SEM-DSM hybrid method
User Manual

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Chapter 1

Introduction

Despite computational capability of High Performance Computing (HPC) was being dramatically enhanced, simulating high frequency (e.g. 1Hz or higher) seismic wave propagation at the global scale is still prohibitive. Thus, we develop this software package SEM-DSM-hybrid to efficiently compute teleseismic synthetics with a local 3D structure limited in the source-side, mid-way or receiver-side. Currently, only the source-side SEM-DSM coupling is implemented and carefully benchmarked in this package. A receiver-side SEM-DSM coupling has been implemented by Monteiller et al. [2012]. In the future, we may add the receiver-side and mid-way coupling in this package.

1.1 General background

In this hybrid method, we combine the advantages of SPECFEM3D_Cartesian and DSM to efficiently compute teleseismic synthetics. As a 1D synthetic simulation tool, DSM has the advantage of high accuracy and cheap computational cost [Geller and Ohminato, 1994, Geller and Takeuchi, 1995, Takeuchi et al., 1996, Kawai et al., 2006]; As a 3D Spectral Element method (SEM), SPECFEM3D_Cartesian can handle full 3D velocity structures, topography, fluid/solid interfaces, and complex geometries accurately [Komatitsch and Tromp, 1999, 2002]. If you want to know more about SPECFEM3D and DSM, please read the relevant literature.

Our source-side SEM-DSM coupling is composed of three steps, SEM simulation, DSM computation and the final step of coupling (Fig. 1.1). More details about the coupling theory and benchmark examples are described in Wu et al. [2018]. Our hybrid method is useful for a series of problems in seismology, such as imaging 3D structures of a subducting slab or a mid-ocean ridge and studying source parameters with 3D source-side complexities using teleseismic waveforms.

1.2 Citation

If you use this DSM-SEM hybrid method, please cite Wu et al. [2018].

We have used this method to investigate some earthquakes and you may be also interested in these following articles: Wang et al. [2017, 2018]

1.3 Support

This work was supported by funding from National Basic Research Program of China (973 Program) through grant 2014CB845901. Shengji Wei is supported by the internal grant (M4430255) of Earth Observatory of Singapore.

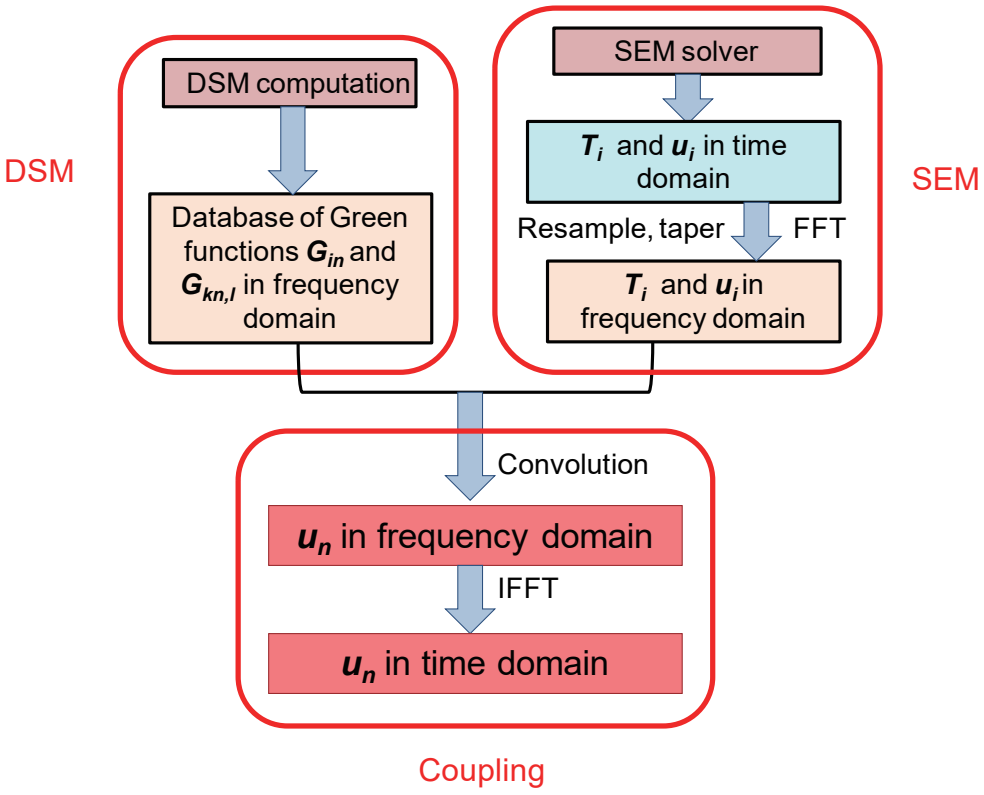


Figure 1.1: Work flow of SEM-DSM coupling at source-side.

Chapter 2

Getting Started

To download the SEM_DSM_hybrid software package, type this:

```
git clone --recursive --branch devel https://github.com/wenbowu-geo/SEM_DSM_hybrid
```

Before compiling the packages, you may need to load all the needed modules (e.g. openmpi, intel et al.). We have successfully compiled this software package on Tiger supercomputer in Princeton University, Fram cluster at SeismoLab of Caltech and TianHe-2 supercomputer in China.

2.1 Compile SPECFEM3D_Cartesian packages

The SPECFEM3D_Cartesian manual provides detailed information of compiling the codes. We modified some subroutines, but most compiling tricks introduced there should also work here. First, you need to go to the SEM root directory `SEM_DSM_hybrid/specfem3d` and run the `configure` shell script to produce the file `Makefile`:

```
>cd SEM_DSM_hybrid/specfem3d/
>./configure FC=ifort CC=icc MPIFC=mpif90 --with-mpi
```

You can replace the Intel compilers above (ifort and icc) with other compilers if you want to; for instance use GNU compilers FC=gfortran and FC=gcc instead.

Finally, type `make all` to compile the codes

```
>make all
```

To be consistent with DSM, we use cubed-sphere coordinates in SEM. We provide tools to convert geographical topography, as a function of latitude and longitude, to that in cubed-sphere coordinates (ξ,η). The first tool `xcubedsphere_topo` helps you convert topography of interfaces in SEM model. The topography is tapered near the boundaries of SEM box and some extremely high and/or low topography/bathymetry could be truncated if necessary. To compile this tool, type

```
>cd SEM_DSM_hybrid/specfem3d/src/cubedsphere_topo/
>make clean
>make
```

Another tool `xcubedsphere_topo_FindOcean` does a similar job, but it does not taper and/or truncate the topography. This tool is needed when you incorporate ocean. To compile this tool, type

```
>cd SEM_DSM_hybrid/specfem3d/src/cubedsphere_topo_FindOcean/
>make clean
>make
```

2.2 Compile DSM codes

To compile DSM, type

```
>cd SEM_DSM_hybrid/DSM/src/
>make
```

Again, you may need to replace the Intel compiler `ifort` with `gfortran` in the `Makefile`.

2.3 Compile coupling codes

We provide two different interpolation schemes to accomplish the final step of coupling (see Chapter 5).

To compile the codes of linear interpolation scheme, type

```
>cd SEM_DSM_hybrid/coupling/Linear_piecewise_interpolation/
>make
```

To compile the codes of Lagrange interpolation scheme, type

```
>cd SEM_DSM_hybrid/coupling/Lagrange_interpolation/
>make
```

Chapter 3

SEPCFEM3D

The same as the original SPECFEM3D-Cartesian, running SEM in our coupling mode is composed of three steps: meshing, generating databases and running solver. The usage of SPECFEM3D-Cartesian in our hybrid method is almost the same as the original code, so we strongly recommend users to read the SPECFEM3D-Cartesian Manual before running this package. However, some changes are made to implement the hybrid method and the following subsections list these changes.

