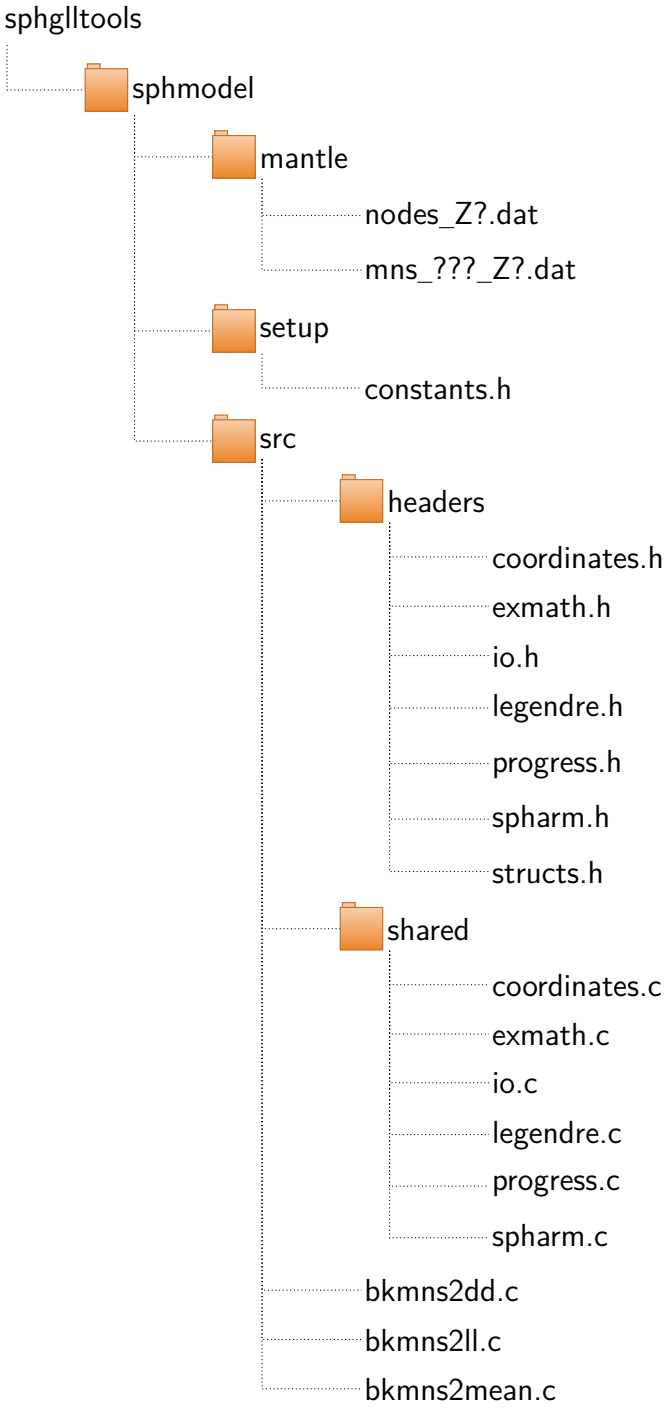
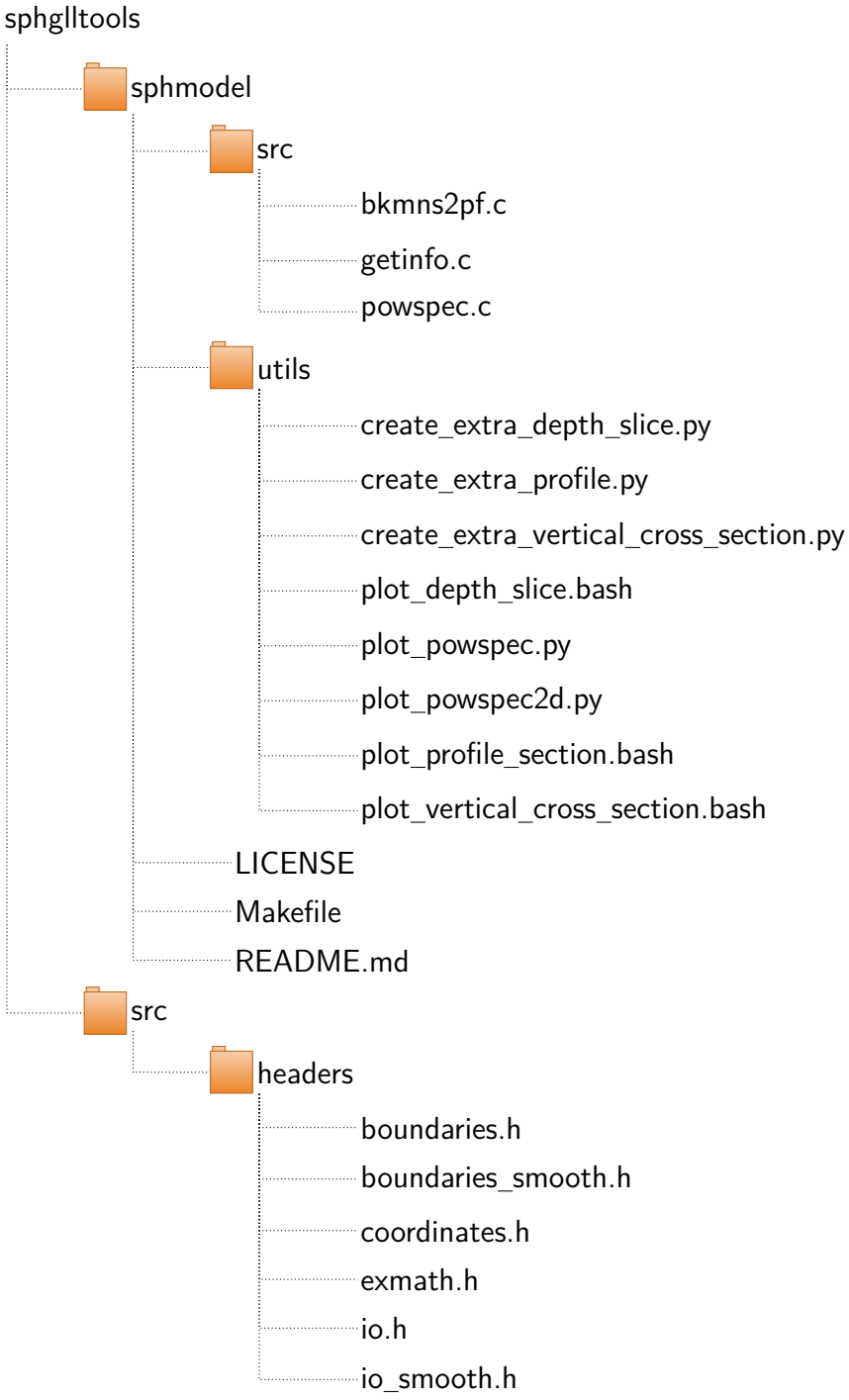
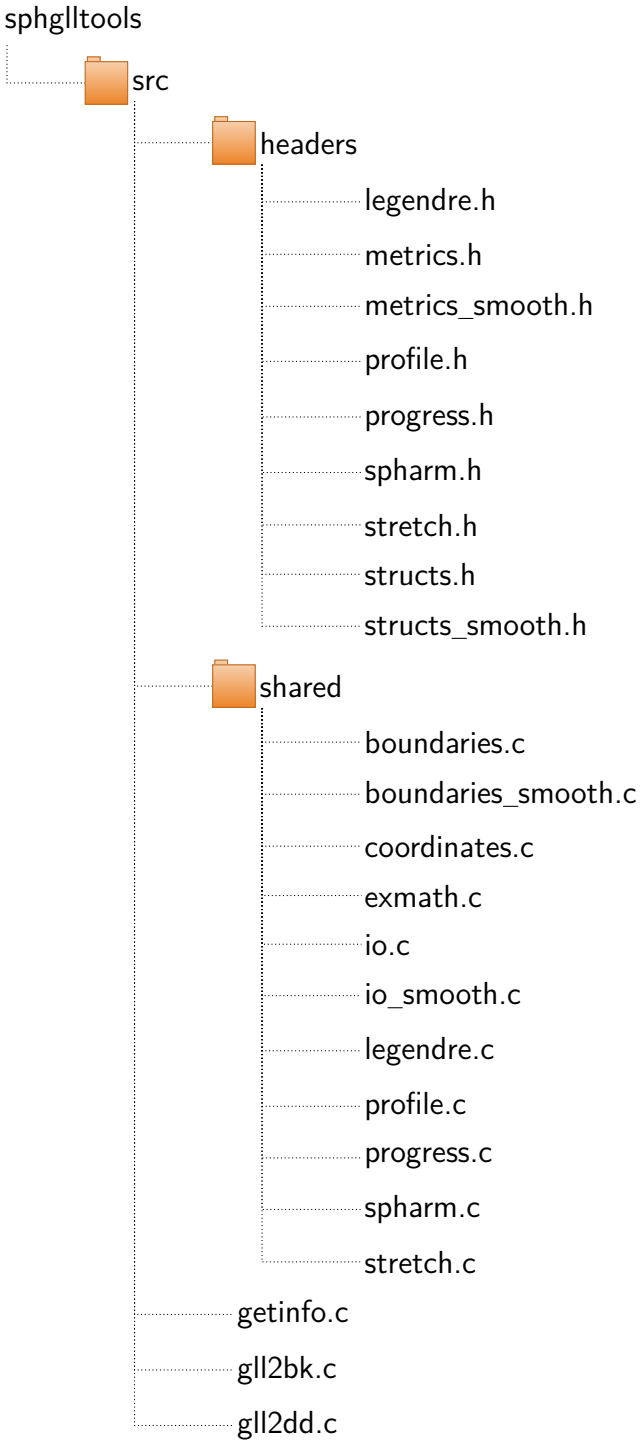
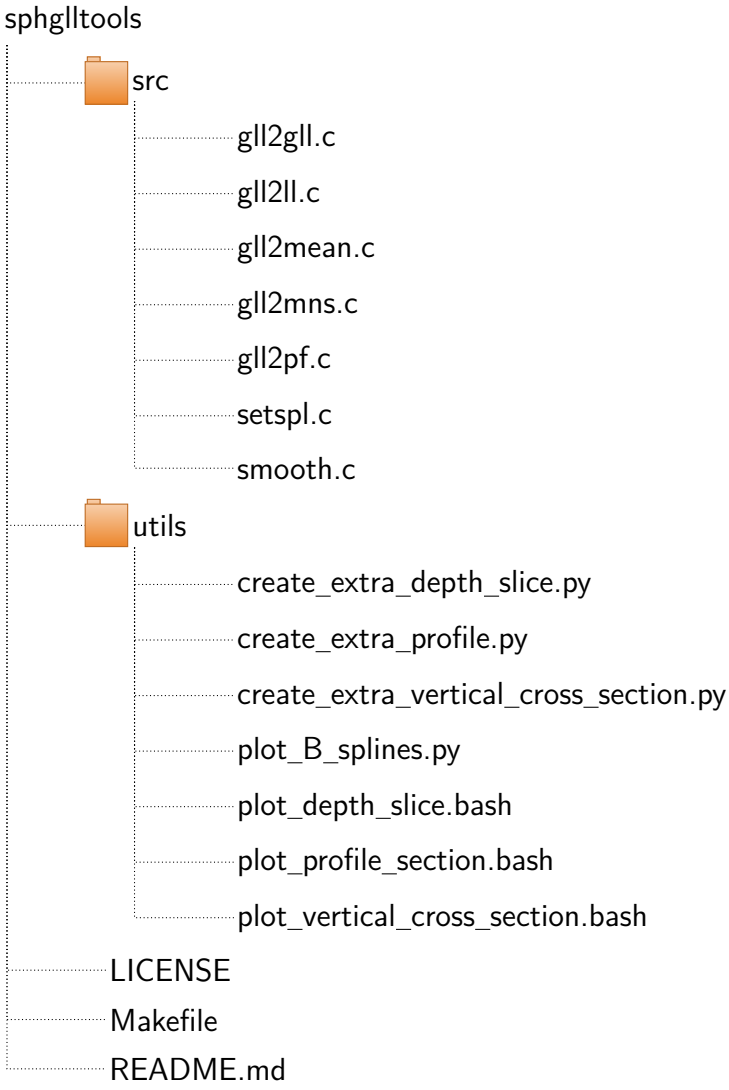
hotspots.dat
plate_boundaries.dat
tomo.cpt


