

Using SPECFEM3D_GLOBE-7.0.0 for ASKI – Analysis of Sensitivity and Kernel Inversion, versions 1.0 to 1.2

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If you use SPECFEM3D_GLOBE for ASKI for your own research, please cite one of our papers [SFL16], or [SF16], as appropriate:

F. Schumacher, W. Friederich and S. Lamara,

”A flexible, extendable, modular and computationally efficient approach to scattering-integral-based seismic full waveform inversion”,

Geophysical Journal International, (February, 2016) 204 (2): 1100-1119

<http://dx.doi.org/10.1093/gji/ggv505>

Schumacher F, Friederich W.

”ASKI: A modular toolbox for scattering-integral-based seismic full waveform inversion and sensitivity analysis utilizing external forward codes”.

SoftwareX 5 (2016) 252–259,

<http://dx.doi.org/10.1016/j.softx.2016.10.005>

This documentation was written in the hope that it will be useful to the user, but it *cannot be assured* that it is accurate in every respect or complete in any sense. In fact, at some places *this manual is work in progress*.

Please do not hesitate to report any inconsistencies by opening (or adding to) an ”issues” topic on https://github.com/seismology-RUB/SPECFEM3D_GLOBE_for_ASKI or to improve this documentation by incorporating your experiences with SPECFEM3D for ASKI and your personal experience of getting used to it (at best by modifying the source and issuing a pull request on gitHub, in any case let us know about it! Thanks).

Furthermore, I am aware of the poor L^AT_EX coding of this document (at the moment, \sloppy is used at the beginning of the document to avoid overfull hboxes in many places). There is a

lot of potential to improve the document style, hence the readability of the manual as a whole, as well as the coding style of the particular `.tex` files. *Please do not hesitate to improve!*

The \LaTeX source files and all related components of this document are available via https://github.com/seismology-RUB/SPECFEM3D_GLOBE_for_ASKI , sub-directory `doc/` of the repository.

Florian Schumacher, Dec 2016

Guide Through This Manual

We assume that you have sufficient knowledge of how to run the regular `SPECFEM3D_GLOBE` software. (i.e. without extension for use with `ASKI`).

For details on how to get started by installing everything required for using `SPECFEM3D_GLOBE` with `ASKI` , refer to section 1 (page 5).

Before you start using the code to produce output for `ASKI` , please consider the general comments in section 2 (page 8).

If you are planning to compute a lot of kernels for source-receiver paths (e.g. doing full waveform inversion) it makes sense to use the automated python script

`run_specfem3dGlobeForASKI_simulations.py` which conducts a lot of simulations in an automated fashion. Please read section 4 (page 9).

If you want to conduct one single simulation (or just a few ones) producing output for `ASKI` , please read section 3 (page 8).

Section 8 (page 17) is intended to be used as a reference section only.

Bracketed comments starting with “**TODO IN THE FUTURE:**” are intended to mark ideas for future work. So please ignore if you are just applying the code.

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1 Installation and Getting Started

This section explains how to install the SPECSEM3D_GLOBE software (http://geodynamics.org/cig/software/specsem3d_globe) in order to be used as a forward method for ASKI. In general, a regularly installed SPECSEM3D_GLOBE version is extended by certain few modifications so it can produce output for ASKI. So, SPECSEM3D_GLOBE for ASKI basically has the same requirements and dependencies as the SPECSEM3D_GLOBE code, except that it needs a bit more memory and weigh more disc space for output. *Load balancing might not be perfect anymore!!* You should, therefore, have sufficient knowledge of how to run the regular SPECSEM3D_GLOBE software.

1.1 Requirements

1. You require an installation of the ASKI main package, available via <https://github.com/seismology-RUB/ASKI>:

```
git clone --depth 1 --branch master https://github.com/seismology-RUB/ASKI
```


The directory created by the `git clone` command will be referred to below as ASKI/
2. You need a functioning installation of the SPECSEM3D_GLOBE code, including modifications for usage with ASKI :
 - You can either use the modified slim version of SPECSEM3D_GLOBE_V7.0.0 that comes with this package (see section 1.3 (page 6)),
 - or use your running installation of SPECSEM3D_GLOBE and extend it for usage with ASKI, as described below in section 1.4 (page 6).

In *both* cases you must install this package (section 1.2 (page 5)).

3. You need basic experience in using the regular SPECSEM3D_GLOBE software!

1.2 Installing this package

Clone the latest version of the master branch of the `github` repository to *the same* directory where you have cloned the ASKI main package to (in the ASKI documentation exemplarily called `/your/programs/`), i.e. execute

```
git clone --depth 1 --branch master https://github.com/seismology-RUB/SPECSEM3D_GLOBE_for_ASKI
```

(in one line, of course) from local path `/your/programs/`. This will create subdirectory `/your/programs/SPECSEM3D_GLOBE_for_ASKI` (also referred to below simply as `SPECSEM3D_GLOBE_for_ASKI/`) containing the code and documentation of the current release of the extension package SPECSEM3D_GLOBE for ASKI.

Alternatively, go to https://github.com/seismology-RUB/SPECSEM3D_GLOBE_for_ASKI and download the content of the master branch as a `.zip` or try executing

```
wget https://github.com/seismology-RUB/SPECSEM3D_GLOBE_for_ASKI/archive/master.zip
```

(in one line, of course) and extract it in such a way that the code files are contained in `/your/programs/SPECSEM3D_GLOBE_for_ASKI/`.

Furthermore you need to compile few more ASKI binaries following these step:

- In `SPECFEM3D_GLOBE_for_ASKI/Makefile`, set `COMPILER` appropriately, adjust `FFLAGS` if required and set the variables `BLAS`, `LAPACK`, just as you did in `ASKI/Makefile` when installing the `ASKI` main package.
- Execute the command `make all` from path `SPECFEM3D_GLOBE_for_ASKI/`

After that, `SPECFEM3D_GLOBE_for_ASKI/../../ASKI/bin/` should contain the new binaries.