3.1 Meshing with `xmeshfem3D` in a cubed-sphere coordinate system

Meshing is the first step of running SPECFEM3D-Cartesian. The original package provides two ways to do meshing: (1) A professional meshing tool, such as Cubit, Gmesh or other meshing tools, or (2) internal meshing package `xmeshfem3D`. The current version of our SEM-DSM coupling does not support external meshing tools and only allows users to use the internal meshing `xmeshfem3D`. In order to couple SEM with DSM, we made the below changes to the original SPECFEM3D-Cartesian.

First, we use cubed-sphere coordinates, instead of UTM coordinates in the original code. Using the original `xmeshfem3D`, the model must be a regular box, whose edges are aligned with the X, Y and Z axises. In our SEM-DSM coupling method, we modify the subroutines to create a small chunk in a cubed-sphere coordinate system, instead of a X-Y-Z box. By doing that, the curvature of interfaces within the Earth are reserved. Another advantage of cubed-sphere coordinates is making elements at the coupling boundaries have regular geometries, that results in a small number of depths of GLL points and therefore significantly simplifies DSM computation.

Secondly, ocean water, if existing, is incorporated via `xmeshfem3D`. Investigating effects of ocean water on teleseismic waves is one of the major motivations of developing this code, so we write a subroutine named

```
redefine_ocean_land.f90
```

to incorporate ocean water. Running `xmeshfem3D` reads the file `real_bathymetry_topography`, which specifies the real topography/bathymetry as a function of cubed-sphere coordinates (ξ,η), and then define elements as either solid media type or fluid media type.

The two main parameter files in the meshing step are `Par_file` and `Mesh_Par_file`. In the file `Par_file`, we keep all the previously used parameters and add the below new ones:

`CUBED_SPHERE_PROJECTION` You must set this flag to `.true.` when the SEM-DSM coupling mode is enabled.

`COUPLING_TYPE` 1 for source-side coupling, 2 for station-side coupling, 3 for mid-way coupling and 4 for no coupling. The current version of our code only supports source-side coupling mode or no coupling mode, so do not set it to 2 and 3.

Other parameters needed by `xmeshfem3D` are specified in the file `Mesh_Par_file`. The functions of most parameters in this file do not change in our coupling method, except the below ones:

`LATITUDE_MIN` is not functional. Instead, the dimension of SEM box is defined in another file `SEMtoTele_Par_file`.

LATITUDE_MAX is not functional.

LONGITUDE_MIN is not functional.

LONGITUDE_MAX is not functional.

DEPTH_BLOCK_KM has the same meaning as that in the original codes, but its unit is `km`.

UTM_PROJECTION_ZONE is not functional.

SUPPRESS_UTM_PROJECTION is not functional.

INTERFACES_FILE specifies this name of file containing the information of all interfaces. Its format is not changed, but the topography of each individual interface is given in the cubed-sphere coordinates. We provide two executable files `xcubedsphere_topo` and `xcubedsphere_topo_FindOcean` to convert topography (lat,lon) into topography (ξ,η) (see subsections 6.3 and 6.4).

CUBED_SPHERE_PROJECTION is a new parameter in our SEM-DSM code. You must set this flag to `.true.` when the SEM-DSM coupling mode is enabled.

NDOUBLINGS The number of horizontal doubling layers. In our SEM-DSM coupling, it must be set to either `1` or `2` if `USE_REGULAR_MESH` is set to `.true.`. In the original code, it can be larger than `2`.

NZ_DOUBLING_1 The position of the first doubling layer (only interpreted if `USE_REGULAR_MESH` is set to `.true.`).

NZ_DOUBLING_2 The position of the second doubling layer (only interpreted if `USE_REGULAR_MESH` is set to `.true.` and if `NDOUBLINGS` is set to `2`). Doubling layers must be at least `2` layers apart. The layer count starts from the bottom layer.

THICKNESS_OF_X_PML The thickness of PML layer at max_ξ and min_ξ. Different from the original code, the unit in the SEM-DSM coupling mode is `degree` (1 degree $\approxeq$ 111.19 km at the free surface of the Earth). Typically, a 0.1 degrees (roughly 11 km) thick PML layer works well for seismic waves with a period range of 0.5s-100s and 0.2 degrees is sufficiently high. However, you must set it thicker than the size of at least one element on the ξ direction. Otherwise, PML layer has 0 km thickness and therefore does not work well. If irregular meshes are used and `NDOUBLINGS`=1, the final PML thickness must be 2$\times$ a multiple of finer_element_size on the ξ direction, so this parameter must be between 2$\times$M$\times$finer_element_size and smaller than (2$\times$M+1)$\times$finer_element_size. If `NDOUBLINGS`=2, 2$\times$M$\times$finer_element_size is replaced by 4$\times$M$\times$finest_element_size.

THICKNESS_OF_Y_PML The thickness of PML layer at max_η and max_η, in an unit of degree. See more details in the description of the above parameter `THICKNESS_OF_X_PML`.

THICKNESS_OF_Z_PML The thickness of PML layer at the bottom of SEM model, **in unit of meter**. Usually, a value of 10000 - 20000 m is proper. The same as `THICKNESS_OF_X_PML` and `THICKNESS_OF_Y_PML`, you must guarantee the thickness of PML layer larger than one element size on the vertical direction. If irregular meshes are used, the transition from fine to coarse grids usually happens well above the bottom boundary of SEM box, so just set this parameter to a thickness of a few elements at the most bottom.

NREGIONS Do not specify any fluid block here. The ocean water is defined by the file

```
real_bathymetry_topography
```

In addition to the file `Mesh_Par_file` and `Par_file`, another file `SEMtoTele_Par_file` is new in SEM-DSM coupling mode. It contains the following parameters:

ANGULAR_WIDTH_XI_IN_DEGREES The dimension of SEM box along the ξ direction, in an unit of degree. If

```
GAMMA_ROTATION_AZIMUTH=0.0,
```

positive ξ at the central position of SEM box points to the East or longitude direction.

ANGULAR_WIDTH_ETA_IN_DEGREES The dimension of SEM box along the η direction, in an unit of degree. If

```
GAMMA_ROTATION_AZIMUTH=0.0,
```

positive η at the central position of SEM box points to the North direction.

CENTER_LATITUDE_IN_DEGREES Latitude of the central position of SEM box. Usually, it is close to the latitude of the earthquake hypocenter.

CENTER_LONGITUDE_IN_DEGREES Longitude of the central position of SEM box. Usually, it is close to the longitude of the earthquake hypocenter.

GAMMA_ROTATION_AZIMUTH How much the SEM box is counterclockwise rotated, in an unit of degree. Sometimes, rotating the SEM box would save computational costs or simplify the model setup.

nx_TopographyTaper The number of elements used to make the topography tapering along the ξ direction. A number between 4-20 is usually proper.

ny_TopographyTaper The number of elements used to make the topography tapering along the η direction. A number between 4-20 is usually proper.

nx_NoTopography The number of elements on the left side $\xi = max\_\xi$ and right side $\xi = min\_\xi$ of SEM box, where topography is tapered to zero. In the current version, topography is not allowed in the PML absorbing layers and on the coupling boundary, so `nx_NoTopography` must be sufficiently large to satisfy that condition. A number between 4-20 is usually proper, but it also depends on the parameters `THICKNESS_OF_X_PML`, `ix_LowBound` and `ix_HighBound`.

ny_NoTopography The number of elements on left side $\eta = max\_\eta$ and right side $\eta = min\_\eta$ of SEM box, where topography is tapered to zero. In the current version, topography is not allowed in PML absorbing layers and on the coupling boundary, so `ny_NoTopography` must be sufficiently large to satisfy that condition. A number between 4-20 is usually proper, but it also depends on the parameters `THICKNESS_OF_X_PML`, `iy_LowBound` and `iy_HighBound`.

