

Using SPECSEM3D_Cartesian-3.0 for ASKI – Analysis of Sensitivity and Kernel Inversion, versions 1.0 to 1.2

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If you use SPECSEM3D_Cartesian for ASKI for your own research, please cite our paper [SFL16]:

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

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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 by opening (or adding to) an “issues” topic on https://github.com/seismology-RUB/SPECSEM3D_Cartesian_for_ASKI or to improve this documentation by incorporating your experiences with SPECSEM3D 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_EXcoding 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 L^AT_EXsource files and all related components of this document are available via https://github.com/seismology-RUB/SPECSEM3D_Cartesian_for_ASKI , subdirectory doc/ of the repository.

Florian Schumacher, Aug 2016

Guide Through This Manual

We assume that you have sufficient knowledge of how to run the regular `SPECFEM3D_Cartesian` software (i.e. without extension for use with `ASKI`).

For details on how to get started by installing everything required for using `SPECFEM3D_Cartesian` 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_specfem3dCartesianForASKI_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 10 (page 18) 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_Cartesian software (<http://geodynamics.org/cig/software/specsem3d>) in order to be used as a forward method for ASKI. In general, a regularly installed SPECSEM3D_Cartesian version is extended by certain few modifications so it can produce output for ASKI. So, SPECSEM3D_Cartesian for ASKI basically has the same requirements and dependencies as the SPECSEM3D_Cartesian 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_Cartesian 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_Cartesian code, including modifications for usage with ASKI:
 - You can either use the basic extract from the SPECSEM3D_Cartesian master branch (by November 2015) that comes with this package (see section 1.3 (page 6)),
 - or use your running installation of SPECSEM3D_Cartesian 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_Cartesian 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_Cartesian_for_ASKI
```

(in one line, of course) from local path `/your/programs/`. This will create subdirectory `/your/programs/SPECSEM3D_Cartesian_for_ASKI` (also referred to below simply as `SPECSEM3D_Cartesian_for_ASKI/`) containing the code and documentation of the current release of the extension package SPECSEM3D_Cartesian for ASKI.

Alternatively, go to https://github.com/seismology-RUB/SPECSEM3D_Cartesian_for_ASKI and download the content of the master branch as a `.zip` or try executing

```
wget https://github.com/seismology-RUB/SPECSEM3D_Cartesian_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_Cartesian_for_ASKI/`.

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

- In `SPECFEM3D_Cartesian_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_Cartesian_for_ASKI/`

After that, `SPECFEM3D_Cartesian_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_Cartesian_for_ASKI should be consistent with the latest version of the ASKI repository's master branch.

1.3 Using Already Extended Extract of `SPECFEM3D_Cartesian-3.0` Code

`SPECFEM3D_Cartesian_for_ASKI/specfem3d` contains a very basic extract of the git release of `SPECFEM3D_Cartesian` version 3.0 from git repository <https://github.com/geodynamics/specfem3d> (master branch) by 2015 November 7. Some folders like `utils`, `doc` etc. were removed to keep this copy small. Additionally, two important modifications were applied, which were committed to the `devel` branch on 3 September 2015, or are about to be committed by the developers team (see comments by "FS FS"):

- in `src/specfem3d/setup_sources_receivers.f90` , subroutine `setup_sources()`, l.180 :
removing `USE_FORCE_POINT_SOURCE .or. from the if-clause`, i.e. execute (re)definition of `t0` only in case of `USE_RICKER_TIME_FUNCTION == .true.`
- in `src/specfem3d/compute_add_sources_viscoelastic.f90` :
always call function `comp_source_time_function_gauss()` with half duration `hdur_gaussian(isource)` instead of fixed value of `5.d0*DT`

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_Cartesian_for_ASKI/specfem3d/` :

```
> ./configure FC=gfortran MPIFC=mpif90
> make default
```

In order to produce ASKI output in `SPECFEM3D` simulations, copy file `SPECFEM3D_Cartesian_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) and is described in detail in section 10 (page 18).