sphglltools
sphmodel
mantle
nodes_Z?.dat
mns_???_Z?.dat
setup
constants.h
src
headers
coordinates.h
exmath.h
io.h
legendre.h
progress.h
spharm.h
structs.h
shared
coordinates.c
exmath.c
io.c
legendre.c
progress.c
spharm.c
bkmns2dd.c
bkmns2ll.c
bkmns2mean.c


sphglltools
sphmodel
src
bkmns2pf.c
getinfo.c
powspec.c
utils
create_extra_depth_slice.py
create_extra_profile.py
create_extra_vertical_cross_section.py
plot_depth_slice.bash
plot_powspec.py
plot_powspec2d.py
plot_profile_section.bash
plot_vertical_cross_section.bash
LICENSE
Makefile
README.md
src
headers
boundaries.h
boundaries_smooth.h
coordinates.h
exmath.h
io.h
io_smooth.h


sphglltools
src
headers
legendre.h
metrics.h
metrics_smooth.h
profile.h
progress.h
spharm.h
stretch.h
structs.h
structs_smooth.h
shared
boundaries.c
boundaries_smooth.c
coordinates.c
exmath.c
io.c
io_smooth.c
legendre.c
profile.c
progress.c
spharm.c
stretch.c
getinfo.c
gll2bk.c
gll2dd.c



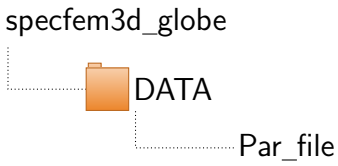
As pictured above, inside the main package, there is a subpackage called *sphmodel*. That is a stand-alone set of routines designed to share a model represented onto spherical harmonics with other researchers. SphGLLTools provide all the programs needed to carry out the expansion.

6 Basic visualization with SphGLLTools

SphGLLTools is composed of two main sets of routines: those who work using interpolation and those related to the spherical harmonics expansions. The first ones can handle both surface and internal topographies, but the second ones need a perfectly spherical mesh. None of them, however, can deal with ellipticity. For educational purposes, let's describe a workflow in which we use all routines in conjunction.

Since the package works in conjunction with SPECFEM3D_GLOBE, the first step is creating the mesh and the model files using the mesher.

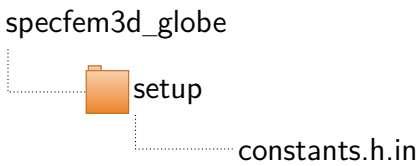
Because we don't want ellipticity, let's turn it off. You can do that under:



In section **# parameters describing the Earth model**, change the **ELLIPTICITY** flag to **false**.

The interpolation routines can handle any number of chunks, but spherical harmonics only make sense in a global mesh. So, set **NCHUNKS** = 6. For performance reasons, use a low-resolution mesh by setting **NEX_XI** = **NEX_ETA** = 64 and **NPROC_XI** = **NPROC_ETA** = 2. For the model, choose S362ANI (Kustowski et al., 2008) + CRUST2.0 (Bassin, 2000) by setting **MODEL** to s362ani_crust2.0. Lastly, you need to set **SAVE_MESH_FILES** as **true** and **ADIOS_ENABLED** as **false** (this last one is important because SphGLLTools cannot handle the ADIOS format yet).

The next step is disabling the topography of the seismic-velocity discontinuities at depths of 410 and 650 km. That is mandatory for the spherical harmonics expansion and advisable for the interpolation. You can do that under:



Set the **SUPPRESS_INTERNAL_TOPOGRAPHY** flag to **false**. Afterward, reconfigure the package to update constants.h:

```
$ ./configure FC=mpif90 CC=mpicc MPIFC=mpif90 MPICC=mpicc FCFLAGS
  ='-g -O3' CFLAGS='-g -O3'
```

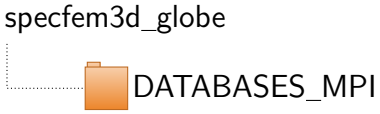
Now, you can compile everything with:

```
$ make -j4 all
```

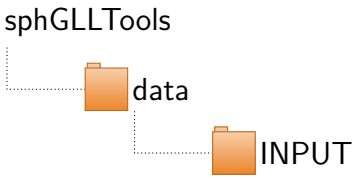
Run the mesher:

```
$ mpiexec -n 24 ./bin/xmeshfem3D
```

The mesher will save both the topological and the model files to the "DATABASES_MPI" directory:

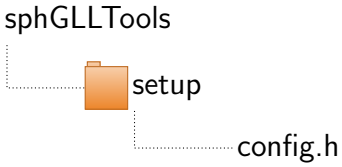


Copy the topological files "proc0000??_reg1_solver_data.bin" and the model files "proc0000??_reg1_[vp,vs,rho].bin" to "data/INPUT" directory:



Within "specfem3d globe/OUTPUT FILES/" there is a header file called "values from mesher.h". The flag **NSPEC_CRUST_MANTLE** (on line 78) is the number of spectral elements in each mesh slice, and the flag **NGLOB_CRUST_MANTLE** (on line 82) is the total number of points on each mesh slice. These values are necessary to set up SphGLLTools.