ix_LowBound The left position of coupling boundary, in unit of number of elements. This parameter must be properly set to make the coupling boundary within the no topography band and outside the PML layer (see subsection 6.1 and Fig. 6.1). If regular meshes are used, the number must be a multiple of 2 for `NDOUBLINGS`=1 and a multiple of 4 for `NDOUBLINGS`=2.

ix_HighBound The right position of coupling boundary, in unit of number of elements. This parameter must be properly set to make the coupling boundary within the no topography band and outside the PML layer. If regular meshes are used, the number must be a multiple of 2 for `NDOUBLINGS`=1 and a multiple of 4 for `NDOUBLINGS`=2.

iy_LowBound The upper position of coupling boundary, in unit of number of elements. This parameter must be properly set to make the coupling boundary within the no topography band and outside the PML layer. If regular meshes are used, the number must be a multiple of 2 for `NDOUBLINGS`=1 and a multiple of 4 for `NDOUBLINGS`=2.

iy_HighBound The lower position of coupling boundary, in unit of number of elements. This parameter must be properly set to make the coupling boundary within the no topography band and outside the PML layer. If regular meshes are used, the number must be a multiple of 2 for `NDOUBLINGS`=1 and a multiple of 4 for `NDOUBLINGS`=2.

ir_BoundTop The top of coupling boundary, in unit of number of elements. For source-side SEM-DSM coupling, this number must be equal to NZ, the total number of elements on the vertical direction.

ir_BoundBot The bottom position of coupling boundary, in unit of number of elements. A number between 3-5 is usually good, but you must ensure the coupling boundary is above the PML layer (see Fig. 6.1).

LOW_RESOLUTION Choose low or high spatial resolution coupling mode. If .True., only the central GLL points of coupling faces are used. If .False., the displacement and strain on all the coupling GLL points are saved to get more accurate results, but it needs much more disk storage and slows down the SEM computation.

NSTEP_BETWEEN_OUTPUTBOUND How many time steps we save out the displacement and traction on the coupling GLL points. By doing so, we do not need to allocate variables with large size, that could exceed the maximum allowed memory size and/or slow down the running. Note that 'time step' here is after decimating.

DECIMATE_COUPLING Resampling rate of the displacement and traction. Resampling the displacement and traction helps us save disk storage, but resampling them down could bring in large errors. Thus, you should avoid too much information missed by resampling, e.g. ensure at least eight points per source duration. However, when you use Dirac delta source time function or the specified source duration is smaller than the minimum period resolved, resampling rate must be 1. Otherwise, DECIMATE_COUPLING>1 could cause large errors.

NPOINTS_PER_PACK The number of GLL points in one output package. In order to avoid files with large size, we divide the coupling GLL points into a number of groups and the output results of each group are saved in individual file. A number between 200-1000 is usually good.

Some output files after running xmeshfem3D are:

```
OUTPUT_FILES/DATABASES_MPI/proc??????_Database
OUTPUT_FILES/DATABASES_MPI/proc??????_TeleEle_rBot.info
OUTPUT_FILES/DATABASES_MPI/proc??????_TeleEle_rTop.info
OUTPUT_FILES/DATABASES_MPI/proc??????_TeleEle_xHigh.info
OUTPUT_FILES/DATABASES_MPI/proc??????_TeleEle_xLow.info
OUTPUT_FILES/DATABASES_MPI/proc??????_TeleEle_yHigh.info
OUTPUT_FILES/DATABASES_MPI/proc??????_TeleEle_yLow.info
```

Among the above files, the first one is from the original code and other files contain the information of coupling elements.

3.2 Generating databases

Running xgenerate_databases is also almost the same as the original package, except the process of assigning seismic structure. In the current version of our code, a 1D velocity model provided in the file DATA/dsm_model_input is read and assigned to each GLL points. This file is also the input of DSM computation (see section 4). In the examples of subsections 6.3 and 6.4, we show how to incorporate topography and ocean water in SEM model. To incorporate more complex 3D velocity structure, you need to modify the code, basically the subroutine model_tomography in the file model_tomography.f90.

After running xgenerate_databases, the depths of all the coupling GLL points are collected and saved in the files

OUTPUT_FILES/DATABASES_MPI/depth_table_acoustic_innerbound

and

OUTPUT_FILES/DATABASES_MPI/depth_table_elastic_innerbound. The depths in the former file (elastic coupling GLL points) will be used in the DSM computation. The depths in the later file might be useful in mid-way coupling (i.e. outer core), but not in the source-side coupling.

The parameters depth_id, media type, normal vector, Jacobian and Cartesian coordinates associated each coupling GLL point are saved in the file

`OUTPUT_FILES/DATABASES_MPIiproc????/disp_pack??????`
These parameters are used in the final step of coupling (5).

3.3 Running the solver

This step is the same as the original package. The manual of SPECFEM3D_Cartesian explains the input parameters in the file `DATA/Par_file` in detail, but you should be careful to set up `NSTEP`. A complete 3D SEM wavefield is critical for accurate source-side coupling [see Wu et al., 2018], so you need to use a sufficiently large `NSTEP` to ensure that all waves are well absorbed. Once the solver starts, the displacement and traction on the coupling GLL points are continuously saved at every `NSTEP_BETWEEN_OUTPUTBOUND` time steps. The displacement and traction are saved in the files

`OUTPUT_FILES/DATABASES_MPIiproc????/disp_pack??????`
and
`OUTPUT_FILES/DATABASES_MPIiproc????/traction_pack??????`

Chapter 4

DSM computation

After running SEM, the next step is to compute the Green's functions using DSM.

4.1 Main parameter file

The main input parameters are specified the file `dsm_model_input`. Most of these parameters are the same as the original DSM code, except some new ones listed at the end of the file. For example, the file `dsm_model_input` used in the example of `iasp91_1D_benchmark` (see subsection 6.1) is as follow:

```
4096.0     512          #time series length, number of frequency
1.1d-3              #imaginary omega for artificial attenuation
60000     0     28000          #number of grids on the radius direction, minimum angular order,
                                 maximum angular order
11          #number of structure zone
0.0     1217.1     13.0885     0.0000     -8.8381     0.0000     #zone1 - inner core: r_min, r_max, coef1_density,
                                                                   coef2_density, coef3_density, coef4_density
11.2409     0.0000     -4.0969     0.0000                        #coef1_Vpv, coef2_Vpv, coef3_Vpv, coef4_Vpv
11.2409     0.0000     -4.0969     0.0000                        #coef1_Vph, coef2_Vph, coef3_Vph, coef4_Vph
3.56454     0.0000     -3.4524     0.0000                        #coef1_Vsv, coef2_Vsv, coef3_Vsv, coef4_Vsv
3.56454     0.0000     -3.4524     0.0000                        #coef1_Vsh, coef2_Vsh, coef3_Vsh, coef4_Vsh
1.0000     0.0000     0.0000     0.0000     84.6     1327.7     #coef1_eta, coef2_eta, coef3_eta, coef4_eta,
                                                                   Qmu, Qkappa
1217.1     3482.0     12.5815     -1.2638     -3.6426     -5.5281     #zone2 - outer core: r_min, r_max, coef1_density,
                                                                        coef2_density, coef3_density, coef4_density
10.0390     3.7567     -13.6705     0.0000                        #coef1_Vpv, coef2_Vpv, coef3_Vpv, coef4_Vpv
10.0390     3.7567     -13.6705     0.0000                        #coef1_Vph, coef2_Vph, coef3_Vph, coef4_Vph
0.0000     0.0000     0.0000     0.0000                          #coef1_Vsv, coef2_Vsv, coef3_Vsv, coef4_Vsv
0.0000     0.0000     0.0000     0.0000                          #coef1_Vsh, coef2_Vsh, coef3_Vsh, coef4_Vsh
1.0000     0.0000     0.0000     0.0000     -1.0     57823.0     #coef1_eta, coef2_eta, coef3_eta, coef4_eta,
                                                                   Qmu, Qkappa
...
...
0.01     0.00     90.00     2          #source depth, source latitude, source longitude, source type
                                          (1 for moment tensor and 2 for single force)*
20     1.0     0.0     0.0     0.0     0.0     0.0          #nexp, moment tensor (six components) or force (only
                                                             the first three components f_r, f_θ and f_φ are functional)*
depth_solid_list          # output of SEM*
dist_solid_list          # output of SEM*
```

```
depth_fluid_list          # output of SEM*
dist_fluid_list          # output of SEM*
1          #save velocity (1) or displacement seismograms (2)*
end
```

The parameters marked with "*" are new variables in our SEM-DSM method.