1.4 Extend Your Own `SPECFEM3D_Cartesian-3.0` Code to Produce Output for ASKI

You can use your own running installation of `SPECFEM3D_Cartesian` and extend it in the following way for usage with ASKI , provided it has the required functionality. This procedure

was tested for SPECSEM3D_Cartesian git master by 2015 Nov 7, extended by the two modifications described above in section 1.3 (page 6):

1. install SPECSEM3D_Cartesian on your system and make it run, gain experience in using it (below, the installation path is referred to as specsem3d/).
2. Copy file SPECSEM3D_Cartesian_for_ASKI/specsem3d_for_ASKI.f90 to specsem3d/src/specsem3D/
3. Replace file specsem3d/src/generate_databases/model_external_values.f90 by SPECSEM3D_Cartesian_for_ASKI/model_external_values.f90
4. Append content of file SPECSEM3D_Cartesian_for_ASKI/parallel_ASKI.f90 to file specsem3d/src/shared/parallel.f90
5. Append content of file SPECSEM3D_Cartesian_for_ASKI/specsem3D_par_ASKI.f90 to file specsem3d/src/specsem3D/specsem3D_par.f90
6. In specsem3d/src/specsem3D/rules.mk : add the following line into the definition of specsem3D_OBJECTS (e.g. before line with \$ (EMPTY_MACRO))
[tab_character]\$O/specsem3d_for_ASKI.spec.o \
(be aware that the above line *must* start with an actual TAB character in order to conform to the GNU-make syntax)
7. In specsem3d/src/specsem3D/prepare_timerun.F90 in subroutine prepare_timerun :
add the following line at the end of the subroutine, before the statistics output is written to main output file by rank 0:
call prepare_timerun_ASKI()
8. In specsem3d/src/specsem3D/iterate_time.F90 in subroutine iterate_time :
add the following line just before the "enddo" of the time loop
call write_ASKI_output()
9. In specsem3d/src/specsem3D/finalize_simulation.f90 in subroutine finalize_simulation :
add the following line just before the main output file is closed at the end of the subroutine
call save_ASKI_output()
10. Set USE_SOURCES_RECVS_Z = .true. in specsem3d/setup/constants.h (or wherever your file constants.h is located).
11. Recompile all SPECSEM3D binaries, possibly by issuing make in directory specsem3d/
12. In order to produce ASKI output in SPECSEM3D simulations, copy file SPECSEM3D_Cartesian_for_ASKI/Par_file_ASKI to your respective DATA/ path (which is e.g. specsem3d/EXAMPLES/my_example/DATA/ , or specsem3d/DATA/). This file must be adjusted for any specific simulation (just as all other parameter files) and is described in detail in section 10 (page 18).

If you have a newer version of `SPECFEM3D_Cartesian` 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 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 10.2 (page 19). 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, e.g. all kernels in your specific iteration step of an inversion). It may, hence, be sensible to use the same MPI Databases for all `SPECFEM3D` for `ASKI` simulations (adjust your script `process.sh` in such a way, that you do not always recompile and decompose `MESH`, but only call the solver again, with changed parameter files and source files).
- Green tensor simulations are done using the third coordinate in the station definition as the `FORCESOLUTION` depth value, in order to allow receivers to be located not only on the surface. It, hence, is strongly recommended to thoroughly use `USE_SOURCES_RECVS_Z = .true.` in `specfem3d/setup/constants.h`.
- When using the provided `SPECFEM3D` version in subdirectory `SPECFEM3D_Cartesian_for_ASKI/specfem3d`, or using file `SPECFEM3D_Cartesian_for_ASKI/model_external_values.f90` for extending your own `SPECFEM3D` version, the functionality controlled by flag `COUPLE_WITH_EXTERNAL_CODE` does not work anymore, so `COUPLE_WITH_EXTERNAL_CODE` should be switched to `.false.` in `Par_file`. If you want to produce `ASKI` output with `COUPLE_WITH_EXTERNAL_CODE` switched on, you need to incorporate the coupling functionality into `model_external_values.f90` accordingly.
- As coordinates of wavefield points (and, hence, inversion grid coordinates) `SPECFEM3D` for `ASKI` uses:
First coordinate = X, second coordinate = Y, third coordinate = Z.
- 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`).

3 One Single Simulation

As usual, you need to do (external or internal) meshing for the appropriate (current) background model. See section 5 (page 11) for details on how to import the current model of an inversion (the inverted model of the last iteration step) into `SPECFEM3D`.

Set the regular SPECFEM3D files `Par_file`, `CMTSOLUTION` / `FORCESOLUTION` and `STATIONS` (standard SPECFEM3D functionality; only if you want to record any seismograms).