Under:



Set **NC** (number of cores) to 24, **NEL** (number of spectral elements) to 8896 and **NG** (total number of points) to 592913. Also, enable the parameters V_P, V_S and ρ. Then, just run the Makefile to recompile all the routines.

All the ASCII and binary files created in the following examples that are not too big are within the directory "examples". They are useful to check your results.

6.1 Creating depth slices

To create depth slices directly from the model parameters, use the routine GLL2LL. All routines have a help menu that shows up wherever you run them with no or with a wrong number of command-line parameters. The same menu is also at the beginning of each source code. For example, if we run the routine GLL2LL with no parameters, a message similar to the one in Fig. 1 will show up:

```
1 $ ./bin/gll2ll
```

For performance reasons, all the interpolating routines should be run in parallel, using MPIRUN or MPIEXEC. The ideal number of cores for many routines, including GLL2LL, is only constrained by your hardware and should be set according to the size of your problem. In this example, we picked 12. The larger the mesh resolution and/or the resolution of the output files, the more memory and cores you should request. Some routines, though, must be run with the same number of cores used to create the mesh. Those are GLL2GLL, SETSPL, GLL2MNS, and SMOOTH.

Following the example suggested in the help menu, you can create a depth slice of the model at 300 km depth with a 0.5° resolution by running:

```
1 $ mpiexec -n 12 bin/gll2ll 300 0.5 data/INPUT/ .
```

The above command should create three output files on your local directory: "vp_300_DS.dat", "vs_300_DS.dat" and "rho_300_DS.dat".

```
Error: wrong number of parameters on the comand line...

 GLL2LL

 USAGE
    mpiexec -n 12 bin/gll2ll DEPTH HORIZONTAL_RESOLUTION INPUT_DIRECTORY OUTPUT_DIRECTORY

 EXAMPLE
    mpiexec -n 12 bin/gll2ll 300 0.5 data/INPUT/ .

 COMMAND LINE ARGUMENTS
    DEPTH                  - depth in which the depth slice will be created
    RESOLUTION             - spatial distance (in degrees) between both latitude and longitude
                             grid points of the depth slice
    INPUT_DIRECTORY        - directory containing the input files
    OUTPUT_DIRECTORY       - directory where the routine will write the output files

 DESCRIPTION
    Reads the depth, the horizontal grid spacing, the input, and output directory names from
    the command line and creates a block model for the desired parameters (defined in 'config.h').
    The routine writes the output to files called PARAMETER_DEPTH_DS.dat.

--------------------------------------------------------------------------
MPI_ABORT was invoked on rank 0 in communicator MPI_COMM_WORLD
with errorcode 1.

NOTE: invoking MPI_ABORT causes Open MPI to kill all MPI processes.
You may or may not see output from other processes, depending on
exactly when Open MPI kills them.
--------------------------------------------------------------------------
```

Figure 1: Help menu for GLL2LL, printed when the user calls the routine with a wrong number of command-line parameters.

6.2 Plotting depth slices

Once you created the desired depth slices, you can easily plot any of them using the provided GMT6 scripts (see the result in Fig. 2):

```
1 $ ./utils/plot_depth_slice.bash vs 300
```

GLL2LL can only create depth slices for the available model parameters. However, you can use those parameters to derive others, such as the V_P/V_S ratio, T_i (transverse isotropy, requires V_{SV} and V_{SH}), and the bulk sound speed (C_{Bulk}) using the Python script CREATE_EXTRA_DEPTH_SLICE. For example, since you have the depths slices for V_P and V_S already, to create a depth slice for the bulk sound speed, just run:

```
1 $ ./utils/create_extra_depth_slice.py cb 300
```

To plot the result:

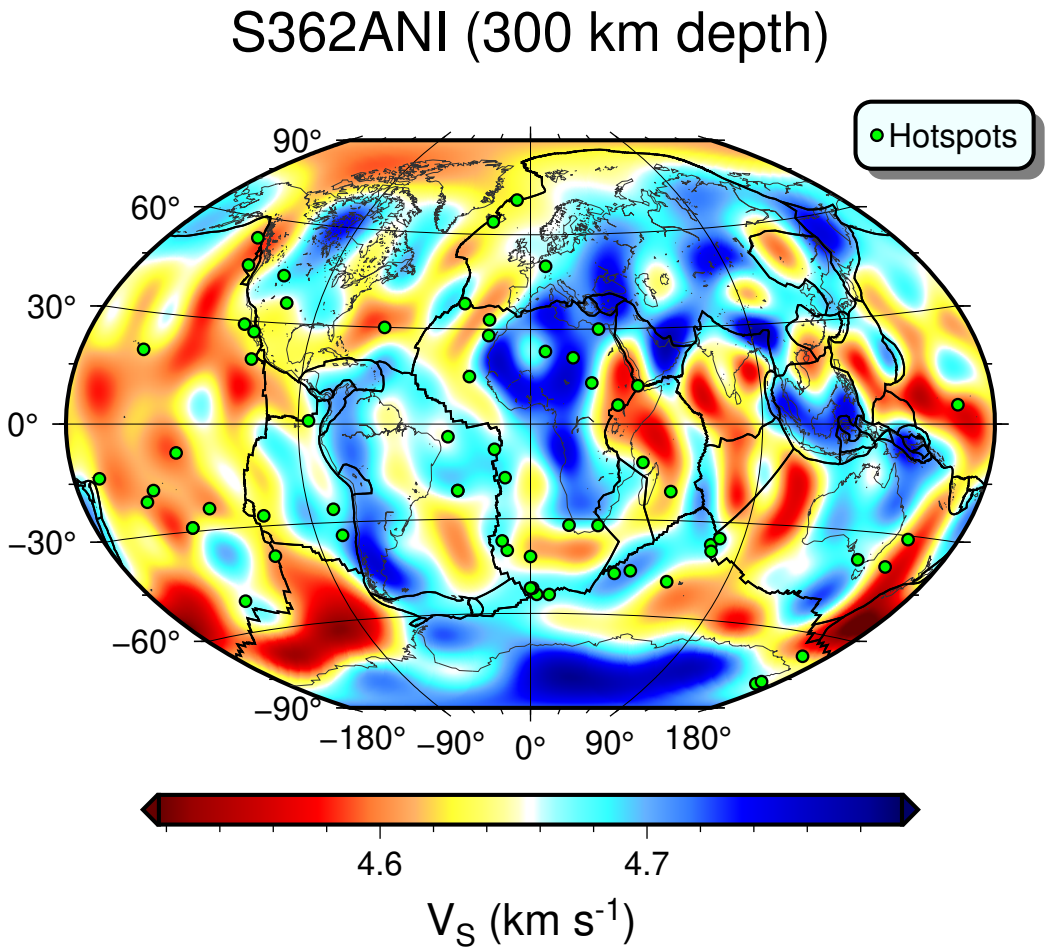


Figure 2: Depth slice at 300 km for V_S. The plate boundaries were extracted from DeMets et al. (1990).

```
$ ./utils/plot_depth_slice.bash cb 300
```

Fig. 3 shows the result.