DSM code uses the cubic polynomials to describe the 1D model, the same as PREM [Dziewonski and Anderson, 1981]. For example, the Vp of the inner core in the above IASP91 model is $V_p = 11.2409 + 0.0 * a - 4.0969 * a^2 + 0.0 * a^3$ km/s, where $a = r/R_{Earth} = r/6371.0$.

For source-side coupling,

1. The source must be a single force (source type=1).
2. The unit of force is $dyne$. For example, the above line "20 1.0 0.0 0.0 0.0 0.0 0.0" represents a vertical single force $f_r = 1.0 * 10^{20}\ dyn = 1.0 * 10^{15}\ N$.

   Note that, Green's function corresponds to an unit force of $1\ N = 10^5 dyn$. However, we usually use a proper number of nexp (i.e. 20) to keep high numerical precision. Otherwise, too small variables in the code would give rise to large numerical errors. Consequently, the final hybrid synthetics needs to be corrected back (i.e. multiply them with 10^{-15}).
3. The files "depth_solid_list" and "depth_fluid_list" are automatically generated when running SEM. Just copy them to your DSM work directory.
4. the files "dist_solid_list" and "dist_fluid_list" contains the distances, where we want to compute Green's functions (see subsection 4.3).
5. save Green's functions of velocity seismograms rather than displacement.

4.1.1 The parameters you may need to change for source-side coupling

1. `time series length`: We have tested many cases and found a time length of $4096\ s$ works well for the direct P, S saves and other body wave phases (e.g. PcP, ScP, PKP, ScS, SKKS etc). If you really want to change it, do not use a too small number (i.e. $<$1024 s), because the artificial and real attenuation needs sufficiently long time to attenuate the late seismic waves. Otherwise, the wrap-around effects of these late waves would give rise to large errors. A longer time length allows attenuation to attenuate late waves better, but it increases computation costs.
2. `number of frequency`: This parameter together with `time series length` determines the maximum frequency of DSM synthetics. For example, a combination of `number of frequency`=512 and `time series length`=4096.0 means a maximum frequency of DSM synthetics of 0.125 Hz. Usually, we use a power of two (i.e. 256, 512, 1024, 2048, and so on) for this parameter.
3. `1D Earth model`: If you want to use other 1D model, you need to convert it to DSM format.
4. f_r, f_θ and f_ϕ: If only vertical components of hybrid synthetics are of concern, you only need to run the case of $f_r = 1.0$, $f_\theta = 0.0$ and $f_\phi = 0.0$. If all the three components are of concern, you have to run each case individually and save their Green's functions in separate folders (see subsection 6.2).
5. `dist_solid_list`: refer to subsection 4.3

4.2 The depth tables `depth_solid_list` and `depth_fluid_list`

These two depth tables contain the depths of the coupling grids of SEM elements. They are automatically generated when run SEM, so you can just simply copy them from the SEM output folders into your DSM work folder. This depth table file is like:

2.0000000E-02 35 #depth_shift_add_nodes (shift this small depth to add new radial nodes), number of depths
4.9999999E-03 # depth_separation_tolerance.
5 #number of GLL points on a coupling face of SEM element
0.000000000000000E+000 11 #depth0, izone_this_depth
1.72673164646048 11 #depth1, izone_this_depth
5.00000000000000 11 #depth2, izone_this_depth
8.27326835353952 11 #depth3, izone_this_depth
10.0000000000000 11 #depth4, izone_this_depth
...
70.0000000000000 9 #depth33, izone_this_depth
73.2732683535395 9 #depth34, izone_this_depth
74.9999999999991 9 #depth35, izone_this_depth

For most cases, you can simply copy them from the SEM output and do not need to change the above parameters. The only two parameters you are allowed to change are `depth_shift_add_nodes` and `depth_separation_tolerance`. In order to accurately compute stress, we add one new radial nodes above and another one below the target depth, that give us more accurate strain on the radial direction. The small variable `depth_shift_add_nodes` is the depth shift of the two new nodes relative to the target depth. In addition to that, we also need to add a new node for the target depth itself. However, if there is an preexisting node sufficiently close to the node awaiting to be created, it is not necessary to add it. The criteria is `depth_separation_tolerance`, so `depth_separation_tolerance` must be smaller than `depth_shift_add_nodes`. Again, the values of these two parameters in the above table have been confirmed to work well for many test cases, so you may just use them.

Similarly, the table `depth_fluid_list` corresponds to fluid media. Basically, this table is designed for mid-way coupling across core mantle boundary or inner core boundary. Thus, they are not used in source-side or receiver-side coupling. In the future, it could be used in a source-side or receiver-side coupling, in which ocean water is fully incorporated in both local and global simulation (e.g. hybrid method combining SPECFEM3D_GLOBE and SPECFEM3D_Cartesian).

4.3 The distance tables `dist_solid_list` and `dist_fluid_list`

These two files contain evenly spaced distance tables, where Green's function are computed and stored. The file `dist_solid_list` is like:

100 #number of distances for depth0
25 #distance0
25.1 #distance1
25.2 #distanc2
...
34.8 #distacne99
34.9 #distance100
100 #number of distances for depth1
25 #distance0

```
25.1 #distance1
25.2 #distance2
...
34.8 #distacne99
34.9 #distance100
...
100 #number of distances for depth35
25 #distance0
25.1 #distance1
25.2 #distance2
...
34.8 #distacne99
34.9 #distance100
```

You may notice that each depth has the same distance table and the information is highly redundant. They can be easily simplified to just four parameters: number of depths, number of distances, minimum distance and distance space. However, we still use this redundant table, because a future version of SEM-DSM hybrid method may use unevenly spaced distance table.

Similarly, `dist_fluid_list` contains a distance table corresponding to fluid media (the Earth's outer core). For source-side coupling, the current version of code does not support coupling SEM elements in the ocean, so this table is not used.

4.3.1 How to generate a distance table?

The key to make the distance table is using a proper distance range and distance space. The distance range should be sufficiently large to cover all the distances needed in the final step of coupling. For example, supposing that the SEM box has dimensions of $5^o \times 5^o$ and its horizontal center is 20^o away from the target teleseismic receiver, a distance table spanning a range of $16^o - 24^o$ must cover all the distances needed in coupling. Of course, a very large distance range is always safe, but it takes more computational costs.

We use interpolation to obtain Green's functions at target distances in the final step of coupling, so a small distance space is important for accurate interpolation. However, a very small distance space may cause a large dimension of distance table and therefore significantly increases computational costs. Basically, a higher maximum frequency of concern requires a smaller distance space. More details about this issue are discussed in [Wu et al., 2018].

4.4 Output of DSM computation

If you successfully run DSM, you will see a file "Green_Par_forConvolution" and other subdirectories in the directory "OUTPUT_GREENS/". For source-side coupling, the relevant subdirectories are only "velo_solid/" and "sigma/", where Green's functions of velocity and stress in solid media are stored.