The latest version of the master branch of gitHub repository https://github.com/seismology-RUB/SPECFEM3D_GLOBE_for_ASKI should be consistent with the latest version of the `ASKI` repository's master branch.

1.3 Using Already Extended Copy of `SPECFEM3D_GLOBE-7.0.0` Code

`SPECFEM3D_GLOBE_for_ASKI/specfem3d_globe` contains a copy of the release version `SPECFEM3D_GLOBE-V7.0.0` (released 10 July 2015) that was extended by the steps 2.–9. as in section 1.4 (page 6) in order to produce output for `ASKI`. Furthermore, `utils` and `documentation` (not required for use with `ASKI`) were removed in order to keep the directory `SPECFEM3D_GLOBE_for_ASKI/specfem3d_globe` small.

Re-configure and compile the software on your system according to the compilers you are using etc., e.g. by executing the following commands from path `SPECFEM3D_GLOBE_for_ASKI/specfem3d_globe/`:

```
> ./configure FC=gfortran MPIFC=mpif90
> make xmeshfem3D xspecfem3D
```

In order to produce `ASKI` output in `SPECFEM3D` simulations, copy file `SPECFEM3D_GLOBE_for_ASKI/Par_file_ASKI` to your respective `DATA/` path (which is e.g. `specfem3d_globe/EXAMPLES/my_example/DATA/`, or `specfem3d_globe/DATA/`). This file must be adjusted for any specific simulation (just as all other parameter files) and is described in detail in section 8 (page 17).

1.4 Extend Your Own `SPECFEM3D_GLOBE-7.0.0` code to produce output for `ASKI`

If you have a regular `SPECFEM3D_GLOBE` installation which has not significantly different functionality compared with `SPECFEM3D_GLOBE` release version 7.0.0 (2015-07-10), you can extend it for `ASKI` by the following steps:

1. Install `SPECFEM3D_GLOBE` on your system and make it run, gain experience in using it (below, the installation path is referred to as `specfem3d_globe/`).
2. Append content of file `SPECFEM3D_GLOBE_for_ASKI/specfem3D_par_ASKI.f90` to file `specfem3d_globe/src/specfem3D/specfem3D_par.F90`
3. In `specfem3d_globe/src/specfem3D/prepare_timerun.F90` in subroutine `prepare_timerun`:
add the following line at the beginning of the subroutine, after the `use ...` statements:
`use specfem_for_ASKI_par`
add the following line close to the end of the subroutine, before `synchronize_all()`

is called:

```
call prepare_timerun_ASKI()
```

4. In `specfem3d_globe/src/specfem3D/iterate_time.F90` in subroutine `iterate_time`:
add the following line at the beginning of the subroutine, after the `use ...` statements:
`use specfem_for_ASKI_par`
add the following line just before the `enddo` of the main time loop:
`call write_ASKI_output()`
5. Append content of file `SPECFEM3D_GLOBE_for_ASKI/ASKI_external_model.f90` to file `specfem3d_globe/src/meshfem3D/meshfem3D_par.f90`
6. In `specfem3d_globe/src/meshfem3D/setup_model.f90` in subroutine `setup_model`:
add the following line at the beginning of the subroutine, after the `use ...` statements:
`use ASKI_external_model`
add the following line just before info output is written to `IMAIN`, after the 3D models are broadcasted:
`call broadcast_ASKI_external_model(myrank)`
7. In `specfem3d_globe/src/meshfem3D/get_model.F90` in subroutine `get_model`:
add the following line at the beginning of the subroutine, after the `use ...` statements:
`use ASKI_external_model`
add the following lines just before define elastic parameters in the model (i.e. setting all arrays `rhostore`, `kappavstore`, `muvstore`, ...), just after all other get model routines:

```
call values_ASKI_external_model(iregion_code, xmesh, ymesh,
                                zmesh, r, &
                                vpv, vph, vsv, vsh, rho, Qmu, Qkappa, eta_aniso, dvp, &
                                c11, c12, c13, c14, c15, c16, c22, c23, c24, c25, &
                                c26, c33, c34, c35, c36, c44, c45, c46, c55, c56, c66)
```
8. Append content of file `SPECFEM3D_GLOBE_for_ASKI/parallel_ASKI.f90` to file `specfem3d_globe/src/shared/parallel.f90`
9. Recompile the relevant `SPECFEM3D` binaries by issuing
`make xmeshfem3D xspecfem3D` in directory `specfem3d_globe/`
10. In order to produce `ASKI` output in `SPECFEM3D` simulations, copy file `SPECFEM3D_GLOBE_for_ASKI/Par_file_ASKI` to your respective `DATA/` path (which is e.g. `specfem3d_globe/EXAMPLES/my_example/DATA/`, or `specfem3d_globe/DATA/`). This file must be adjusted for any specific simulation (just as all other parameter files) and is described in detail in section 8 (page 17).

If you have a newer version of `SPECFEM3D_GLOBE` which does not work with `ASKI` as thus described, we are happy to hear about it. Please feel free to get in touch with the `ASKI` developers (via <https://github.com/seismology-RUB> or <http://www.rub.de/aski>).