6.3 Creating vertical cross-sections

The routine GLL2DD is analogous to GLL2LL, but instead of depth slices, it can create vertical cross-sections. For example, to write a vertical cross-section from 80 to 2891 km depth, connecting the points with coordinates

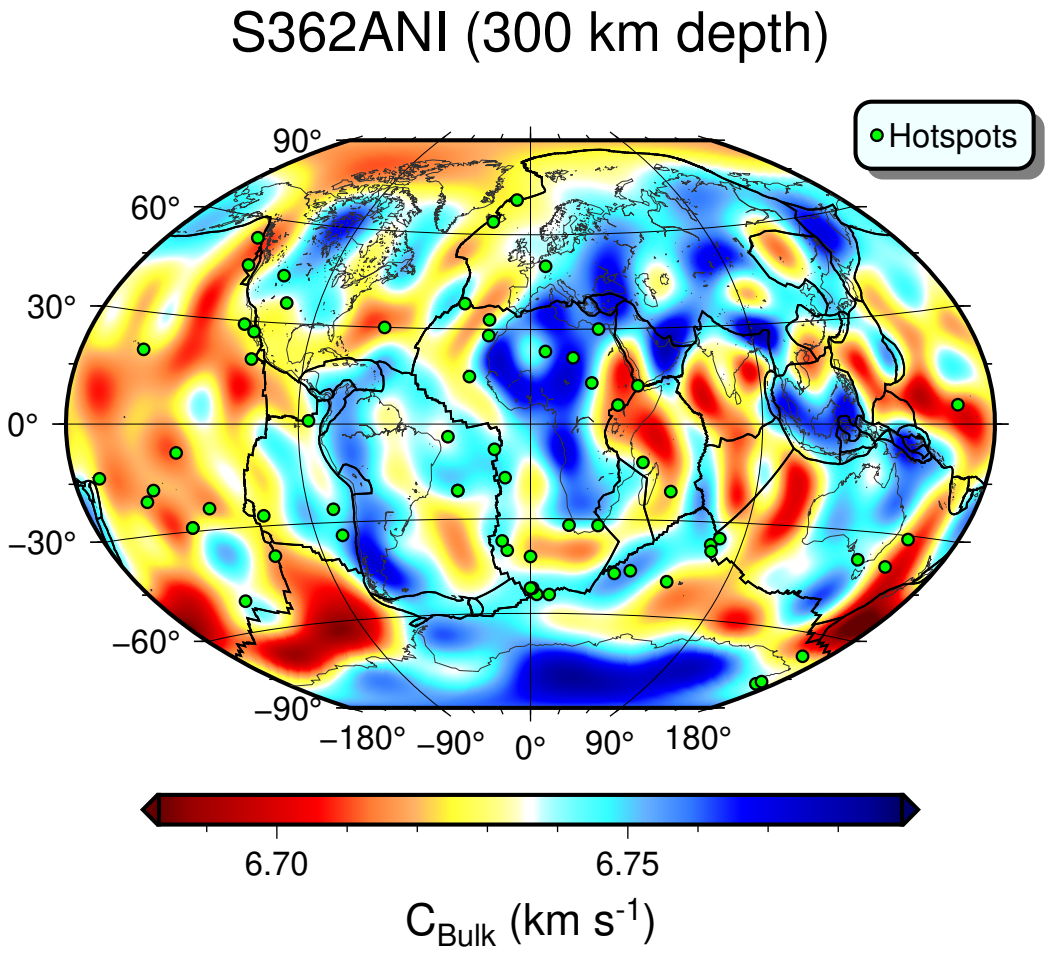


Figure 3: Depth slice at 300 km for the bulk sound speed.

(1.4S, 25.1W) and (23.7N 51.3E) along a geodesic (great circle) with 0.1° of horizontal grid spacing and 1 km of vertical grid spacing, you should run:

```
1 $ mpiexec -n 12 bin/gll2dd 80 2891 -1.4 -25.1 23.7 51.3 0.1 5 data/INPUT/ .
```

6.4 Plotting vertical cross-sections

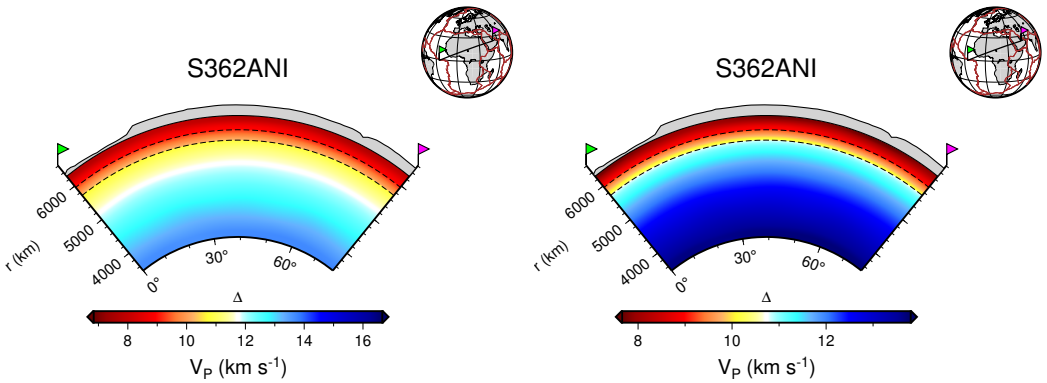
Like the depth slices, there is also a GMT6 routine for plotting vertical cross-sections:

```
$ ./utils/plot_vertical_cross_section.bash vp
```

If no limits are given, the routine tries to set them automatically by using the mean and standard deviation. However, if the result is not satisfying, you can manually set them. From the output of the first plot, we know that the V_P values range between 7.66 and 13.8 km/s. So, you can recreate the figure with:

```
$ ./utils/plot_vertical_cross_section.bash vp 7.66 13.8
```

See the results in Fig. 4:



(a) (b)

Figure 4: a) Vertical cross-section for V_P along the great circle illustrated on the inset map (upper-right corner) using the automatic color bar limits. b) Same figure but with limits manually set.

You can also compute the V_P/V_S ratio (Fig. 5):

```
$ ./utils/create_extra_vertical_cross_section.py vpvs
$ ./utils/plot_vertical_cross_section.bash vpvs
```

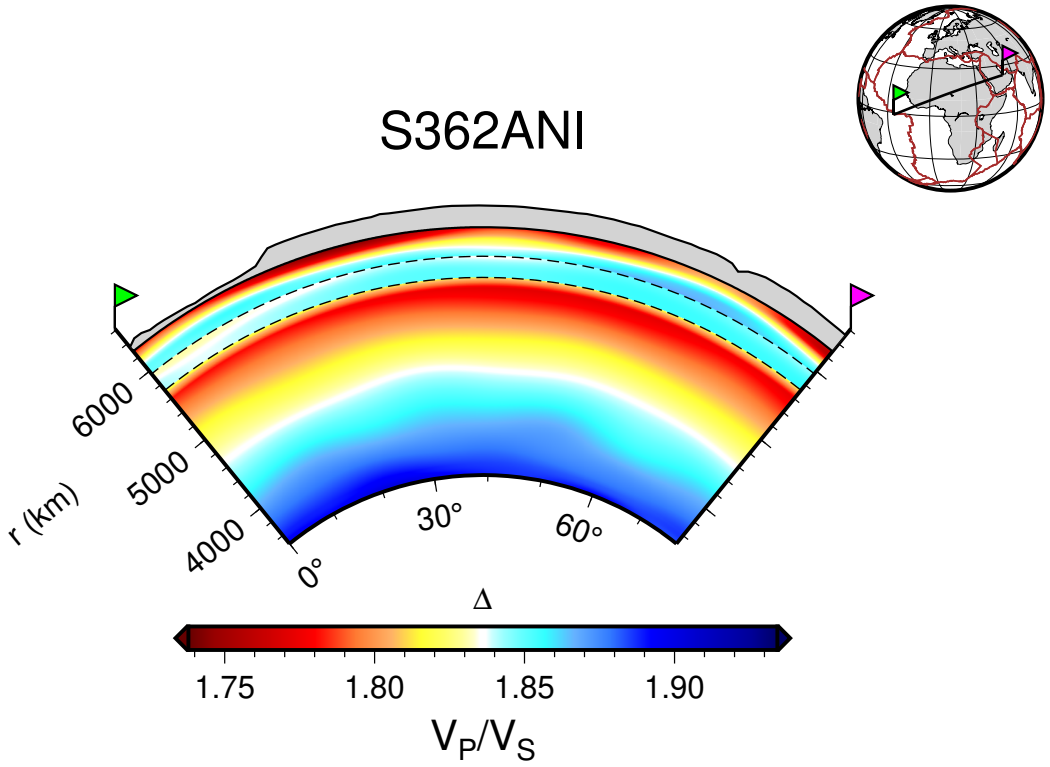


Figure 5: Vertical cross-section for the V_P/V_S ratio.

6.5 Creating one-dimensional profiles

The third visualization routine is for creating one-dimensional profiles at any point on Earth. That routine is serial, so it always uses a single core, no matter how many are requested. However, for compatibility reasons, it should also be run using MPI. The following example creates the profiles for a location in Australia, from the sea level down to the CMB, using a grid spacing of 1 km:

```
1 $ mpiexec -n 1 bin/gll2pf 0 2891 -28 140 1.0 data/INPUT/ .
```

6.6 Plotting one-dimensional profiles

There is also a third GMT6 script for plotting these profiles (see Fig. 6):

```
$ ./utils/plot_profile.bash rho
```

For all of those routines, it is possible to plot the perturbations instead of absolute values. For that, you can run the Python scripts with a letter "d" preceding the code of the parameter (e.g. ds to compute the V_S perturbations) and then plot the resulting files in the same way. The following commands will create and make a plot of the vertical cross-section for the V_S perturbations:

```
$ ./utils/create_extra_vertical_cross_section dvs
$ ./utils/plot_vertical_cross_section dvs
```

However, to compute the perturbations, you first need to calculate the mean model using the GLL2MEAN routine.