Chapter 5

Running the Coupling

Now that You have successfully obtained the boundary information (displacement and traction) from SEM simulations and Green's functions from DSM computation, it is ready to couple them and compute hybrid teleseismic synthetics. We provide two different interpolation schemes for the coupling. You can choose either linear interpolation or Lagrange interpolation scheme to compute accurate Green's functions. The Lagrange polynomial interpolation is computationally slower, but has higher accuracy than linear interpolation. These two schemes use the same input parameters, so you can keep the same input setups, run both of them and compare their differences. If significant differences between them are seen, you should be ware that large errors must be present in the results of linear interpolation and possibly also in Lagrange interpolation. If that, you need to use a small distance space to recompute the Green's functions.

The following subsections explain the input files for a source-side coupling. **Only the main parameter file `DATA/Par_file` needs to be manually edited. All other input files described in subsections 5.2 and 5.3 are automatically produced by SEM and DSM, you can simply copy them to the right directories.**

5.1 Main parameter file

The main parameter file `DATA/Par_file` is as follow

```
npoints_taper_SEM = 100
vertical_component= .true.
radial_component= .false.
transverse_component= .false.
```

npoints_taper_SEM gives the length of tapers applied on SEM displacement and traction, in an unit of `deltat_SEM`. Note that the `deltat_SEM` here is the time step after decimating (see 5.2), rather than the original time step in the SEM solver. Ideally, the displacement and traction on SEM coupling grids should be close to zero at the very late time. However, real cases are not always ideal. For example, some SEM coupling grids might be close to the source and therefore have large static displacement; Absorbing boundaries do not absorb waves well, due to too short time length (see 3.3), too thin PML layers (see 3.1) and/or other reasons. In this situation, tapering the ends of traction and displacement are useful.

vertical_component Do coupling for vertical component if set it to `.true.`. If .true., make sure you have computed the Green's functions associated with the vertical single force f_r.

radial_component Do coupling for radial component if set it to `.true.`. If .true., make sure you have computed the Green's functions associated with two horizontal single forces f_θ and f_ϕ.

transverse_component Do coupling for transverse component if set it to `.true.`. If .true., make sure you have computed the Green's functions associated with two horizontal single force f_θ and f_ϕ.

If only vertical component is of concern (e.g. direct P-waves), you do not need to compute the Green's functions associated with f_θ and f_ϕ, because vertical component is independent on them [see the eq. 9 in Wu et al., 2018]. Similarly, the two horizontal components, radial and transverse, are independent on Green's functions associated with f_r. However, you have to compute Green's functions of both f_θ and f_ϕ, even you are only interested in one of the two horizontal components.

5.2 input files from SEM

The input information from SEM simulation includes `package_list`, `SEM_Par_Coupling` and other variables (i.e. geometry information, media type, traction and displacement) on coupling grids. These files are automatically generated when you run SEM, so you can simply copy them from SEM outputs into the directory `SEM_input/`.

5.2.1 `package_list`

The structure of `package_list` is as follow

```
1    0    1    300    # ipackage_global, iproc_SEM, ipackage_this_proc, npoints_per_pack_SEM
2    0    2    300
3    0    3    300
4    0    4    300
...
27    0    27    300
28    0    28    300
29    1    1    300
30    1    2    300
...
105    3    23    300
106    3    24    300
107    3    25    225
```

5.2.2 `SEM_Par_Coupling`

The file `SEM_Par_Coupling` includes the below parameters

npackage_SEM is the number of lines of the file `SEM_input/package_list`.

npoints_per_pack_SEM is the `NPOINTS_PER_PACK` in the SEM input file `SEMtoTele_Par_file` (see section 3.1).

nstep_each_section_SEM is `NSTEP_BETWEEN_OUTPUTBOUND` in the SEM input file `SEMtoTele_Par_file` (see section 3.1).

total_nstep_SEM is the number of time steps of SEM displacement and traction. It equals

`total_nstep_SEM=nstep_SEM_original/DECIMATE_COUPLING`.

`nstep_SEM_original` is the `NSTEP` in the SEM main parameter file `Par_file` and `DECIMATE_COUPLING` can be found in `SEMtoTele_Par_file` (see section 3.1)

nsection_SEM is the number of sections in each package of SEM displacement and traction. It is equal to right-round `total_nstep_SEM/nstep_each_section_SEM`, where 'right-round' means the nearest integer larger than `total_nstep_SEM/nstep_each_section_SEM`.

deltat_SEM equals `delta_SEM_original`×`DECIMATE_COUPLING`. `delta_SEM_original` is the `DT` in the SEM main parameter file `Par_file` and `DECIMATE_COUPLING` can be found in `SEMtoTele_Par_file` (see section 3.1).

5.2.3 Variables associated with each coupling grid

The geometry information (i.e normal vector, Jacobian, X-Y-Z coordinates), media type, traction and displacement on coupling grids from each CPU processor are stored in the corresponding directories `SEM_input/iproc????`.

5.3 input files from DSM

Input information from DSM computation includes the Green's functions and parameter file `Green_Par`. They are stored in the directory `DSM_input`.

The structure of file `DSM_input/Green_par` is as below

```
512 #number of frequency
0.0     0.1     0     #min_dep_acoustic, ddep_acoustic, ndepth_acoustic
0.0     0.1     35     #min_dep_solid, ddep_solid, ndepth_solid
25.0     0.1     100     #min_distance, distance_space, number of distances
4096.0     #time length
1.1E-003     #artificial attenuation coefficient - imaginary_omega
```

In the above parameters, `min_dep_acoustic`, `ddep_acoustic`, `min_dep_solid` and `ddep_solid` are not used in source-side coupling.

The Green's functions corresponding to f_r, f_θ, f_ϕ are stored in the directories `DATA/zcomp`, `DATA/rcomp` and `DATA/tcomp` respectively.

5.4 Output hybrid synthetics

When the coupling is completed, hybrid synthetics are stored in the directory `seismograms`. Note that

(1) The seismograms are displacement and the unit is 10^{-15} meter (see subsection 4.1). Thus, you need to multiply them with 10^{-15} to get an unit of meter.

(2) Do not use very low frequency waveforms (i.e. <0.01 Hz). There might be large errors at very low frequencies, due to errors from series of sources, including SEM computation, local wavefield approximation and tapering SEM synthetics.

(3) The maximum resolved frequency of hybrid synthetic seismograms is the lower one between that of SEM and DSM. Usually, applying a band-pass filter to synthetics is necessary when comparing synthetic seismograms to data.

(4) If ocean is present and truncated at the boundaries of SEM box, you must be ware that only the direct P-waves are valid. Do not use the waves after the direct P-waves, unless you have carefully checked them. Because the ocean is truncated at the boundaries of SEM box, large errors might be present in the late waves (see the example in subsection 6.4).

Chapter 6

Examples

For a source-side coupling, you need to run the three steps of SEM, DSM and coupling one by one, because the following step is dependent on the previous one. We provide four examples to show how to run a SEM-DSM source-side coupling. In each example, you can see an `README` file, which contains some useful information and descriptions of how to run that example. Among the three steps, creating a good SEM model is critical and contains many user-specified parameters, so we mostly focus on how to set up SEM model in the below subsections.