2 General Things to Consider

- parameters `FILE_KERNEL_REFERENCE_MODEL` and `FILE_WAVEFIELD_POINTS` of the `ASKI` parameter file for a specific iteration step must be set to some main `ASKI` output file, which is the basefile name of `ASKI_outfile` extended by `.main`, see 8.2 (page 18). Use the main `ASKI` output file of some arbitrary `ASKI` output, e.g. the kernel displacement output of the first source or some kernel green tensor output.
- As there is a fixed order assumed of the `ASKI` wavefield points (by procs and local element numbering), the computation of many kernels (e.g. for many source-receiver paths in an inversion) can only be consistent, if the *same* mesh decomposition and the *same* number of procs is used at all times (for those kernels you want to use together in some analysis, e.g. all kernels in your specific iteration step of an inversion). It may, hence, be sensible to run the mesher *once* before all simulations are conducted (only re-setting the source mechanism and `Par_file_ASKI` before a specific simulation, adjust your script `run_mesher_solver.bash` appropriately). Such a mechanism is supported by the automated python script through flag `use_different_command_in_first_simulation`.
- You must use `PRINT_SOURCE_TIME_FUNCTION = .true.` in the `SPECFEM3D Par_file` in order to ensure correct functionality (relevant for cases `ASKI_DECONVOLVE_STF = .true.` in `Par_file_ASKI`).
- You must set `ROTATE_SEISMOGRAMS_RT = .false.` in the `SPECFEM3D Par_file` in order to ensure that synthetic data (or measured data for synthetic studies) can be transformed to the spectral `ASKI` format correctly (by programs as in sections 6 (page 13), 7 (page 14)).
- In file `constants.h`, you must set `ASSUME_PERFECT_SPHERE = .true.` in order to assure proper functionality for `ASKI`, as `ASKI` interprets spherical event and station coordinates w.r.t. a sphere and the spherical `ASKI` inversion grids are based on perfect spheres. For the extended `SPECFEM` version in `SPECFEM3D_GLOBE_for_ASKI/specfem3d_globe/`, this functionality is already assured by modification of file `SPECFEM3D_GLOBE_for_ASKI/specfem3d_globe/setup/constants.h.in`.

3 One Single Simulation

As usual, you need to set the mesh according to the needs of your seismic problem, e.g. the resolved highest frequency etc. You need to choose a `SPECFEM3D` background model (defined in `Par_file` as usual). For details on how to import the current model of an inversion (the inverted model of the last iteration step) into `SPECFEM3D`, see section 5 (page 11). Refer to the same section on how to set a different 1D background model or superimpose a checkerboard / spike-test model.

Set the regular `SPECFEM3D` files `Par_file`, `CMTSOLUTION` and `STATIONS` (standard `SPECFEM3D` functionality).

Additionally, you need to set file `Par_file_ASKI` to desired values. The file is described in detail in section 8 (page 17).

After that, you are ready to run the code. Since all relevant information for producing ASKI output are read on runtime, you do not need to recompile the SPECfEM3D code every time you run a SPECfEM3D simulation for ASKI, you just need to set the above listet parameter files.

4 Using Automated Python Script for Doing Several Simulations

As usual, you need to set the mesh according to the needs of your seismic problem, e.g. the resolved highest frequency etc. You need to choose a SPECfEM3D background model (defined in `Par_file` as usual). For details on how to import the current model of an inversion (the inverted model of the last iteration step) into SPECfEM3D, see section 5 (page 11). Refer to the same section on how to set a different 1D background model or superimpose a checkerboard / spike-test model.

Python script `run_specfem3dGlobeForASKI_simulations.py` (provided in directory `SPECfEM3D_GLOBE_for_ASKI/`) conducts the specified kernel simulations (as described inside the script on the top) by running SPECfEM3D simulations one after another, setting all parameter files before each simulation appropriately. You need to edit the parameters in the first part of the script and set all variables defined there to appropriate values, as described in the comments in the script

(**TODO IN THE FUTURE:** maybe it is better to have an input (file?) mechanism to this script. But then: more overhead/extra requirements (packages, arguments handling) to cope with on cluster machines ...)

The python script may not be suitable for the HPC system you are using. If you are not able to adapt it in a way which makes it possible to be used, you might have to figure out an analogous way yourself how to perform the tasks done by this script.

In case of using the provided python script `run_specfem3dGlobeForASKI_simulations.py`, some parameters in SPECfEM3D files `CMTSOLUTION`, `Par_file` and in file `Par_file_ASKI` are automatically changed, while the script conducts the SPECfEM3D simulations one after another.

In the following, only those parameters/lines are listed, which, if necessary, need to be set *manually* before running this python script. All other parameters are set by the script.

4.1 Manually Setting `Par_file_ASKI`

The following `Par_file_ASKI` parameters need to be set manually before running the python script, since they are not changed/set by the script.

- `USE_ASKI_BACKGROUND_MODEL, FILE_ASKI_BACKGROUND_MODEL`
- `IMPOSE_ASKI_INVERTED_MODEL, FILE_ASKI_INVERTED_MODEL`
- `ASKI_INVERTED_MODEL_INTERPOLATION_TYPE, ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS`
- `IMPOSE_ASKI_CHECKER_MODEL, FILE_ASKI_CHECKER_MODEL`

- ASKI_MAIN_FILE_ONLY (must be set to `.false.`, otherwise no ASKI wavefield output will be produced!)
- OVERWRITE_ASKI_OUTPUT
- ASKI_DECONVOLVE_STF (strongly recommended to set to `.true.` always)
- ASKI_DFT_double
- ASKI_DFT_apply_taper, ASKI_DFT_taper_percentage
- in case of `define_ASKI_output_volume_by_inversion_grid = False` in the python script, you need to manually set all parameters concerning the inversion grid, i.e. ASKI_type_inversion_grid, ASKI_nchunk, ASKI_(c/w) (lat/lon), ASKI_rot_gamma, ASKI_r (min/max)

It is important to notice, that the flag ASKI_DECONVOLVE_STF is not changed by the automated python script. Although it is required for Green functions (“gt” simulations) to use ASKI_DECONVOLVE_STF = `.true.` in order to get the displacement field w.r.t. a Dirac impulse source-time function, the situation might arise, that for the forward wavefields (“displ” simulations) emanated by the seismic events you want to use a pre-defined source wavelet (e.g. Ricker wavelet) that *should not* be deconvolved from the wavefields. For now, This can only be realized by doing two separate runs with the python script, one for all “gt” simulations (setting ASKI_DECONVOLVE_STF = `.true.`) and one for the “displ” simulations (setting ASKI_DECONVOLVE_STF = `.false.`).