7 Computing mean models

Creating a one-dimensional model from a three-dimensional one requires averaging its values at different depths using a reasonable sampling rate. That is a computationally intensive task and requires a long time unless you can afford to use a relatively large number of cores. Even using that low-resolution mesh, to create a 1D profile every 1 km by sampling each depth at 0.5° resolution may take more than one hour, even using 36 cores. So, if you are running these examples on a cluster, you can choose a larger number of cores to speed up the calculations.

In the example below, −5 denotes a starting depth at 5 km above the sea level:

```
$ mpiexec -n 36 bin/gll2mean -5 2891 0.5 1.0 data/INPUT/ .
```

8 Remeshing

When carrying out an adjoint tomography with SPECFEM3D_GLOBE, it is usual that, eventually, we need to increase or decrease the mesh resolution or

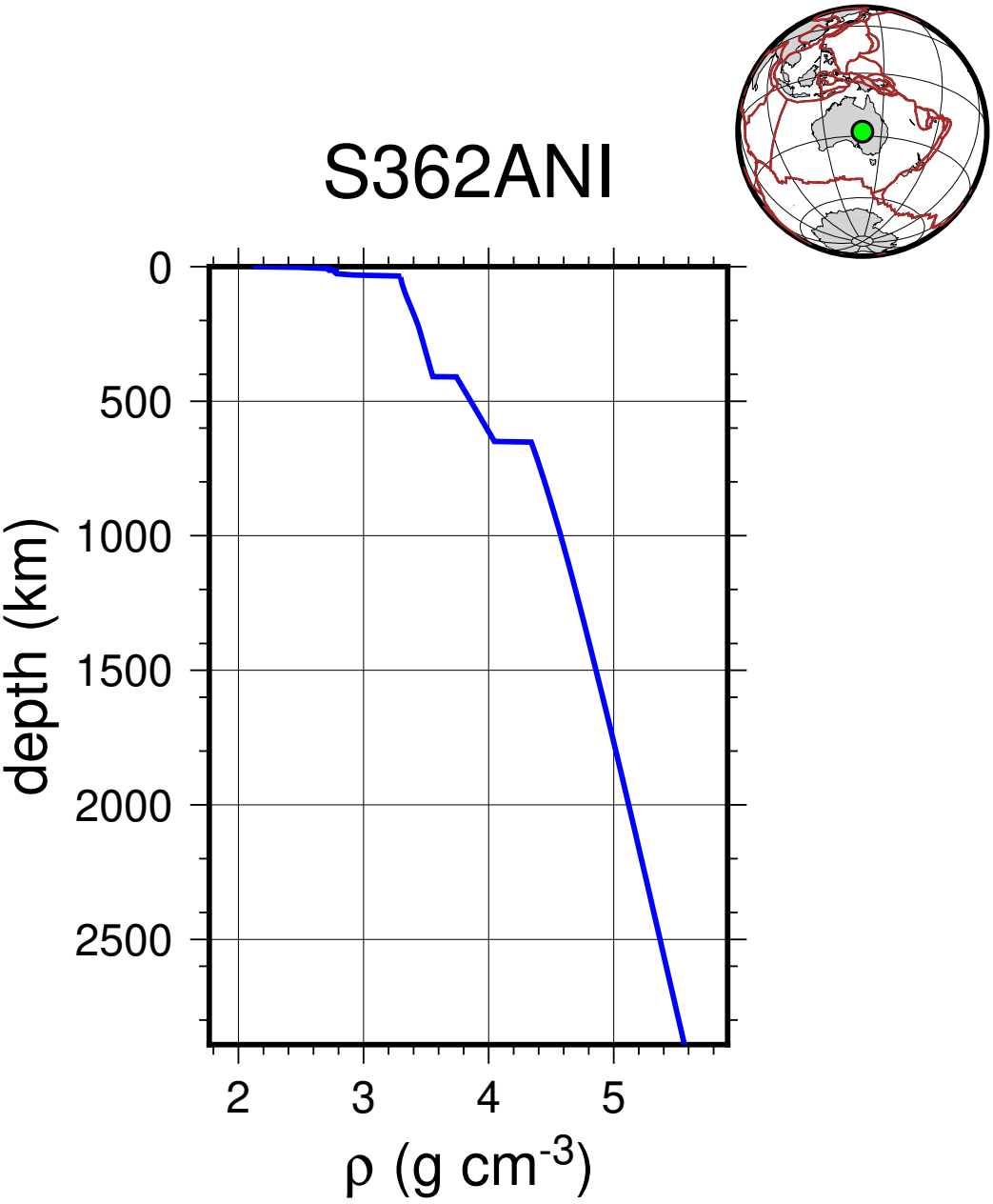
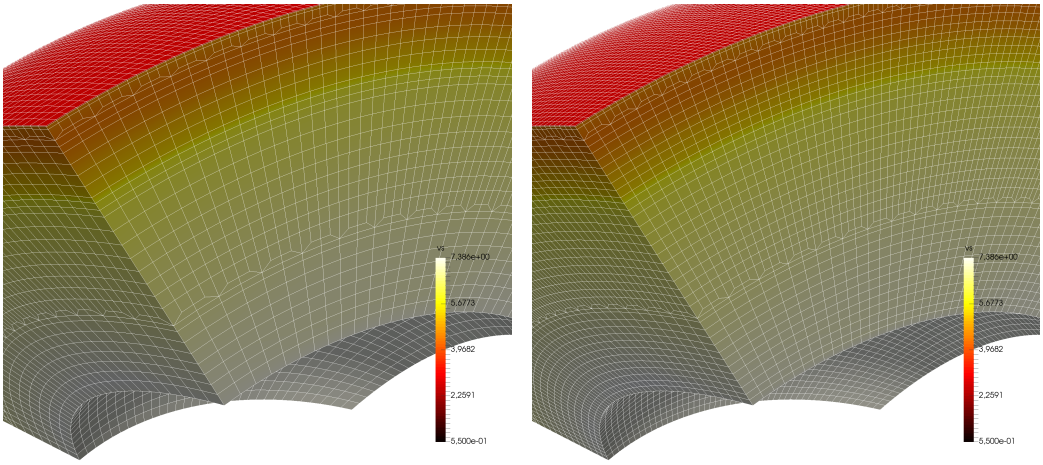


Figure 6: One-dimensional density profile in Australia.

the number of cores for various reasons. That task is way more complicated than it may seem at first glance, as accurately interpolating spectral elements

is far from trivial. Nevertheless, using routine GLL2GLL, you can easily accomplish that. Fig. 7 shows two meshes with different resolutions.



(a) NXI = NETA = 128 (b) NXI = NETA = 192

Figure 7: a) Low-resolution mesh with 128 spectral elements on each side. b) Intermediate-resolution mesh with 192 elements on each side. In both figures, the color palette denotes S-wave velocity (V_S). Extracted from Ciardelli et al., 2020.

To interpolate from one mesh to another, you must set the "config.h" file again. All you need to do is to specify the number of spectral elements a total number of points of both the input and output meshes. Set the **NEL1** flag to 8896 and the **NG1** flag to 592913.

The input topological and model files are under "data/INPUT" already. Put the topological files of the new mesh under "data/OUTPUT". The GLL2GLL routine will create the interpolated model files in "data/OUTPUT" too.

The output mesh may have any number of slices and resolution. Its number os spectral elements and points, as expected, should be provided on **NEL2** and **NG2**. The only requirement to run the routine, like for any other in the package, is that you have enough memory on your machine. In case your memory is limited, you can interpolate one model parameter at a time. Just V_S, for instance.

To run the routine, just do:

```
$ mpiexec -n 24 bin/gll2gll data/INPUT/ data/OUTPUT/
```

Remeshing is useful for changing the mesh resolution, but it is also a critical step for expanding 3D Earth models onto spherical harmonics, as you shall see in section 10.1.

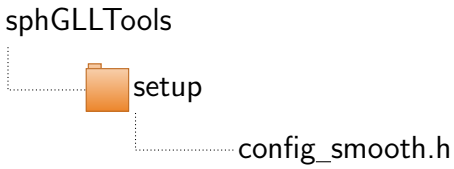
9 Smoothing

Smoothing is equivalent to applying a low-pass spatial filter to the mesh. The SMOOTH routine uses a 3D-Gaussian filter to low-pass any desired model parameter. If you have enough memory, you can smooth all the desired parameters at once. That dramatically speeds up the computations.