Additionally, you need to set file `Par_file_ASKI` to desired values. The file is described in detail in section 10 (page 18).

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 do (external or internal) meshing for the appropriate (current) background model. See section 5 (page 11) for details on how to import the current model of an inversion (the inverted model of the last iteration step) into SPECFEM3D.

Python script `run_specfem3dCartesianForASKI_simulations.py` (provided in directory `SPECFEM3D_Cartesian_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 first lines 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_specfem3dCartesianForASKI_simulations.py`, some parameters in SPECFEM3D files `CMTSOLUTION`, `FORCESOLUTION`, `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`
- `ASKI_MAIN_FILE_ONLY` (must be set to `.false.!`)

- `OVERWRITE_ASKI_OUTPUT`
- `ASKI_DECONVOLVE_STF`
- `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_(cw) (xyz), ASKI_rot_(XYZ)`

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 **FORCESOLUTION**

The python script *always* automatically sets “latorUTM:”, “longorUTM:”, “depth:”, “factor force source:”, “component dir vect source E:”, “component dir vect source N:”, “component dir vect source Z_UP:”. In case of “displ” and “gt” simulations, additionally “f0:” is set to $5 \times DT$. So, if you wish to do a “data” simulation for single force sources, using a different “f0:” value, you should conduct those in a separate run of the python script.

It is strongly recommended (if not necessary) to use `USE_SOURCES_RECVS_Z = .true.` in `specfem3d/setup/constants.h`, see comment in section 2 (page 8).

4.3 Manually Setting **CMTSOLUTION**

The python script *always* automatically sets “latorUTM:”, “longorUTM:”, “depth:”, “Mrr:”, “Mtt:”, “Mpp:”, “Mrt:”, “Mrp:”, “Mtp:”. In case of “displ” simulations, additionally “half duration:” is set to “0.”. So, if you wish to do a “data” simulation for moment tensor sources using a different “half duration:” value, you should conduct those in a separate run of the python script.

It is strongly recommended (if not necessary) to use `USE_SOURCES_RECVS_Z = .true.` in `specfem3d/setup/constants.h`, see comment in section 2 (page 8).

4.4 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 SPECSEM3D STATIONS file, you must provide it manually. The standard SPECSEM3D STATIONS file should contain the definition of stations as in the ASKI file FILE_STATION_LIST, in consistend SPECSEM3D notation, i.e. coordinate columns being lat (= Y, third column of STATIONS and fourth column of FILE_STATION_LIST) and lon (= X, fourth column of STATIONS and third column of FILE_STATION_LIST) and elev (= Z, 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!

It is strongly recommended (if not necessary) to use USE_SOURCES_RECVS_Z = .true. in specsem3d/setup/constants.h, see comment in section 2 (page 8).

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

There are two types of external models that can be put (in combination) into SPECSEM3D, using a special implementation of the SPECSEM3D module model_external_values:

Simple 1D layered gradient background models can overwrite the default background model (coming from the mesher, e.g. Trelis). Exported .kim files (as produced by ASKI program exportKim with option -otxt) may be superimposed onto the background model (default Trelis model or ASKI 1D background model) and used as a model for the new iteration of full waveform inversion of ASKI .

These two types of external models are explained in the following. To be able to use *any* of the two (or both in combination), you *must* set MODEL = external in Par_file !

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_Cartesian 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 (or rather Z). *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_Cartesian_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 line contains one real value defining the maximum Z value z_{\max} of the model domain (since internally, Z values are processed and there is no knowledge about “depth”, hence the Z-value of the following depth nodes are computed as $z_{\text{node}} = z_{\max} - \text{depth}_{\text{node}}$).

the third and fourth 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 third 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 fourth line contains as many integer values (separated by white space) as there are layers (as defined by line three) and gives for each layer the number of nodes. must contain the number of nodes inside each layer.

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 [Kg/m³] vp [m/s] vs [m/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.

6 Preparing Synthetic Data as Expected by ASKI

Use executable `transformSpecfem3dCartesianSyntheticData`, 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 `transformSpecfem3dCartesianSyntheticData` the basic requirements for an iteration step are initiated (compare `ASKI` manual, section “Initiate Basic Requirements”).