4.2 Manually Setting CMTSOLUTION

The python script *always* automatically sets “latitude:”, “longitude:”, “depth:”, “Mrr:”, “Mtt:”, “Mpp:”, “Mrt:”, “Mrp:”, “Mtp:”. In case of “gt” *and* “displ” simulations, “half duration:” is set to “0.” ASKI follows the idea to also compute “displ” wavefields with an impulsive source-time function (setting ASKI_DECONVOLVE_STF = `.true.`) and apply filters afterwards. For simulations of type “data”, however, “half duration:” is *not* modified by the python script! So, if you wish to do a “data” simulation using a “half duration:” value different from “0.”, you should conduct those in a separate run of the python script (not mixing with “displ” or “gt” simulations).

4.3 Manually Setting STATIONS

In the upper part of the python script, the flag `create_specfem_stations` can be set to `True`. In this case, the SPECFEM3D STATIONS file is automatically generated from the ASKI file `FILE_STATION_LIST`.

If you do not use this flag to automatically generate the SPECFEM3D STATIONS file, you must provide it manually. The standard SPECFEM3D STATIONS file should contain the definition of stations as in the ASKI file `FILE_STATION_LIST`, in consistend SPECFEM3D notation, i.e. coordinate columns being lat (third column of STATIONS and fourth column of `FILE_STATION_LIST`) and lon (fourth column of STATIONS and third column of `FILE_STATION_LIST`) and elev (sixth column of STATIONS and fifth column of `FILE_STATION_LIST`).

You must also assure to use the very same station names and network codes in file STATIONS as in ASKI file FILE_STATION_LIST!

5 Importing external models into SPECSEM3D , e.g. simple background model or currently inverted model for next iteration step

There are three types of external models that can be put (in combination) into SPECSEM3D, using the additional module ASKI_external_model:

Simple 1D layered spline-interpolation models can overwrite the SPECSEM3D model chosen in Par_file. Exported .kim files (as produced by ASKI program exportKim with option -otxt) may be superimposed onto the background model (default SPECSEM3D model or ASKI 1D background model) and used as a model for the new iteration of full waveform inversion of ASKI. After that, a checkerboard / spike-test model can be superimposed onto the resulting model, imposing relative model perturbations in a checkerboard or spike-like fashion that can be used for resolution analysis.

These three types of external models are explained in the following. The use of any of these is controlled by respective flags in Par_file_ASKI.

5.1 Overwrite background model by simple 1D layered gradient model

The logical flag USE_ASKI_BACKGROUND_MODEL in Par_file_ASKI indicates whether SPECSEM3D_GLOBE should use the 1D reference model as defined in the text file with name given by FILE_ASKI_BACKGROUND_MODEL, relative to DATA/. This mode will overwrite model values on all GLL points, dependent on depth. *A model like this will not affect the meshing of spectral elements or any internal boundaries created by the meshing process!*

The 1D model is defined by a list of model values at given depth nodes between which a spline interpolation is done. A template of such a background model file, containing documenting commentary, is given by file SPECSEM3D_GLOBE_for_ASKI/ASKI_background_model_template. The specific format of this text file is described now in the following:

the first line is ignored, this line may contain a short description of the model or can be empty.

the second and third line simply define the characteristics of the depth nodes which are defined in the table (for convenience when reading the file by the program):

The second line must contain the number of layers, between which discontinuities are allowed in the 1D model. At the boundary of any two layers, there should be a “double node”, i.e. two lines with *same* depth. There is no spline interpolation done accross any layer boundaries, i.e. over any double node. Different model values on either side of a double node will be interpreted as a discontinuity in the model. You can also set the same model value on either side of a double node, e.g. if you want to have a half space of the same model values as a gradient coming from above, etc.

The third line contains as many integer values (separated by white space) as there are layers (as defined by line two) and gives for each layer the number of nodes.

starting from line 4, each line defines a depth node giving (isotropic) model values at this depth. The columns are separated by white space and assume the meaning:

depth [m] density [g/cm³] vp [km/s] vs [km/s] Qmu Qkappa

The depth is assumed to be monotonically *increasing*, the first line should have depth 0.

Everything below the expected number of lines is ignored, so you can also add commentary below the model definition.

5.2 Impose exported .kim model onto background model

This functionality is controlled by logical flag `IMPOSE_ASKI_INVERTED_MODEL` along with the parameters `FILE_ASKI_INVERTED_MODEL`, `ASKI_INVERTED_MODEL_INTERPOLATION_TYPE`, `ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS` in `Par_file_ASKI`.

`FILE_ASKI_INVERTED_MODEL` provides the filename (relative to directory `DATA/`) of the exported .kim file (text file as produced using option `-otxt` of `ASKI` executable `exportKim`).

`ASKI_INVERTED_MODEL_INTERPOLATION_TYPE` and `ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS` control the method of interpolating the given inverted model (defined on an `ASKI` internal inversion grid) onto the GLL points used in your `SPECFEM3D` simulation. At the moment, an unstructured 3D interpolation after Shepard [She68] is supported which is founded on inverse-distance weighting and accounts for issues of nearby points, direction and slope. `ASKI_INVERTED_MODEL_INTERPOLATION_TYPE` can be either set to `shepard_standard` or to `shepard_factor_radius`.

In case of type `shepard_factor_radius`, the factor given by `ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS` controls the influence of neighbouring control nodes on the interpolation (larger factor will include more control nodes (further away) for the interpolation). For a particular GLL point, first the closest control node of the inverted model (center of inversion grid cell) is found. Then this distance is multiplied by `ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS` to yield a radius within which all contained control nodes of the inverted model will be taken into account to compute the interpolated value for that GLL point.