6.1 1D synthetic (vertical component) benchmark using the IASP91 model

In this example, we simply run a 1D model without any 3D heterogeneities. The 1D model is IASP91 velocity model and PREM attenuation model. In the SEM part, part of the parameters (see more detailed descriptions in subsection 3.1) are

Mesh_Par_file :

```
DEPTH_BLOCK_KM                  = 105.d0
...
NEX_XI                          = 30
NEX_ETA                         = 30
...
THICKNESS_OF_X_PML              = 0.24
THICKNESS_OF_Y_PML              = 0.24
THICKNESS_OF_Z_PML              = 25000.0
...
NREGIONS                        = 1
# define the different regions of the model as :
#NEX_XI_BEGIN #NEX_XI_END #NEX_ETA_BEGIN #NEX_ETA_END #NZ_BEGIN #NZ_END #material_id
1  30  1  30 1 11 2
```

SEMtoTele_Par_file :

```
ANGULAR_WIDTH_XI_IN_DEGREES    = 3.0d0
ANGULAR_WIDTH_ETA_IN_DEGREES   = 3.0d0
...
nx_NoTopography=5
ny_NoTopography=5
ix_LowBound=4
ix_HighBound=26
iy_LowBound=4
iy_HighBound=26
```

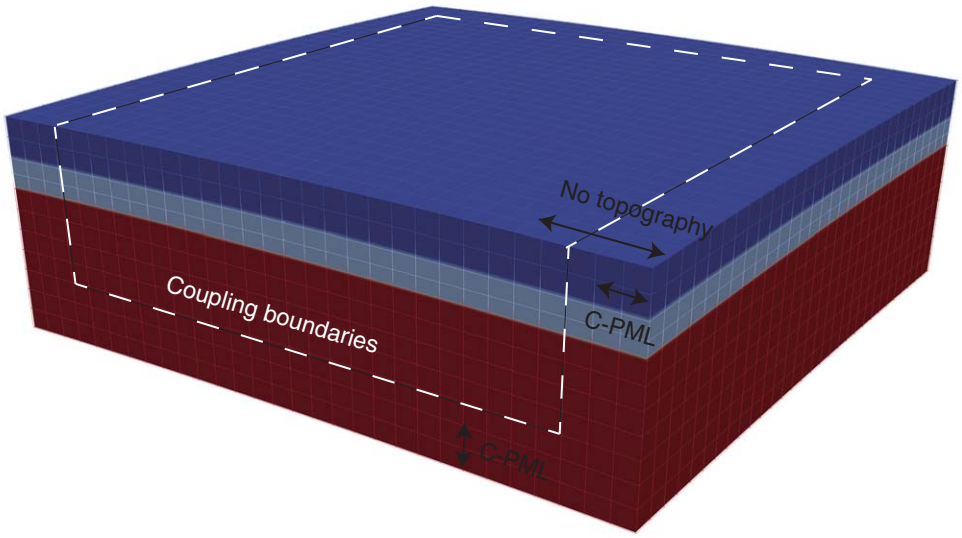


Figure 6.1: Screenshot of mesh of the 1D synthetic benchmark. The white dashed lines indicate the coupling interfaces, where seismic displacement and traction are stored and used in the final step of SEM-DSM coupling. The black arrow on the top interface shows the width of no topography region on the right boundary of SEM box, which is a length of five elements. The other two arrows show the C-PML absorbing boundaries with a width of two elements on the right and bottom boundaries of SEM box.

```
ir_BoundTop=11
ir_BoundBot=4
...
```

Based on the above parameters, the internal mesh tool `xmeshfem3D` produces meshes shown in Fig. 6.1. The dimensions of one element are $9.55\,km$ ($105\,km/11$, vertical) $\times 0.1^o$ ($3.0^o/30$, horizontal ξ) $\times 0.1^o$ ($3.0^o/30$, horizontal η). Thus, `THICKNESS_OF_X_PML=0.24` produces C-PML absorbing boundaries with a width of two elements at $\xi = min\_\xi$ and $\xi = min\_\xi$. The widths of C-PML layers at the bottom, $\eta = min\_\eta$ and $\eta = max\_\eta$ are also two elements (Fig. 6.1).

Although there is no topography in this 1D SEM box, we still need to specify the parameters `nx_NoTopography` and `ny_NoTopography`. We set `nx_NoTopography` and `ny_NoTopography` to 5. It means that the outermost five elements must be flat (Fig. 6.1). As we mentioned in subsection 3.1, the coupling interface must be inside the no topography region and outside the C-PML band (Fig. 6.1). If this condition is not satisfied, error report is raised.

Please read the three `README` files in the corresponding SEM, DSM and coupling directories, which tells you how to run this example. Basically, you just follow the below steps to run the executable bash command files.

```
(1) Read section 2 and compile the software packages.
(2) run SEM
    >cd SEM_DSM_hybrid/specfem3d/EXAMPLES_COUPLING/iasp91_1D_benchmark
    >./run_SEM.sh
(3) run DSM
    >cd SEM_DSM_hybrid/DSM/example/iasp91_1D_benchmark
    >./run_DSM.sh
(4) run the coupling step
    >cd SEM_DSM_hybrid/coupling/example/iasp91_1D_benchmark
    >./run_coupling.sh
(5) check the hybrid synthetics in the directory
    SEM_DSM_hybrid/coupling/example/iasp91_1D_benchmark/seismograms.
```

Note that only vertical components are valid, because we only compute the Green's functions of vertical single force to save computational cost.

6.2 1D synthetic (three components) benchmark using the IASP91 model

In the above example of 1D synthetic benchmark, we only compute the vertical components. Here, the radial and transverse components are also computed. To accomplish that, we need to run DSM for all the three single forces f_r, f_θ and f_ϕ.

How to run this example?

```
(1) Read section 2 and compile the software packages.
(2) run SEM
    >cd SEM_DSM_hybrid/specfem3d/EXAMPLES_COUPLING/iasp91_1D_benchmark_three_components
    >./run_SEM.sh
(3) run DSM
    >cd SEM_DSM_hybrid/DSM/example/iasp91_1D_benchmark_three_components
    >./run_DSM.sh
(4) run the coupling step
    >cd SEM_DSM_hybrid/coupling/example/iasp91_1D_benchmark_three_components
    >./run_three_single_forces.sh
(5) check the hybrid synthetics in the directory
    SEM_DSM_hybrid/coupling/example/iasp91_1D_benchmark_three_components/seismograms.
```

6.3 A simple sinusoidal shape topography model (no attenuation)

In this example, we duplicate the case shown in Fig.5 of Wu et al. [2018], where a sinusoidal shape topography is introduced in the SEM box. Because we use cubed-sphere coordinates in SEM simulation, topography as a function of latitude and longitude needs to be converted to that in cubed-sphere coordinates (ξ, η). The below command does coordinate conversion and save the output results in `DATA/meshfem3D_files/real_bathymetry_topography`, which will be read by `xmeshfem3D` to define ocean water.

```
../../bin/xcubedsphere_topo_FindOcean ./DATA/meshfem3D_files/latlon_surf_topo.dat
320 320 -0.1 -0.1 0.01d0 0.01d0
```

The first parameter `./DATA/meshfem3D_files/topo_surf.dat` is the file name of topography model in longitude-latitude coordinates.

The second and third parameters (320 and 320) are the numbers of points along ξ and η respectively.

The fourth and fifth parameters (-0.1 and -0.1) are minimum ξ and η. Note that, these two parameters must be smaller than 0.0 to fully cover the simulated region.

The last two parameters (0.01d0 and 0.01d0) are spacing between points.

The SEM model of this example contains three interfaces (from bottom to top: Moho, upper crust and free surface discontinuities). We assume no topography on the upper crust and Moho interfaces, so it is easy to produce these interfaces (see details in `run_SEM.sh`). The topography of free surface in cubed-sphere coordinates is formed by the bellow command.

```
../../bin/xcubedsphere_topo 3 ./DATA/meshfem3D_files/latlon_surf_topo.dat 0.0
-20000.0 30000.0
```

The first parameter "3" indicates that we are working on the third interface listed in the file `INTERFACES_FILE` (see subsection 3.1). The other two interfaces are upper-crust and Moho discontinuity.

The second parameter `./DATA/meshfem3D_files/topo_surf.dat` is the file name of topography model in longitude-latitude coordinates.

The third parameter 0.0 is the basement value of the free surface topography. The topography on the boundaries of SEM box are tapered to the basement value (see more interpretations in the example of next subsection 6.4).

The last two parameters -20000.0 and 30000.0 are the minimum and maximum allowed topography. Any topography out of this range are truncated. The peak topography in this model is 10000 m, so max_allowed_topography=30000.0 does not truncate any topography.