Executing `transformSpecfem3dCartesianSyntheticData` (without arguments) will print a help message how to use it and will list the required positional arguments and mandatory options and optional options. Those are described in more detail in the following:

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

-bicode band_instrument_code `band_instrument_code` is a character string consisting of bandcode 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?.semf”

-ori orientation `orientation` is either “NEZ” or “XYZ”, indicating the component characters following `band_instrument_code`.

-dt time_step Gives the time step of the `SPECFEM3D` seismograms (as in the `SPECFEM3D Par_file`).

-nstep number_of_time_steps Defines the number of samples `NSTEP` as in the `SPECFEM3D Par_file`

-ocomp "comp_1 ... comp_n" Vector of station components for which synthetic data 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

-event_id `event_id` indicates a single event for which synthetic data is produced, otherwise synthetic data is produced for *all* events (as defined by the `ASKI FILE_EVENT_LIST`).

-dconv If set, the source time function will be deconvolved from the SPECFEM3D seismograms. This option is consistent with setting `ASKI_DECONVOLVE_STF = .true.` in `Par_file_ASKI`.

-bin Indicates whether the SPECFEM3D trace files are binary files or not. For ascii output simply do not set option `-bin`.

-ext extension *This option is not needed for standard functionality, only use this if you know what your're doing.* Standard functionality (i.e. *not* setting `-ext`) will produce *displacement* spectra. If `-ext` is set, however, the specific file extension `extension` is forced to be used. `extension` represents *anything* following the orientation character, including *all* dots etc., e.g. “.semv” if the filenames that should be used look like “network.staname.FX?.semv”.

-diffTs *This option is not needed for standard functionality, only use this if you know what your're doing.* Standard functionality (i.e. *not* setting `-diffTs`) will produce *displacement* spectra. If set, the time series will be differentiated (by simple first order central differences) before further processing.

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” simulations (e.g. produced by automated python script, 4 (page 9)) will produce these data in standard SPECFEM 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 (e.g. choosing seismic Unix output for the SPECFEM simulations, or 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 `transformSpecfem3dCartesianMeasuredData`, 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!

Executing `transformSpecfem3dCartesianMeasuredData` (without arguments) will print a help message how to use it and will list the required positional arguments and mandatory options and optional options (described in more detail in the following). Note that only necessary things will be read/initialized on the basis of the ASKI main parameter file given (e.g. everything not needed, like integration weights, inversion grid, will *not* be initialized at this point, i.e. those quantities are not required to exist already! Hence, you may use this executable before starting to solve the forward problem in the first iteration of ASKI FWI).

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

-bicode band_instrument_code `band_instrument_code` is a character string consisting of bandcode 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?.semd”

-ori orientation `orientation` is either “NEZ” or “XYZ”, indicating the component characters following `band_instrument_code`.

-dt time_step Gives the time step of the SPECSEM3D seismograms (as in the SPECSEM3D `Par_file`).

-nstep number_of_time_steps Defines the number of samples NSTEP as in the SPECSEM3D `Par_file`

-ocomp "comp_1 ... comp_n" Vector of station components for which measured data 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

-ext extension *This option is not needed for standard functionality, only use this if you know what your’re doing.* Standard functionality (i.e. *not* setting `-ext`) will produce *displacement* spectra. If `-ext` is set, however, the specific file extension `extension` is forced to be used. `extension` represents *anything* following the orientation character, including *all* dots etc., e.g. “.semv” if the filenames that should be used look like “network.staname.FX?.semv”.

-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 `transformSpecfem3dCartesianMeasuredData`! 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 event_id event_id indicates a single event for which measured data is produced, otherwise measured data is produced for *all* events (as defined by the `ASKI_FILE_EVENT_LIST`).

-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 source time function will be deconvolved from the `SPECFEM3D` seismograms. This option is consistent with setting `ASKI_DECONVOLVE_STF = .true.` in `Par_file_ASKI`.

-diffts *This option is not needed for standard functionality, only use this if you know what your're doing.* If set, the time series will be differentiated (by simple first order central differences) before further processing.

-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.

-bin Indicates whether the `SPECFEM3D` trace files are binary files or not. For ascii output simply do not set option `-bin`.

8 Create `ASKI` filter file from source time function file

Using the executable `createSpectralFilters` contained in the `ASKI` main package, spectral filter files as required by `ASKI` can be produced from a time-domain trace file (e.g. the output txt file `plot_source_time_function.txt`). This functionality may be useful for synthetic tests: After producing “measured” data by simulation with a specific source-time function (e.g. a Ricker wavelet), spectral filters containing the source-time-function information should be used in `ASKI`.