Method `shepard_standard` is the same as using `shepard_factor_radius` with `ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS = 2.0`. This factor proved to be a good choice. When setting the method to `shepard_standard`, any value given for `ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS` is ignored.

5.3 Impose checkerboard/spike-test model onto the resulting model

A checkerboard/spike-test model as described in this section is only supported for 1-chunk simulations!

Onto the “final” resulting model (i.e. the chosen `SPECFEM3D` model, after possibly overwriting by an `ASKI` 1D background model (or not), after possibly superimposing a .kim inverted model (or not)), relative checkerboard / spike-test anomalies can be superimposed in order to conduct resolution analysis tests.

These anomalies are defined by their width and gaps between them (in km on the surface), in both, lat and lon direction of the chunk (i.e. the XI and ETA directions), as well as the depth locations and thicknesses of checker layers. The anomalies are defined by positive percentages

which alternate in sign throughout the checker grid. A template of such a model file, containing documenting commentary, is given by file `SPECFEM3D_GLOBE_for_ASKI/ASKI_checker_model_template`. The specific format of this text file is described now in the following:

the first line is ignored, this line may contain a short description of the model or can be empty.

the second and third line define the lateral distribution of checkers and background gaps in between in lat and long direction of the model chunk. The given sizes [km] at the surface of the Earth are projected into depth and distributed equi-angularly on the model chunk.

the fourth line gives the number of depth layers in which there should be checker patterns. Must be a positive integer.

the fifth line defines the depth values [km] of the upper boundaries of the checker layer.

the sixth line defines the thicknesses [km] of the checker layers.

the seventh line finally contains 5 percentage values separated by white space, defining the relative model anomaly values [positive percentage] of the 5 isotropic parameters density, v_p , v_s , Q_{μ} , Q_{κ} . The anomalies will be alternating in sign, i.e. varying +anomaly -anomaly, etc.

Everything below the expected content is ignored. Also, from each of the above described lines, only the expected content is read (e.g. just two numbers are read from lines 2-3) and everything behind is ignored. This way, you may add arbitrary commentary to a file.

6 Preparing Synthetic Data as Expected by ASKI

Use executable `transformSpecfem3dGlobeSyntheticData`, as described below.

It is assumed that a copy of the content of the `OUTPUT_FILES` directory (without the `MPI_DATABASES` files etc...) of all involved `SPECFEM3D` simulations (which contain the standard seismograms files) can be found at the path as choosen by the automated python script (see 4 (page 9)), i.e. filename of the kernel displacement file for the respective event with the extension `_OUTPUT_FILES`. The synthetic data then is written in the required form to path `PATH_SYNTHETIC_DATA/`, where the filenames are by convention `synthetics_EVENTID_STATIONNAME_COMPONENT`. Make sure that the `ASKI` frequency discretization as defined by the `ASKI` main parfile and iter parfile is correctly set! Also, all other objects used for an `ASKI` iteration step (like wavefield points file, inversion grid etc.) must be in place, since for executing `transformSpecfem3dGlobeSyntheticData` the basic requirements for an iteration step are initiated (compare `ASKI` manual, section “Initiate Basic Requirements”).

The executable `transformSpecfem3dGlobeSyntheticData`

Transforms standard `SPECFEM3D_GLOBE_7.0.0` output to `ASKI 1.0-1.2` spectral data in synthetic-data format.

It is assumed that seismograms were written as `NEZ`, and *not* as `ZRT`, i.e. `ROTATE_SEISMOGRAMS_RT = .false.`

It is assumed that text files were written, one file per seismogram, i.e. `OUTPUT_SEISMOS_ASCII_TEXT = .true.`, `SAVE_ALL_SEISMOS_IN_ONE_FILE = .false.`, `USE_`

```
BINARY_FOR_LARGE_FILE = .false..
```

Executing `transformSpecfem3dGlobeSyntheticData` (without arguments) will print a help message how to use it and will list the required positional arguments and mandatory options and optional options (listed in the following with a short description).

positional arguments of executable `transformSpecfem3dGlobeSyntheticData`

main_parfile Main parameter file of inversion.

mandatory options

-bicode band_instrument_code `band_instrument_code` must be two characters, band code and instrument code i.e. the first two characters before the component in seismogram filename. E.g. “LH” if your filenames look like “network.staname.LH*.sem”.

-dt time_step `time_step` is the real number defining the time step of the seismograms as given in files `output_mesher.txt`, `output_solver.txt`

-nstep number_of_time_samples `number_of_time_samples` is the number of samples NSTEP as given in file `output_solver.txt`

-ocomp output_components `output_components` is a vector of receiver components for which synthetic data output is produced. Valid components are CX , CY , CZ , N , S , E , W , UP , DOWN (also see ASKI user manual, section on “Data in ASKI ”).

optional options

-evid eventID If set, `eventID` indicates the single event for which synthetic data is produced. Otherwise, synthetic data is produced for all events (as defined in `FILE_EVENT_LIST` given in the ASKI main parfile).

-dconv If set, the normalized and differentiated source time function will be deconvolved from the differentiated synthetics. It is assumed that the source time function (error function) was written to file `plot_source_time_function.txt`, i.e. flag `PRINT_SOURCE_TIME_FUNCTION` was set to `.true.` in `SPECFEM3D Par_file`. `-dconv` is consistent with `ASKI_DECONVOLVE_STF = .true.` in `Par_file_ASKI`. In case `ASKI_DECONVOLVE_STF` was `.true.`, here flag `-dconv` should be set for consistency!