Executing the above command produces the file `DATA/meshfem3D_files/topo_surf.dat`. You can see the above two commands and more detailed interpretations in the file `run_SEM.sh` in the corresponding SEM directory. Then, the internal mesh tool `xmeshfem3D` reads `topo_surf.dat` to create the free surface. Then the file `real_bathymetry_topography` is read to classy each SEM elements to either acoustic ocean or solid media. Any element with a central GLL point above the bathymetry given in `real_bathymetry_topography` is classified to acoustic media.

Note that the dimensions of region described in `real_bathymetry_topography` and all the interfaces listed in `INTERFACES_FILE` should be sufficiently large to cover the SEM region. Otherwise, the codes cannot properly build up the model you want. For example, the ranges of dimensions in the above command are -0.1 deg to 3.1 deg along ξ and η, which fully cover the SEM box (0 deg to 3.0 deg). There is no ocean in this example, so the topography/bathymetry described in `real_bathymetry_topography` and `topo_surf.dat` are the same. In the example of next subsection 6.4, we will discuss how to use the real topography/bathymetry data to incorporate the ocean water.

How to run this example?

```
(1) Read section 2 and compile the software packages.
(2) run SEM
    >cd SEM_DSM_hybrid/specfem3d/EXAMPLES_COUPLING/
    >cd iasp91_sinusoidal_topography_no_attenuation
    >./run_SEM.sh
(3) run DSM
    >cd SEM_DSM_hybrid/DSM/example/iasp91_sinusoidal_topography_no_attenuation
    >./run_DSM.sh
(4) run the coupling step
    >cd SEM_DSM_hybrid/coupling/example/iasp91_sinusoidal_topography_no_attenuation
    >./run_coupling.sh
(5) check the hybrid synthetics in the directory
SEM_DSM_hybrid/coupling/example/iasp91_sinusoidal_topography_no_attenuation/seismograms.
```

6.4 Simulating the P-waves from the 2016/10/27 Mw6.0 South America earthquake

This example duplicates the synthetics in Fig. 11b in Wu et al. [2018]. We use the 30 arc-second resolution topography/bathymetry data to incorporate the ocean and land topography. First, the topography/bathymetry data in geographical coordinates needs to be converted to that in cubed-sphere coordinates.

```
../../bin/xcubedsphere_topo_FindOcean ./DATA/meshfem3D_files/SA_real_topo.dat
540 540 -0.2 -0.2 0.01 0.01
```

The above command is executed when you run the script `run_SEM.sh` in the corresponding SEM directory. The converted topography/bathymetry is stored in `real_bathymetry_topography` (Fig. 6.2).

Then we need to prepare the topography files of the four interfaces (Moho, upper crust, ocean bottom and free surface). Comparing to the example of sinusoidal topography in subsection 6.3, another interface of ocean bottom is needed to incorporate the ocean. The ocean bottom interface is formed using the below command.

```
../../bin/xcubedsphere_topo 3 ./DATA/meshfem3D_files/SA_real_topo.dat -3878.0
-20000.0 -1500.0
```

We have explained what each parameter does in subsection 6.3. The minimum allowed bathymetry of -20000.0 meters is deeper than any bathymetry in the world, that means no deep bathymetry truncated. The output results are stored in the file `topo_botOC.dat` (Fig. 6.3a). Similarly, the topography of the free surface is formed by the below command and stored in `topo_surf.dat` (Fig. 6.3b).

```
../../bin/xcubedsphere_topo 4 ./DATA/meshfem3D_files/SA_real_topo.dat 0.0 0.0
30000.0
```

Based on these two interface, `xmeshfem3d` creates and meshes the top layer, where the ocean is incorporated (Fig. 6.4). This layer is meshed using three elements along vertical direction and the element size are proportional to the layer's thickness. Using proper input parameters to make ocean bottom and free surface is important to generate high quality elements. For example, we use a maximum allowed bathymetry of -1500 m to produce the ocean bottom. This value makes most deep bathymetry features exactly honoured (Fig. 6.4) and generates elements with good qualities (e.g. good aspect ratios). In some extreme cases (e.g. rapidly varying topography/bathymetry), properly truncating and/or smoothing the topography/bathymetry is necessary to avoid highly skewed elements.

Running this example needs moderate computational costs (e.g. 10-20 hours using hundreds of CPU processors),

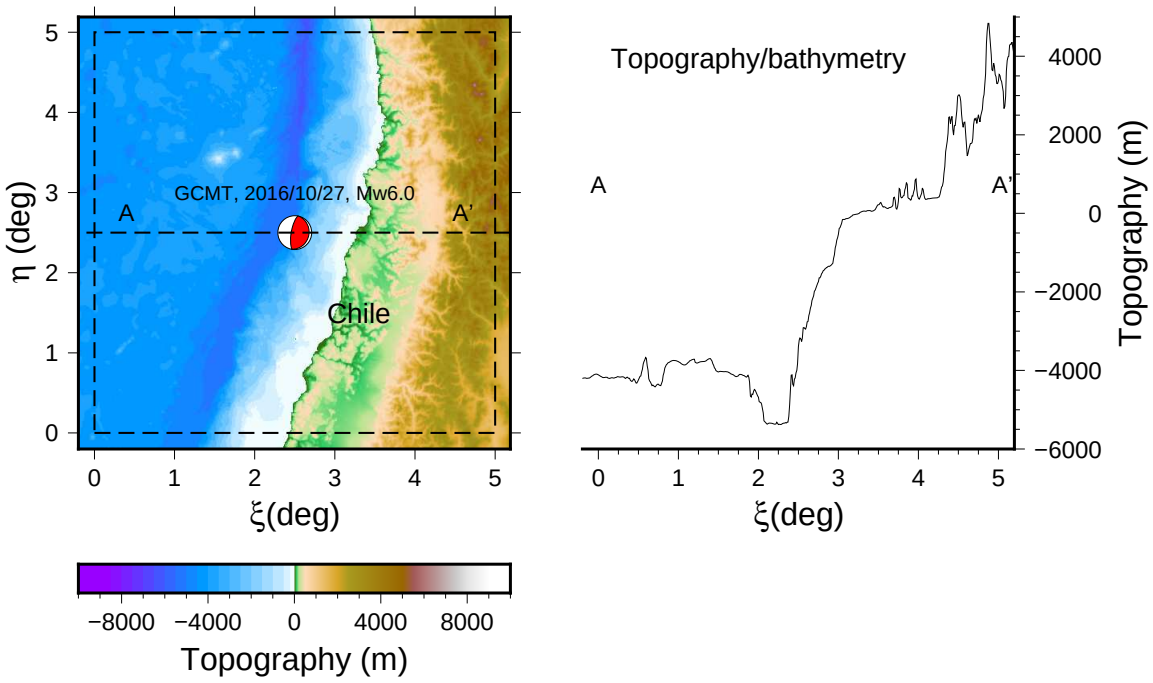
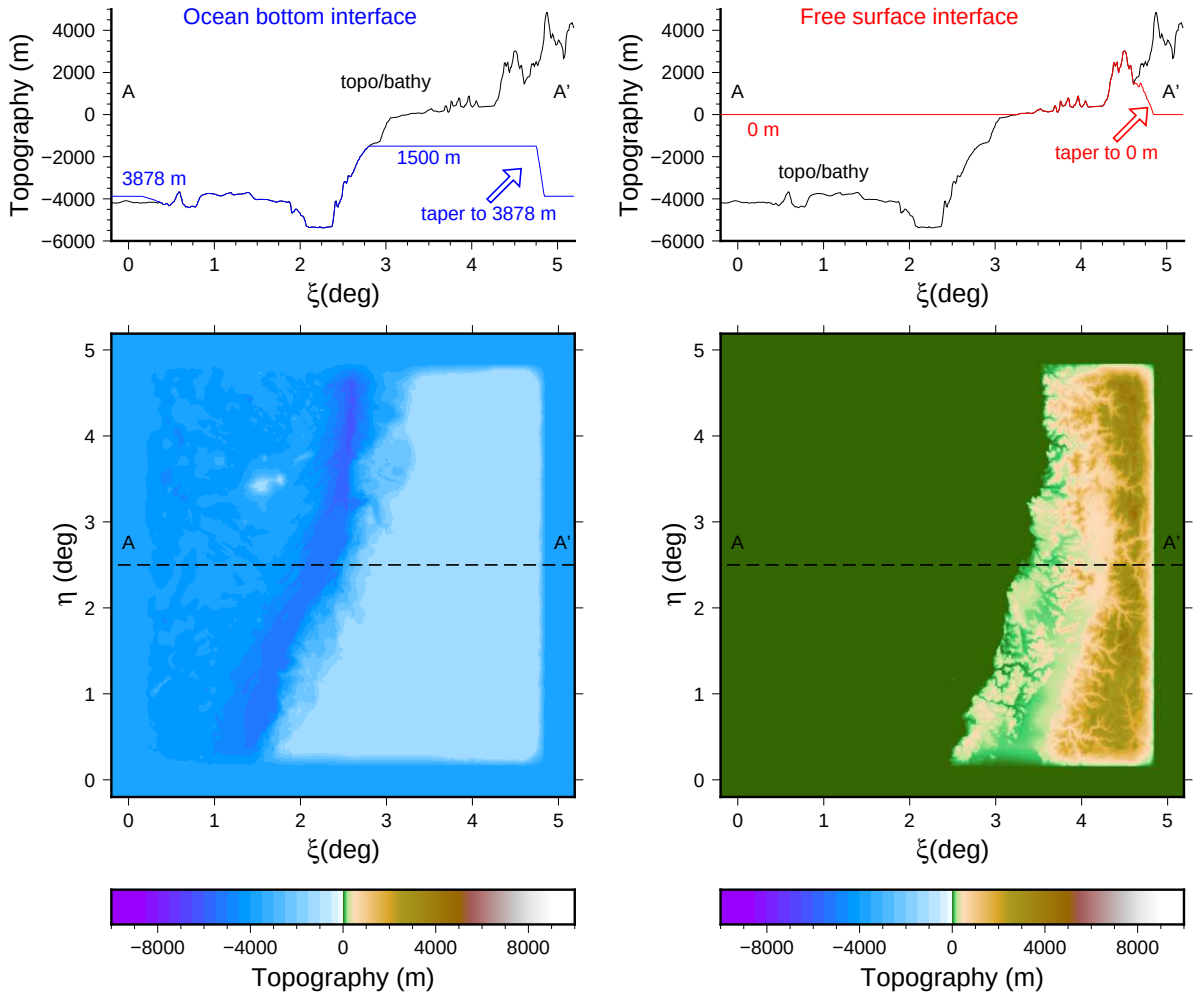


