Using SPECFEM3D_GLOBE-7.0.0 for ASKI - Analysis of Sensitivity and Kernel Inversion, version 1.0

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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 via `http://www.rub.de/aski` or to improve this documentation by incorporating your experiences with `SPECFEM3D for ASKI` and your personal experience of getting used to it (plus, let us know about it! Thanks).

I am aware of the poor LaTeXcoding of this document. 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 LaTeXsource files and all related components of this document are available via `http://www.rub.de/aski`

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Guide Through This Manual

We assume that you have sufficient knowledge of how to run the regular SPECFEM3D_GLOBE software.

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

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

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.

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

Section 8 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 SPECFEM3D_GLOBE software (http://geodynamics.org/cig/software/specfem3d_globe) in order to be used as a forward method for ASKI . In general, a regularly installed SPECFEM3D_GLOBE version is extended by certain few modifications so it can produce output for ASKI . So, SPECFEM3D_GLOBE for ASKI basically has the same requirements and dependencies as the SPECFEM3D_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 SPECFEM3D_GLOBE software.

1.1 Requirements

1. You need a functioning installation of the SPECFEM3D_GLOBE code, including modifications for usage with ASKI :

   - You can either download and install the modified SPECFEM3D version SPECFEM3D_GLOBE_V7.0.0_extended_for_ASKI.tar.gz, available via http://www.rub.de/aski, which already includes modifications for ASKI (see section 1.4),
   - or use your running installation of SPECFEM3D_GLOBE and extend it for usage with ASKI , as described below in section 1.5.

   In *both* cases you must install the package SPECFEM3D_GLOBE_for_ASKI_1.0.tar.gz!

2. You need basic experience in using the regular SPECFEM3D_GLOBE software!

3. Also you require an installation of the ASKI 1.0 main package available via http://www.rub.de/aski . The ASKI installation directory will be referred to below as ASKI_1.0/

1.2 Download and Extract `tar` ball

You must download the tar ball SPECFEM3D_GLOBE_for_ASKI_1.0.tar.gz from http://www.rub.de/aski. Please extract it in such a way, that the directory SPECFEM3D_GLOBE_for_ASKI is contained in the ASKI installation directory ASKI_1.0/

1.3 Installation

You need to compile few more ASKI binaries following these step:

- In ASKI_1.0/SPECFEM3D_GLOBE_for_ASKI/Makefile , set COMPILER appropriately, adjust FFLAGS if required and set the variables BLAS, LAPACK, just as you did in ASKI_1.0/Makefile when installing main package ASKI_1.0
- Issue the command make all from directory ASKI_1.0/SPECFEM3D_GLOBE_for_ASKI/

After that,
ASKI_1.0/bin should contain the new binaries transformSpecfem3dGlobeSyntheticData, transformSpecfem3dGlobeMeasuredData.

1.4 Using Already Extended Copy of SPECFEM3D_GLOBE-7.0.0 Code

Download SPECFEM3D_GLOBE_V7.0.0_extended_for_ASKI.tar.gz, available via http://www.rub.de/aski. This is a copy of package SPECFEM3D_GLOBE_V7.0.0.tar.gz which is extended by the steps 2.–9. as in section 1.5.

Extract the tar ball somewhere and re-configure and compile the software on your system according to the compilers you are using etc., e.g. by issuing the following commands from the installation directory:

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

In order to produce ASKI output in SPECFEM3D simulations, copy file ASKI_1.0/SPECFEM3D_GLOBE_for_ASKI/Par_file_ASKI to your respective DATA/ path (which is e.g. SPECFEM3D/EXAMPLES/my_example/DATA/ , or SPECFEM3D/DATA/). This file must be adjusted for any specific simulation (just as all other parameter files), refer to the documentation or examples on how to use it.