7 Preparing Synthetically Computed “Measured” Data as Expected by ASKI

For synthetic tests, you might want to treat synthetic data computed by SPECFEM w.r.t. some perturbed earth model as (noise-free) measured data. SPECFEM3D for ASKI “data” simula-

tions (e.g. produced by automated python script, 4 (page 9)) will produce these data in standard SPECSEM time-domain output formats. In order to transform these time series to frequency-domain measured data files in the form required by ASKI there are two possibilities:

First of all, the ASKI executable `transformMeasuredData` can be utilized for this purpose after appropriately renaming the text output trace files as required for input of `transformMeasuredData` option `-txt`).

As an alternative (providing more possibilities of data processing like scaling, filtering, differentiating), you can use executable `transformSpecfem3dGlobeMeasuredData`, as described below. It is assumed that a copy of the content of the `OUTPUT_FILES` folder (without the `MPI_DATABASES` files etc...) of the “data” simulations (which contain the standard seismograms files) can be found in respective directory `PATH_MEASURED_DATA/data_EVENTID_OUTPUT_FILES`. The measured data files then are written in the required form to path `PATH_MEASURED_DATA/`, where the filenames are by convention `data_EVENTID_STATIONNAME_COMP`. Make sure that the frequency discretization of ASKI measured data as defined by the ASKI main parfile is correctly set, as well as the measured data path!

The executable `transformSpecfem3dGlobeMeasuredData`

Transforms standard `SPECSEM3D_GLOBE_7.0.0` output to ASKI 1.0-1.2 spectral data in measured-data format.

It is assumed that seismograms were written as NEZ, and *not* as ZRT, i.e. `ROTATE_SEISMOGRAMS_RT = .false.`).

It is assumed that text files were written, one file per seismogram, i.e. `OUTPUT_SEISMOS_ASCII_TEXT = .true.`, `SAVE_ALL_SEISMOS_IN_ONE_FILE = .false.`, `USE_BINARY_FOR_LARGE_FILE = .false.`.

Executing `transformSpecfem3dGlobeMeasuredData` (without arguments) will print a help message how to use it and will list the required positional arguments and mandatory options and optional options (listed in the following with a short description).

positional arguments of executable `transformSpecfem3dGlobeMeasuredData`

main_parfile Main parameter file of inversion.

mandatory options

-bicode band_instrument_code `band_instrument_code` must be two characters, band code and instrument code i.e. the first two characters before the component in seismogram filename. E.g. “LH” if your filenames look like “`network.staname.LH*.sem`”.

-dt time_step `time_step` is the real number defining the time step of the seismograms as given in files `output_mesher.txt`, `output_solver.txt`

-nstep number_of_time_samples `number_of_time_samples` is the number of samples `NSTEP` as given in file `output_solver.txt`

-ocomp output_components `output_components` is a vector of receiver components for which measured data output is produced. Valid components are CX , CY , CZ , N , S , E , W , UP , DOWN (also see ASKI user manual, section on “Data in ASKI ”).

optional options

-filter If set, the respective event filters and station (component) filters as defined by the ASKI main parfile will be applied to the spectra before writing them to file. I.e. if in the ASKI main parfile any filtering is switched off (by respective flags), *no* filtering will be applied by executable `transformSpecfem3dGlobeMeasuredData` ! If in ASKI main parfile, only event filters are enabled, then this option `-filter` will cause the executable only to apply the event filters etc.

-evid eventID If set, `eventID` indicates the single event for which measured data is produced. Otherwise, measured data is produced for all events (as defined in `FILE_EVENT_LIST` given in the ASKI main parfile).

-cfreq forward_method Instead of the ASKI standard definition of real-valued frequencies by $f_k = k \cdot \Delta f$ (for frequency indices k and frequency step Δf), the data is produced w.r.t. complex frequencies consistent with the given forward method `forward_method`. For instance, setting `-cfreq GEMINI` will produce Gemini-consistent spectral data at complex frequencies with additional constant imaginary part $\sigma = -5\Delta f/2\pi$, thus implicitly using the actual frequencies $f_k = k \cdot \Delta f + i \cdot \sigma$ (with i being the imaginary unit, also see ASKI user manual, section on “Data in ASKI ”). Any filter values (in case of `-filter` is set) are assumed to be given at those complex frequencies, too!

-dconv If set, the normalized and differentiated source time function will be deconvolved from the differentiated seismograms. It is assumed that the source time function (error function) was written to file `plot_source_time_function.txt`, i.e. flag `PRINT_SOURCE_TIME_FUNCTION` was set to `.true.` in `SPECFEM3D Par_file`. `-dconv` is consistent with `ASKI_DECONVOLVE_STF = .true.` in `Par_file_ASKI`. When producing “measured data” that is to be modelled by (filtered) waveforms w.r.t. an impulsive source, it is recommended to set `-dconv` here and use `-filter`.

-diffths If set, the time series will *additionally* be differentiated (in the frequency domain after Fourier transform). This option is sensible to set when you require velocity seismograms (spectra).

-scale ts_scale_factor If set, the time series are scaled with factor `ts_scale_factor` (must be different from 0) after reading in, before transforming to frequency domain.

8 File `Par_file_ASKI`

File `Par_file_ASKI` is, just like the file `Par_file`, located in directory `DATA/` of your current `SPECFEM3D` example. It basically controls `ASKI` functionality if used along with an `ASKI` extended `SPECFEM3D` installation. If in such an extended `SPECFEM3D` version the file `Par_file_ASKI` is not present, no `ASKI` output is produced and `SPECFEM3D` runs with standard functionality.

In the following, we give a short description of the functionality of parameters defined in file `Par_file_ASKI`.

8.1 `ASKI` external model

First the `SPECFEM3D` model is set, as defined by standard `SPECFEM` mechanisms (i.e. by flag `MODEL` in file `Par_file`). Then, *only if indicated* by flag `USE_ASKI_BACKGROUND_MODEL`, this model is overwritten by the `ASKI` 1D background model at all depths where this background model is defined (see 5.1 (page 11)).