Figure 6.2: Topography/bathymetry in cubed-sphere coordinates (ξ, η). The left figure shows the topography/bathymetry described in `real_bathymetry_topography`. The beach ball represents the GCMT solution [Global Centroid Moment Tensor, Ekström et al., 2012] of this earthquake. The dashed line box shows the simulated SEM box with dimensions of 5 deg $\times$ 5 deg). The topography/bathymetry on the profile A-A' is plotted in the right figure. Note the different scales on x- and y-axis (1 degree is equivalent to $\sim$111.19 km).

that cannot be accomplished by a few CPUs. If you successfully run this example, the synthetic seismograms are stored in the directory `SEM_DSM_hybrid/coupling/example/SouthAmerica_Earthquake_161027/seismograms`. We note that only the direct P-waves in the first $\sim$60 seconds (maybe a little longer, e.g. 120 seconds) have been checked. Because the ocean is truncated at the boundaries of SEM box, large errors might be present in the very late waves [see Wu et al., 2018, , especially the Fig. S9].

How to run this example?

```
(1) Read section 2 and compile the software packages.
(2) run SEM
>cd SEM_DSM_hybrid/specfem3d/EXAMPLES_COUPLING/SouthAmerica_Earthquake_161027
>./run_SEM.sh
(3) run DSM
>cd SEM_DSM_hybrid/DSM/example/SouthAmerica_Earthquake_161027
>./run_DSM.sh
(4) run the coupling step
>cd SEM_DSM_hybrid/coupling/example/SouthAmerica_Earthquake_161027
>./run_coupling.sh
(5) check the hybrid synthetics in the directory
SEM_DSM_hybrid/coupling/example/SouthAmerica_Earthquake_161027/seismograms.
```



(a) (b)

Figure 6.3: The topography of the ocean bottom and free surface interfaces in the SEM box. (a) The ocean bottom interface described in `topo_botOC.dat`. This interface is truncated at -1500 m towards the land and tapered to 3480 m near the boundaries. The upper panel shows the bathymetry on the A-A' profile. (b) The free surface topography described in `topo_surf.dat`. The topography is fixed to 0 m in the ocean. The upper panel shows the topography on the A-A' profile.

6.5 Run your own example

In the above examples, we show how to run models of 1D structure, 3D topography and 3D ocean. You can use even more complex model to create your own example. If you want to model effects of topography/bathymetry and ocean, the 30 arc-second resolution global topography/bathymetry model can be freely downloaded from General Bathymetric Chart of the Oceans (GEBCO, https://www.gebco.net/); To incorporate 3D velocity model in SEM (e.g. sediment, slab or tomography 3D model), you may need to write some new routines or modify the subroutine `model_tomography` in the Fortran file `SEM_DSM_hybrid/specfem3d/src/generate_databases/model_tomograph`

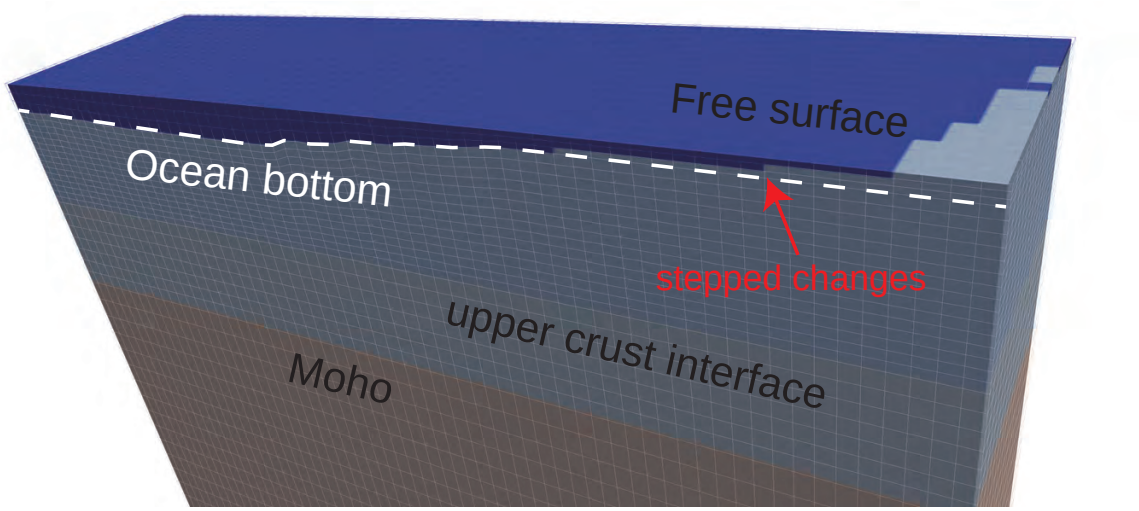


Figure 6.4: Part of meshes. The dark blue region represents the ocean. The white dashed line shows the ocean bottom interface. The deep bathymetry (i.e. <-1500 m) is exactly honoured and the shallower bathymetry is approximated by stepped grids.

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