Usually, it is essential to smooth sensitivity *kernels*. As explained in the SPECFEM3D_GLOBE manual, even filtering the adjoint sources, the *kernels* often present numerical noise in the form of high-frequency artifacts. Low-pass filtering them is critical before computing the gradients for the model update.

However, in case your model has numerical noise already (perhaps because you didn't filter the *kernels* of the last updates enough), SMOOTH can also be used to get rid of these numerical artifacts. Smoothing your model may also be useful to prevent aliasing when interpolating it to a lower-resolution mesh.

The smoothing routine has a separated configuration file:

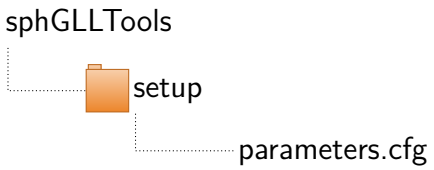


As in the previous cases, just set **NC** to the number of cores (24, in our case), **NEL** to the number of spectral elements (8896), and **NG1** to the number of points (592913).

If you set **SEPARATE_ZONES** as **true**, the routine will smooth the upper mantle, the transition zone, and the lower mantle separately. That is useful if you are filtering a model parameter and want to preserve the 410

and 650 km discontinuities. For kernels, however, you should set that flag as **false**.

The SMOOTH routine can apply different filters in the horizontal direction and the vertical direction. And those filters can also vary with depth. These parameters should be set under:



For example:

```
 1 #Number of layers in the profile
 2 #Smoothing radius for the profile (km)
 3 #Depth of the top of the layer (km)  sigma_h (km)  sigma_v (km)
 4 9
 5 100
 6 -10   100   5
 7 100   100   10
 8 200   100   20
 9 300   100   30
10 410   110   40
11 520   120   50
12 650   130   60
13 1000  140   80
14 2000  150  100
```

Figure 8: Example of smoothing parameters.

In the fourth line, we write the number of layers in the smoothing profile, which is 9, in our example.

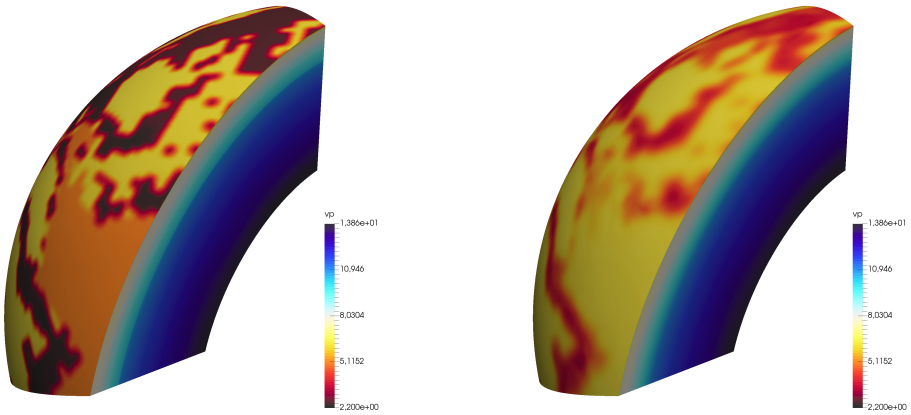
Sharp changes in smoothing with depth can create artificial discontinuities in the model. To prevent this from happening, the smoothing profile itself is convolved with a Gaussian kernel. We specify the width of this filter in the tenth line (100).

From lines 6 to 14, we write the layers. The first layer begins 10 km above the sea level and goes down to 100 km depth. The horizontal smoothing σ_h for this layer is 100 km, and the vertical smoothing σ_v is just 5 km. The last layer begins at 2000 km depth and goes all the way down to the CMB. Notice that if set the starting depth of the first layer at 20 km depth, for instance, the routine will ignore any spectral element above that depth.

After setting all the parameters, run the routine with:

```
$ mkdir smooth
$ mpiexec -n 24 bin/smooth data/INPUT/ smooth/
```

Fig. 9 shows the upper chunk for V_P before and after smoothing:



(a) (b)

Figure 9: a) Model S362ANI + CRUST2.0 with no smoothing. b) The Same model after smoothing with the parameters of Fig. 8.

10 Converting a GLL model to spherical harmonics

Expanding a model onto spherical harmonics facilitates visualization and sharing a lot, but also allows for further analysis, like computing power spectra.

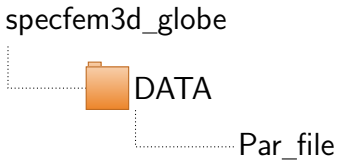
Converting the model from the GLL basis to a spherical harmonics basis is very challenging. However, SphGLLTools has many tools that allow you to do that.

10.1 Remeshing before the expansion

To expand the model onto spherical harmonics, we need a spherical mesh. Disabling the ellipticity and the internal discontinuities are enough to make the lower mantle and the transition zone spherical, but the crust and the upper mantle remain distorted due to the surface topography. Switching off the surface topography is possible but creates other problems as it moves the spectral elements along the radial direction, creating artifacts in the upper mantle. Besides, three-dimensional models have a doubling layer right beneath the crust that extends down to 120 km depth.

The proper way of dealing with the upper mantle is interpolating it to a perfectly spherical mesh. The right choice is STW105 (Kustowski et al., 2008), which is the 1D reference model for S362ANI. Choosing the correct reference model is crucial, as different models may have internal discontinuities at different depths.

To create the new mesh, go back to:

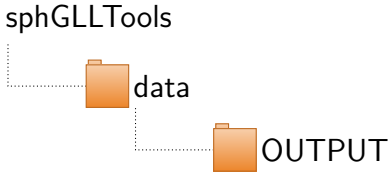


Change **MODEL** to 1D_ref and **TOPOGRAPHY** to **false**. You can also set **SAVE_MESH_FILES** as **false**, as the new model files will be created by the interpolation routine.

Then, run the following commands to recompile and create the new mesh:

```
$ make clean
$ make -j4 all
$ mpiexec -n 24 bin/xmeshfem3D
```

Copy the new topological files (proc000???_reg1_solver_data.bin) to:



In the "config.h" file, set **NEL2** to 8896 and **NG2** to 592913. As you can see, the STW105 mesh has the same number of spectral elements and points as the S362ANI mesh. Also, make sure of enabling the interpolation of V_P, V_S, and ρ.

Run the interpolation routine:

```
$ mpiexec -n 24 bin/gll2gll data/INPUT/ data/OUTPUT/
```

Taking some depth slices from the original model and the interpolated one to compare is always a good practice to make sure that everything looks fine.

10.2 Setting up the B-splines

The radial basis is made of cubic B-splines, whose knots must be carefully set to achieve good results. SphGLLTools provide examples of knots files that were fine-tunned for S362ANI, called "knots_Z?.dat". Each region has its own set of splines because B-splines cannot handle discontinuities properly. They strongly oscillate wherever a zero-order discontinuity is present (Fornberg and Flyer, 2007). That's why we must expand each region separately. Besides, the upper mantle requires more spherical harmonics coefficients to be properly represented than the transition zone and the lower mantle.

Each "knots_Z?.dat" file is composed of the number of knots, the degree of the B-splines, approximate the minimum, and the maximum radius of the region, and the knots.

All values are normalized by the Earth's radius. Therefore, 0.900 corresponds to a radius of 3440 km (2930 km depth). The code will use these minimum and maximum values to select the spectral elements of each region. After it selects all of them, it will calculate the exact radial boundaries of the zones.

The routine responsible for fine-tuning the B-splines is SETSPL. It requires the "knots_Z?.dat" files and the mean model of the parameter used for the fine-tuning. You may use "vs.dat", created by GLL2MEAN in section 7.

To check the knots for the three zones, use:

```
$ mpiexec -n 24 bin/setspl vs 2 data/OUTPUT/ .
$ mpiexec -n 24 bin/setspl vs 3 data/OUTPUT/ .
$ mpiexec -n 24 bin/setspl vs 4 data/OUTPUT/ .
```

For each region, SETSPL calculates a misfit between the mean model provided and the B-splines radial expansion. You can move the position of the knots or add/remove more splines to try to decrease the misfit. It's also useful to visualize the quality of the fitting. For that, SETSPL writes out the "vs_Z?_KC.dat" files.