After that, *only if indicated*, by flag `IMPOSE_ASKI_INVERTED_MODEL` an `ASKI` inverted model is superimposed to the then existing model values (will set absolute model values, but at the boundaries of the inversion domain it will smooth out to the existing model, see 5.2 (page 12)).

Yet after that, ONLY IF INDICATED BELOW, one can superimpose a checkerboard by relative model anomalies. By setting the respective flags to `.false.`, this checkerboard can be superimposed to any standard `SPECFEM` model, as well as the `ASKI` background model or the `ASKI` inverted model.

`USE_ASKI_BACKGROUND_MODEL`, `FILE_ASKI_BACKGROUND_MODEL`

Logical flag `USE_ASKI_BACKGROUND_MODEL` indicates whether at all to use a 1D background model and

`FILE_ASKI_BACKGROUND_MODEL`, defines a filename relative to `DATA/` from which the 1D model is read. For the required format of this text file, see 5.1 (page 11).

`IMPOSE_ASKI_INVERTED_MODEL`, `FILE_ASKI_INVERTED_MODEL`, `ASKI_INVERTED_MODEL_INTERPOLATION_TYPE`, `ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS`

Logical flag `IMPOSE_ASKI_INVERTED_MODEL` indicates whether at all to impose an `ASKI` inverted model onto the existing model (standard background or standard background plus `ASKI` 1D background).

`FILE_ASKI_INVERTED_MODEL` gives the filename relative to `DATA/` where to find the file containing the the exported `.kim` file (text file as produced using option `-otxt` of `ASKI` executable `exportKim`).

Parameters `ASKI_INVERTED_MODEL_INTERPOLATION_TYPE`, `ASKI_INVERTED_MODEL_FACTOR_SHEPARD_RADIUS` control the way of interpolating the model values given on control nodes of an `ASKI` inversion grid onto the GLL points of the current `SPECFEM3D` mesh. For their meaning see 5.2 (page 12).

IMPOSE_ASKI_CHECKER_MODEL, FILE_ASKI_CHECKER_MODEL

Logical flag `IMPOSE_ASKI_CHECKER_MODEL` indicates whether to impose a relative checkerboard / spike-test model after defining the model by the chosen `SPECFEM3D` model, a possible `ASKI` background model and possible an `ASKI` inverted model.

`FILE_ASKI_CHECKER_MODEL` gives the filename relative to `DATA/` where to find the file containing the definition of the checkerboard / spike grid.

8.2 ASKI output

COMPUTE_ASKI_OUTPUT, ASKI_MAIN_FILE_ONLY, OVERWRITE_ASKI_OUTPUT

Parameter `COMPUTE_ASKI_OUTPUT` controls whether at all `ASKI` output is produced by the `SPECFEM3D` solver (i.e. kernel green tensor kernel displacement main or frequency files).

If `COMPUTE_ASKI_OUTPUT = .true.`, then logical flag `ASKI_MAIN_FILE_ONLY` controls whether to produce only the `.main` output file at the beginning of a simulation and immediately terminate. No frequency output files and no `SPECFEM` seismograms will be produced in this case. This functionality is useful, if you want to check the resolution of wavefield points with regard of your chosen inversion grid or you want to look at the kernel reference model (background model used by `SPECFEM`) *before* running all your simulations for an iteration step of `ASKI` waveform inversion. With one single `.main` output file available, namely, you can execute the `ASKI` executable `initBasics` and check for everything related to your wavefield points and inversion grid.

Logical flag `OVERWRITE_ASKI_OUTPUT` controls if the `ASKI` output files shall be overwritten if existend or not. If set to `.false.` and any of those files exist, the `SPECFEM3D` solver will terminate raising an error message.

Setting `COMPUTE_ASKI_OUTPUT = .false.` will *not* prevent the `SPECFEM3D` mesher from setting an `ASKI` background/external/checker (if indicated by above logical flags) ! So you can use an `ASKI` external model along with a standard `SPECFEM3D` simulation.

ASKI_outfile, ASKI_output_ID

`ASKI_outfile` defines the absolute base file name of `ASKI` output files. The actual output files of this simulation will be this base name appended by file extensions `.main` (for main output file) and `.jf#####` for each frequency (e.g. `.jf000013` for frequency index 13).

`ASKI_output_ID` is a character string of maximum length as defined by parameter `length_ASKI_output_ID` in file

`SPECFEM3D_GLOBE_for_ASKI/specfem3D_par_ASKI.f90` with which all output files of the current simulation will be tagged, and it will be used to check consistency of the files (could be a timestamp, eventID, station name + component etc).

ASKI_DECONVOLVE_STF

Logical flag `ASKI_DECONVOLVE_STF` indicates whether to deconvolve (the derivative of) the source time function from the wavefield spectra before writing them to files. Select `.true.`

for any Green function computations! Even if a Heaviside source time function is used, the velocity field is not exactly a Green function (i.e. displacement wavefield w.r.t. an impulse source time function), since a steep error function is used by SPECSEM to resemble a quasi-Heaviside function. This steep error function, furthermore, is dependent on timestep `DT`! Hence, only by deconvolution of (the derivative of) this quasi-Heaviside source time function, the real Green function (generated by an impulsive Dirac source time function), which is independent of the time step can be computed. *However, for now it is assumed that a quasi-Heaviside is used! Any other actually used source-time-function is not accounted for correctly, when* `ASKI_DECONVOLVE_STF = .true..`

8.3 Definition of back propagation Green function

Since `SPECSEM3D_GLOBE` does not properly support the use of single force sources, the computation of Green functions requires some additional definitions which are required by the `ASKI` extension code to `SPECSEM3D_GLOBE`.

COMPUTE_ASKI_GREEN_FUNCTION, ASKI_GREEN_FUNCTION_COMPONENT

Logical flag `COMPUTE_ASKI_GREEN_FUNCTION` indicates whether this type of `ASKI` output is a Green function wavefield (i.e. a generalized backpropagation from a receiver) or not. Set to `.false.` if this is a forward wavefield computation from some seismic source. The source position and source depth of this Green function (i.e. technically the respective `ASKI` receiver position) must be defined as usual in the `CMTSOLUTION` file.