By option `-eventf` you must provide a parameter file, particularly specifying the wavelet by `STF_FILE`, `STF_COLUMN_OF_TRACE`, `STF_DT`, `STF_NSTEP`. Please refer to the `ASKI` user manual for any details.

9 Experimental feature: Convolution impulsive synthetics with given source-time function

Attention: this is an experimental feature, the executable `convolveWithStf` does not yet produce satisfying results, i.e. it must be debugged!!

The synthetic data computed for an `ASKI` iteration step is computed w.r.t. an impulsive source-time function and the actual source-time function of the measured data is modelled by applying spectral filters to the frequency-domain synthetic data. This, however, does not allow to compare the current data fit in that iteration visually by looking at time series (comparing measured and synthetic data).

The executable `convolveWithStf` (*not yet debugged!!, do not believe its output!*) aims at convolving the synthetic seismograms (produced by `SPECFEM` for an `ASKI` iteration) with a given source time function (e.g. the one which is assumed for the measured data, or the one that was used in synthetic test inversions for computing the measured data). Optionally, the original source time function that was used in the `SPECFEM` simulation for synthetic data (i.e. the “kernel displacement” simulations), which is a thin Gaussian in case of a single force source or a steep error function in case of a moment tensor source, may be deconvolved from the synthetics before convolving with the given source time function.

The idea of this executable is, to enable the user to have a look at the time-domain data fit *without* having to run another forward simulation for each source using the given source-time function (that was used for producing measured data).

However: it is not clear to the author (Florian Schumacher, August 2016) whether such a process can be successful at all when the synthetic data was modelled to be stable only up to a quite low maximum frequency (e.g. in the first iteration steps), since the higher frequencies that are contained in the measured data are *not* stably contained in the synthetic!

(**TODO IN THE FUTURE:** this executable could support to simply apply the `ASKI` spectral filters *but* these are usually given only in a small frequency band and are given in a frequency discretization different from that used for Fast Fourier Transform.)

In the following, there is a short description of the required positional arguments and mandatory options and optional options of executable `convolveWithStf`.

Positional arguments

stf_file File containing the source time function by which the synthetics are to be convolved. It is assumed that it is a text file containing *two* columns: time (first column) and source-time function values (second column). The first column is used to get the time step of the given source time function (by subtracting first from last time value and dividing by the number of time intervals).

main_parfile Main parameter file of inversion.

Mandatory options

-bicode band_instrument_code `band_instrument_code` is a character string consisting of bandcode and instrument code, i.e. the first two characters before the component in seismogram filenames, e.g. “LH” if your filenames look like “network.staname.LH?.semf”

-ori orientation `orientation` is either “NEZ” or “XYZ”, indicating the component characters following `band_instrument_code`.

-dt time_step Gives the time step of the SPECSEM3D seismograms that was used in the current ASKI iteration (as in the SPECSEM3D Par_file).

-nstep number_of_time_Steps Defines the number of samples NSTEP of the SPECSEM3D seismograms that was used in the current ASKI iteration (as in the SPECSEM3D Par_file).

Optional options

-ext extension *This option is not needed for standard functionality, only use this if you know what your're doing.* Standard functionality (i.e. *not* setting `-ext`) will produce *displacement* spectra. If `-ext` is set, however, the specific file extension `extension` is forced to be used. `extension` represents *anything* following the orientation character, including *all* dots etc., e.g. “.semv” if the filenames that should be used look like “network.staname.FX?.semv”.

-evid event_id `event_id` indicates a single event for which the convolution should be done, otherwise it will be done for *all* events (as defined by the ASKI `FILE_EVENT_LIST`).

-bin Indicates whether the SPECSEM3D trace files are binary files or not. For ascii output simply do not set option `-bin`.

-dconv If set, the source time function will be deconvolved from the SPECSEM3D seismograms. This option is consistend with setting `ASKI_DECONVOLVE_STF = .true.` in `Par_file_ASKI`.

-opath output_path If set, the character string `output_path` will be used to write the convolved seismogram files. It is assumed relative to the respective specsem seismograms path, i.e. `path PATH_KERNEL_DISPLACEMENTS/kernel_displ_eventID_OUTPUT_FILES/`. If not set, the default value “convolved/” is used (indicating the subdirectory “convolve/”).