1.5 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 refered to as SPECFEM3D/).
2. Append content of file ASKI_1.0/SPECFEM3D_GLOBE_for_ASKI/specfem3D_par_ASKI.f90 to file SPECFEM3D/src/specfem3D/specfem3D_par.F90
3. In SPECFEM3D/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/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 `ASKI_1.0/SPECFEM3D_GLOBE_for_ASKI/ASKI_external_model.f90` to file `SPECFEM3D/src/meshfem3D/meshfem3D_par.f90`

6. In `SPECFEM3D/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/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 `ASKI_1.0/SPECFEM3D_GLOBE_for_ASKI/parallel_ASKI.f90` to file `SPECFEM3D/src/shared/parallel.f90`

9. Recompile the relevant `SPECFEM3D` binaries by issuing `make xmeshfem3D xspecfem3D` in directory `SPECFEM3D/`

10. In order to produce `ASKI` output in `SPECFEM3D` simulations, copy file `ASKI_1.0/SPECFEM3D_GLOBE_for_ASKI/Par_file_ASKI` to your respective `DATA/` path (which is e.g. `SPECFEM3D/EXAMPLES/my_example/DATA/` , or `SPECFEM3D/DATA/`). This file must be adjusted for any specific simulation (just as all other parameter files), refer to the documentation or examples on how to use it.

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 `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` extendet by `.main`, see 8.2. 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, 7).

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 inverision (the model of the last iteration step) into `SPECFEM3D`, see section 5. 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.

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 inverision (the model of the last iteration step) into `SPECFEM3D`, see section 5. 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)`

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!

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 SPECFEM3D , 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 SPECFEM3D, using the additional module ASKI_external_model:

Simple 1D layered spline-interpolation models can overwrite the SPECFEM3D 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 SPECFEM3D 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 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 SPECFEM3D_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 deph nodes between which a spline interpolation is done. A template of such a background model file, containing documenting commentary, is given by file SPECFEM3D_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/cm^3] 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 controled 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, vp, vs, Qmu, Qkappa. 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`.
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 below with a short description).

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), 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 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..

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 in SPECFEM3D Par_file.

-nstep number_of_time_samples number_of_time_samples is the number of samples NSTEP as in SPECFEM3D Par_file.

-ocomp output_components output_components is a vector of receiver components for which synthetic data output is produced. Valid components:
CX , CY , CZ , N , S , E , W , UP , DOWN

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 consistend 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

You can produce files for measured data in the form required by ASKI from SPECFEM3D for ASKI "data" simulations (e.g. produced by automated python script, 4). This functionality may be used for synthetic tests, in which you must produce data for some perturbed earth model, which is treated as (noise-free) measured data.

Use executable transformSpecfem3dGlobeMeasuredData.
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.

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 SPECFEM3D_GLOBE_7.0.0 output to ASKI 1.0 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. .

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 in SPECFEM3D Par_file.

-nstep number_of_time_samples number_of_time_samples is the number of samples NSTEP as in SPECFEM3D Par_file.

-ocomp output_components output_components is a vector of receiver components for which measured data output is produced. Valid components:
CX , CY , CZ , N , S , E , W , UP , DOWN

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. I.e. if in the ASKI main parfile any filtering is switched off (by respective flags), *no* filtering will by 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).

-gemini If set, *complex* valued frequencies f = jf*df + i*sigma with usual real part jf*df and constant (!) imaginary part sigma = -5*df/2pi are used for the discrete Fourier transform of the SPECFEM3D output seismograms and the filters are also assumed to be given at those frequencies, etc. Use this flag when producing synthetically compputed data for inversion with GEMINI, which computes spectral synthetics and kernels at those kind of complex frequencies.

-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 consistend 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 .

-diffts 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 before further processing.

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 9)).

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 10)).

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 9).

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 10).

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 immendiately 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 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 lenght as defined by parameter length_ASKI_output_ID in file ASKI_1.0/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 SPECFEM 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 SPECFEM3D_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 SPECFEM3D_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. techincally 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^(-i2pi(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*2pi*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` loactes 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 SPECFEM independent more elaborate spherical inverison 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. SPECFEM3D_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, specfem3dInversionGrid 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).

References

[She68] Donald Shepard. A two-dimensional interpolation function for irregularly-spaced data. In *Proceedings of the 1968 23rd ACM national conference*, ACM '68, pages 517–524, New York, NY, USA, 1968. ACM.

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