By `ASKI_GREEN_FUNCTION_COMPONENT`, the direction of the single force source of this Green function is defined (in case of `COMPUTE_ASKI_GREEN_FUNCTION = .true.`). At the moment, the following directions are supported (following the `ASKI` nomenclature for receiver components):

`N`, `E`, `UP` : pointing to local 'N'orth, 'E'ast or 'UP' direction, dependent on source position
`CX`, `CY`, `CZ` : global Cartesian X, Y, Z directions

8.4 Frequency discretization

The double precision `df` [Hz] and integer values `jf` have the following meaning: The spectra are saved for all frequencies $f = jf * df$ [Hz].

ASKI_df, ASKI_nf, ASKI_jf

`ASKI_df` is a predefined frequency step that is used to evaluate the spectrum. In case we want to do an inverse FT in case of time-domain sensitivity kernel computation, we need to choose `ASKI_df` with care as `ASKI_df = 1/length_of_time_series` and suitably high frequency indices (dependent on frequency content). Otherwise we could lose periodicity (if in $\exp^{(-i2\pi (k) (n) / N)}$ N is no integer, these are no roots of 1 anymore). The spectra are saved for frequencies $f = (ASKI_jf) * ASKI_df$ (`ASKI_nf` many).

ASKI_DFT_double

Choose precision of Discrete Fourier Transform. If there is enough memory available, it is highly recommended to use `ASKI_DFT_double = .true.` in which case double complex spectra are hold in memory (single precision is written to file, though, but less roundoffs during transformation). Otherwise choose `ASKI_DFT_double = .false.` in which case single precision spectra will be used in memory. The transformation coefficients $\exp(-i*2\pi*f*t)$ are always in double complex precision!

ASKI_DFT_apply_taper, ASKI_DFT_taper_percentage

Decide whether the (oversampled, noisy, ...) time series should be tapered by a hanning taper (on tail) while applying the discrete fourier transform (on-the-fly). If `ASKI_DFT_apply_taper = .true.`, the value of `ASKI_DFT_taper_percentage` (between 0.0 and 1.0) defines the amount of total time for which the hanning taper will be applied at the tail of the time series.

8.5 Inversion grid

ASKI_type_inversion_grid

ASKI supports several types of inversion grids for `FORWARD_METHOD = SPECFEM3D`.
`ASKI_type_inversion_grid =`

1. (`TYPE_INVERSION_GRID = schunkInversionGrid`)
ASKI internal, but SPECFEM independent simple spherical inverison grid
2. (`TYPE_INVERSION_GRID = scartInversionGrid`)
NOT TO BE USED WITH SPECFEM3D_GLOBE!
ASKI internal, but SPECFEM independent Cartesian inversion grid:
The values for ASKI output are stored at all inner GLL points of spectral elements which lie inside the block volume defined below by parameters `ASKI_(cw)(xyz)`. ASKI locates the coordinates of those points inside the inversion grid cells and computes integration weights for them.
3. (`TYPE_INVERSION_GRID = ecartInversionGrid`)
External inversion grid provided e.g. by Trelis, which may contain tetrahedra, as well as hexahedra. As in case of `ASKI_type_inversion_grid = 2`, ASKI output is stored at all inner GLL points of elements which are inside the volume defined by `ASKI_(cw)(xyz)`. ASKI locates the wavefield points inside the inversion grid and computes weights.
4. (`TYPE_INVERSION_GRID = specfem3dInversionGrid`)
Use SPECFEM elements as inversion grid:
Wavefield points are *all* GLL points of an element for elements which are (at least partly) inside the volume defined by `ASKI_(cw)(xyz)`. Additionally store the jacobians for all wavefield points. Assume `ncell = ntot_wp/(NGLLX*NGLLY*NGLLY)` as the number of inversion grid cells, and the order of wavefield points accordingly (`do k=1, NGLLZ; do j=1, NGLLY; do i=1, NGLLX; ip=ip+1`)

5. (TYPE_INVERSION_GRID = chunksInversionGrid)

ASKI internal, but SPECSEM independent more elaborate spherical inversion grid supporting several chunks

ASKI_nchunk, ASKI_(c/w) (lat/lon), ASKI_r (min/max), ASKI_rot_gamma

Dependent on ASKI_type_inversion_grid, (a selection of) the following parameters may be used to define a volume within which wavefield points are searched for:

ASKI_nchunk defines the number of chunks of a chunk cubed sphere. SPECSEM3D_GLOBE for ASKI supports 1,2,3 and 6 chunks (like the forward code itself). However, not all those values are supported by all types of inversion grids: the schunkInversionGrid only supports ASKI_nchunk = 1, the ecartInversionGrid, specsem3dInversionGrid and chunksInversionGrid support all values 1,2,3,6.

ASKI_clat, ASKI_clon define the center of the first chunks (not used for full sphere with 6 chunks). ASKI_wlat, ASKI_wlon define the width of the chunk, in case of ASKI_nchunk = 1. For ASKI_nchunk = 2, 3, 6, always ASKI_wlon = ASKI_wlat = 90.0 is used. ASKI_rot_gamma defines the azimuthal rotation angle in degrees by which the 1,2 or 3 chunks are rotated (anti-clockwise) about the local vertical axis through the center of the first chunk (not used for ASKI_nchunk = 6).

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Using SPECFEM3D_GLOBE-7.0.0 for ASKI versions 1.0 to 1.2, Aug 2016

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Authors: Florian Schumacher (Ruhr-Universität Bochum, Germany)

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https://github.com/seismology-RUB/SPECFEM3D_GLOBE_for_ASKI/releases/tag/v1.2

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