10 File Par_file_ASKI

File `Par_file_ASKI` is, just like the file `Par_file`, located in directory `DATA/` of your current SPECSEM3D example. It basically controls ASKI functionality SPECSEM3D if used along with an ASKI extended SPECSEM3D installation. If in such an installation file `Par_file_ASKI` is not present, no ASKI output is produced and SPECSEM3D runs with standard functionality.

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

10.1 ASKI external model

The following parameters will *only* have any effect, when you set `MODEL = external` in `Par_file`.

First the `SPECFEM3D` model is set, as defined by standard `SPECFEM` mechanisms. 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)).

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).

10.2 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 produces 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 SPECSEM) *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 SPECSEM3D solver will terminate raising an error message.

Setting `COMPUTE_ASKI_OUTPUT = .false.` will *not* prevent the SPECSEM3D mesher from setting an ASKI external model, if `MODEL = external` in `Par_file` and any external model is defined as described above in section 10.1 (page 19) ! So you can use an ASKI external model along with a standard SPECSEM3D 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

`SPECSEM3D_Cartesian_for_ASKI/specsem3D_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.

Dependent on the type of source mechanism (single force, or moment tensor), SPECSEM uses a Gaussian (single force) or a Heaviside (moment tensor) in case of `USE_RICKER_TIME_FUNCTION = .false..` ASKI takes care about, which wavefield to store and which source wavelet to deconvolve. ASKI always produces displacement spectra w.r.t. a Dirac impulse time function (if `ASKI_DECONVOLVE_STF = .true.`).

10.3 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 $\text{ASKI_df} = 1/\text{length_of_time_series}$ 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 $f = (\text{ASKI_jf}) * \text{ASKI_df}$ (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.

10.4 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)`
NOT TO BE USED WITH SPECFEM3D Cartesian!
ASKI internal, but SPECFEM independent simple spherical inverison grid
2. `(TYPE_INVERSION_GRID = scartInversionGrid)`
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*NGLLZ) 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)

NOT TO BE USED WITH SPECFEM3D Cartesian!

ASKI internal, but SPECFEM independent more elaborate spherical inversion grid

ASKI_(cw) (xyz) , ASKI_rot_(XYZ)

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:

First, ASKI_wx, ASKI_wy, ASKI_wz define the total width of a block which is centered in x=y=z=0 E.g. the total block extension in x-direction covers all points with $x \geq -0.5 \cdot \text{ASKI_wx}$ and $x \leq 0.5 \cdot \text{ASKI_wx}$.

Then, ASKI_rot_X, ASKI_rot_Y, ASKI_rot_Z define rotation angles in degrees by which the block is rotated (anti-clockwise) about the Z, Y and X coordinate axis, before ASKI_cx, ASKI_cy, ASKI_cz define a vector by which the rotated block is shifted (new center of block).

Be aware:

- the parameters for rotation angles ASKI_rot_(XYZ) *must always* be assigned to values! Set to 0. if no rotation should be applied.
- scartInversionGrid only supports ASKI_rot_Z and uses a different definition of the z-coverage.
- ecartInversionGrid and specfem3dInversionGrid use *all* rotation angles ASKI_rot_(XYZ) (again, set angles to zero if no rotation is desired).

References

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History

This is a section on the history of this document, i.e. its previously published versions, as referred to by the GNU Free Documentation License (version 1.3).

Using SPECFEM3D_Cartesian-3.0 for ASKI versions 1.0 to 1.2, Aug 2016

Recognizable snippet from the title page (scaled):

Using SPECFEM3D_Cartesian-3.0 for
ASKI - Analysis of Sensitivity
and Kernel Inversion, versions 1.0 to 1.2
Aug 2016

Title: Using SPECFEM3D_Cartesian-3.0 for ASKI versions 1.0 to 1.2, Aug 2016

Year: 2016

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

This version of this document is provided for download (as of August 2016) at

https://github.com/seismology-RUB/SPECFEM3D_Cartesian_for_ASKI/releases/tag/v1.2

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https://github.com/seismology-RUB/SPECFEM3D_Cartesian_for_ASKI/releases/download/v1.2/SPECFEM3D_Cartesian_for_ASKI_manual_aug-2016.pdf

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December 2015

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Using SPECFEM3D_Cartesian-2.1 for ASKI version 0.3, September 12, 2013

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Year: 2013

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

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