To plot the B-splines, run:

```
$ ./utils/plot_B_splines.py vs
```

Fig. 10 shows the result:

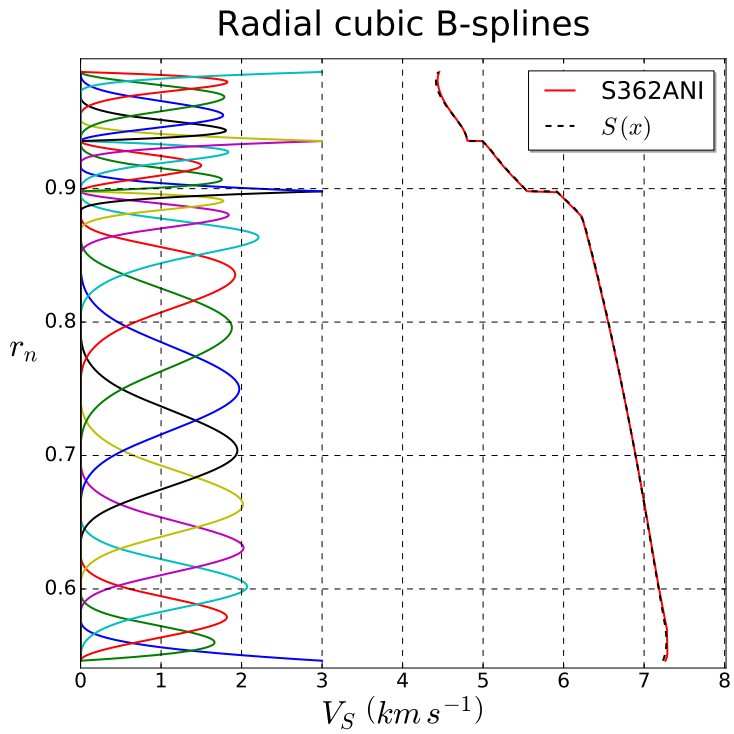


Figure 10: Twenty-five cubic *B-splines* used in the radial direction in the S362ANI expansion. The mean V_S as a function of depth are shown in red. The black dashed line shows $S\,(x)$, the reconstruction of the model from the *B-splines* and the coefficients.

In case you observe a reasonable agreement like the one in Fig. 10, you can proceed to the expansion of the coefficients.

10.3 Expanding onto spherical harmonics

The routine to carry out the spherical harmonics expansion is GLL2MNS. Its input files are also the "knots_Z?.dat".

To expand V_P, V_S and ρ for the three regions, run:

```
$ mpiexec -n 24 bin/gll2mns vp 25 2 data/OUTPUT/ .
$ mpiexec -n 24 bin/gll2mns vp 23 3 data/OUTPUT/ .
$ mpiexec -n 24 bin/gll2mns vp 20 4 data/OUTPUT/ .
$ mpiexec -n 24 bin/gll2mns vs 25 2 data/OUTPUT/ .
$ mpiexec -n 24 bin/gll2mns vs 23 3 data/OUTPUT/ .
$ mpiexec -n 24 bin/gll2mns vs 20 4 data/OUTPUT/ .
$ mpiexec -n 24 bin/gll2mns rho 25 2 data/OUTPUT/ .
$ mpiexec -n 24 bin/gll2mns rho 23 3 data/OUTPUT/ .
$ mpiexec -n 24 bin/gll2mns rho 20 4 data/OUTPUT/ .
```

After the expansion, the routine uses the coefficients to recreate the model and calculates the RMSD between the original model and the expanded version. By checking various degrees and comparing their RMSDs, you can have an idea of the optimal degree for the expansion. Be careful with the lower mantle as it is big and the intermediate part (1500 to 2000 km depth) requires a lower degree than its top and its bottom. Sometimes, the degree that gives you the minimum misfit overall will overshoot the intermediate lower mantle.

Using a degree higher than required create numerical artifacts in the expansion. The ideal degree can also vary from one model parameter to another. That's why the best way of checking your results is, again, comparing some depth slices of the expansion with the original model.

The output files are called "mns_Z?_???.dat".

In section 13, you will learn how to recreate the model from the coefficients.

11 Creating the crustal block model

The crust cannot be expanded onto spherical harmonics and B-splines, as it has many zero-order discontinuities that cannot be avoided. So, one way to represent the crust is by using a block model.

To create a block model from 5 km above the sea level down to 80 km depth, sampling the mesh every 0.5° in the horizontal and 1 km in the vertical, you need to run:

```
$ mpiexec -n 12 bin/gll2bk -5 80 0.5 1.0 data/INPUT/ .
```

Notice that you should create the model from the original mesh to represent the topography properly. The block model is the first region of the model. That's why the upper mantle is called Zone 2.

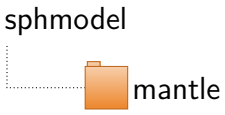
12 Setting up SphModel

The next step requires that you create the files with the accurate positions of the knots. These files are called "knots_Z?.dat" (notice the replacement of Zone? by Z? in the names).

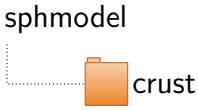
For that, you can use SET_KNOTS:

```
$ ./utils/set_knots.py vs
```

Now, copy the files "knots_Z?.dat" and "mns_Z?_???.dat" to the directory:



Copy the binary files of the block model "???.bin" to:



Enter into the "sphmodel" directory and compile the routines:

```
$ make -j4 all
```

Because SphModel is intended for sharing your spherical harmonics model, it does not use parallelization, as not all users are familiar with OpenMPI. Besides, all the large arrays use dynamic memory allocation, which prevents stack overflow in systems with a small stack size limit.

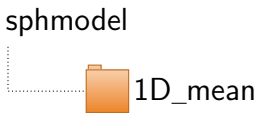
It is advisable to compute the mean models for SphModel using the expansion itself, avoiding the creation of artifacts in the radial direction when plotting the perturbations.

For that, use the BKMNS2MEAN:

```
$ ./bin/bkmns2mean vp -5 2891 0.5 1.0 20
$ ./bin/bkmns2mean vs -5 2891 0.5 1.0 20
$ ./bin/bkmns2mean rho -5 2891 0.5 1.0 20
```

Because that routine is serial, it can take several hours to compute each parameter. One way of speeding up the process is opening multiple tabs in your terminal and running one parameter on each one of them. That is a primitive kind of parallelization, but works.

Then, copy the files "vp.dat", "vs.dat" and "rho.dat" to:



That completes the expansion. Just write the relevant information to your model inside the "README.md" file, and you are ready to share it with other people. You can reduce the final size of your model package by compressing it:

```
$ tar -cvJf your_happy_model.tar.xz sphmodel
```

13 Advanced visualization with SphModel

The following sections will show how you can use SphModel to do a more sophisticated visualization of the model.

13.1 Creating and plotting depth slices

To create a depth slice of the expanded model up to degree 10 run:

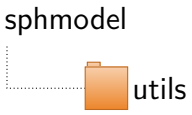
```
$ ./bkmns2ll vs 100 0.5 10
```

The default behavior, if you don't provide the last parameter, is to expand all the coefficients. Notice that limiting the degree of the expansion only makes sense for depth slices below 80 km.

Besides the portability, the possibility of choosing the maximum degree, and the fact that these routines don't require OpenMPI, another convenience is that you can directly compute the perturbations just by adding a "d" before the parameter code. Such as:

```
$ ./bkmns2ll dvs 100 0.5 10
```

To compute V_P/V_S ratios, transverse isotropy and the bulk sound speed, use the create_extra_*.py routines under:



To plot the depth slices, use the GMT scripts in the same directory. They are identical to the GMT scripts used in section 6.

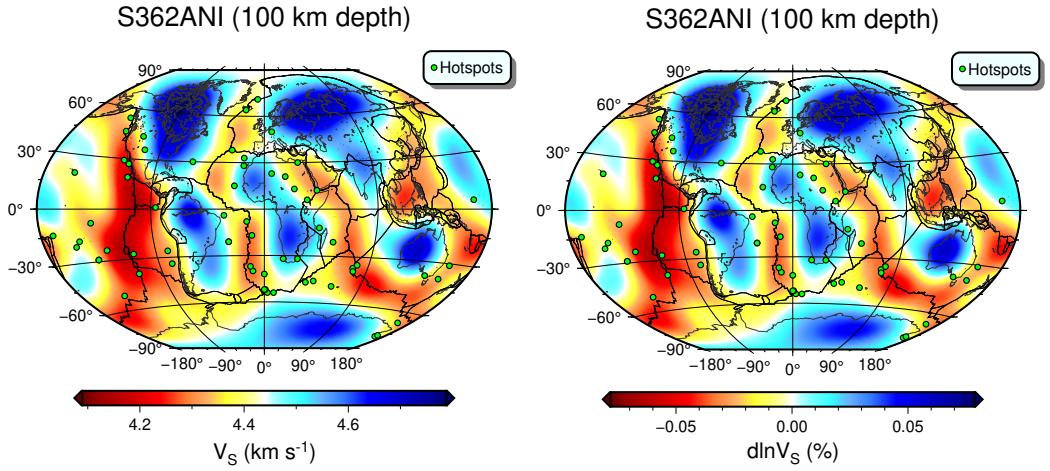
```
$ ./utils/plot_depth_slice.bash vs 100
$ ./utils/plot_depth_slice.bash dvs 100
```

See the results in Fig. 11:

13.2 Creating and plotting vertical cross-sections

To create a vertical cross-section expanding all the coefficients:

```
$ ./bin/bkmns2dd dvs 80 2891 −1.4 −25.1 23.7 51.3 0.1 2.0
```



(a) (b)

Figure 11: a) Depth slice for V_S at 100 km depth. b) Same depth slice, now showing the perturbations.

To plot it (see Fig. 12):

```
$ ./utils/plot_vertical_cross_section.bash dvs
```

13.3 Creating and plotting one-dimensional profiles

Two examples of one-dimensional profiles expanded up to degree 10 are:

```
$ ./bin/bkmns2pf vp 10 2891 0.8 −24.2 1.0 10
$ ./bin/bkmns2pf dvs 10 2891 0.8 −24.2 1.0 10
```

You can plot them with (13):

```
$ ./utils/plot_profile.bash vp
$ ./utils/plot_profile.bash dvs
```

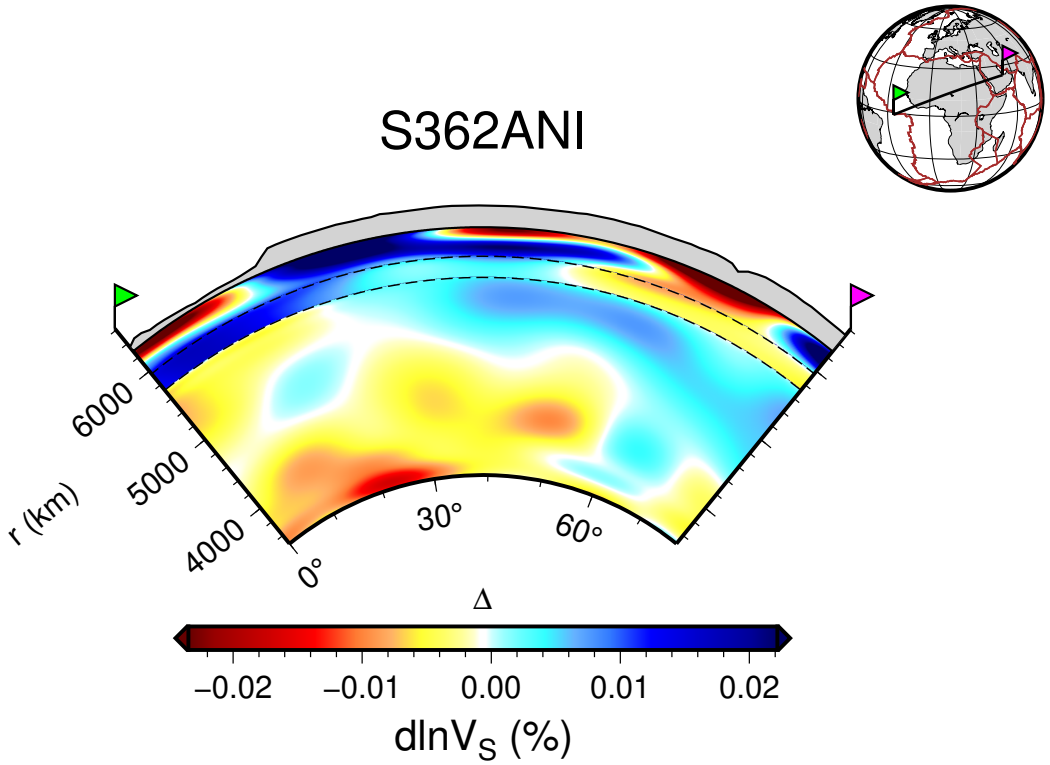


Figure 12: Vertical cross-section showing the V_S perturbations for a great circle crossing North Africa from 80 km depth to the CMB.

13.4 Power spectra

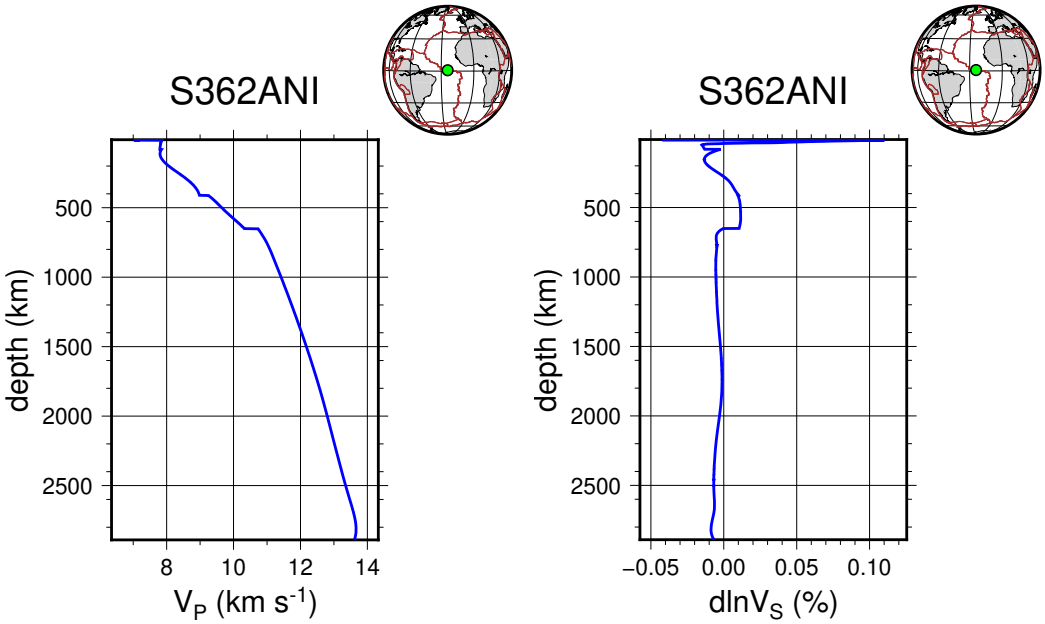
One more analysis that can be carried out using spherical harmonics is power spectra. They are useful for assessing the relative importance of each frequency in the model.

The routine POWSPEC simultaneously creates the one-dimensional power spectrum (power per degree) and the two-dimensional version (power per depth and degree).

Run:

```
1 $ ./bin/powspec vs 20
```

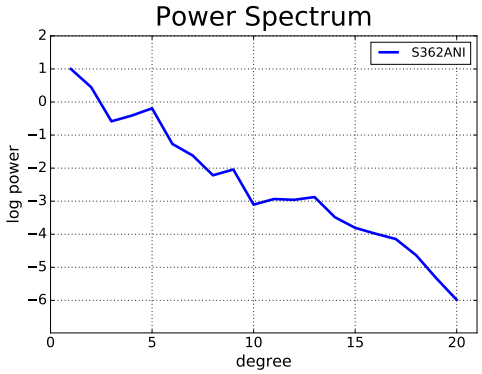
And plot the results using (see Fig. 14):



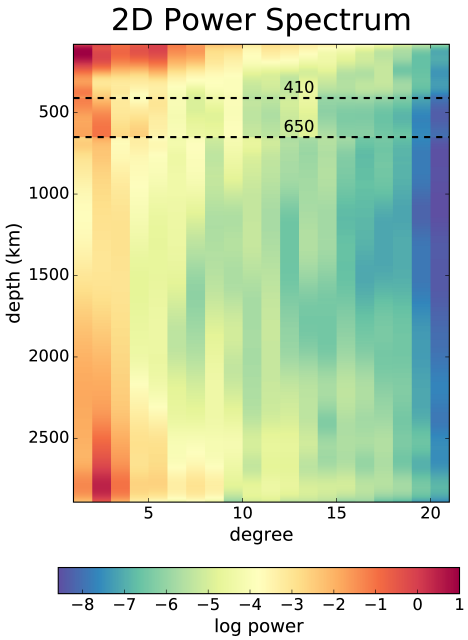
(a) (b)

Figure 13: a) One-dimensional profile for V_P from 10 km depth to the CMB in the Mid-Atlantic Ridge. b) The same profile, but now showing the V_S perturbations.

```
1 $ ./bin/powspec vs 20
```



(a)



(b)

Figure 14: a) One-dimensional power spectrum of V_S for S362ANI. b) Two-dimensional power spectrum of V_S for S362ANI.

List of Figures

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