Using SPECFEM3D_Cartesian-3.0 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*.
lease 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_Cartesian` software.

For details on how to get started by installing everything required for using `SPECFEM3D_Cartesian` 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_specfem3dCartesianForASKI_simulations.py` which conducts a lot of simulations in an automated fashion. Please read section 4.

If you want to conduct one single simulation producing output for `ASKI` , please read section 3.

Section 9 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.

Contents

1 Installation and Getting Started

This section explains how to install the SPECFEM3D_Cartesian software (http://geodynamics.org/cig/software/specfem3d) in order to be used as a forward method for ASKI. In general, a regularly installed SPECFEM3D_Cartesian version is extended by certain few modifications so it can produce output for ASKI. So, SPECFEM3D_Cartesian for ASKI basically has the same requirements and dependencies as the SPECFEM3D_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 SPECFEM3D_Cartesian software.

1.1 Requirements

1. You need a functioning installation of the SPECFEM3D_Cartesian code, including modifications for usage with ASKI:

   - You can either download and install the modified SPECFEM3D version SPECFEM3D_Cartesian_git_master_2015-11-07_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_Cartesian and extend it for usage with ASKI, as described below in section 1.5.

   In *both* cases you must install the package SPECFEM3D_Cartesian_for_ASKI_1.0.tar.gz!

2. You need basic experience in using the regular SPECFEM3D_Cartesian 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_Cartesian_for_ASKI_1.0.tar.gz from http://www.rub.de/aski. Please extract it in such a way, that the directory SPECFEM3D_Cartesian_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_Cartesian_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_Cartesian_for_ASKI/

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

1.4 Using Already Extended Extract of SPECFEM3D_Cartesian-3.0 Code

Download SPECFEM3D_Cartesian_git_master_2015-11-07_extended_for_ASKI.tar.gz, available via http://www.rub.de/aski. This is 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 commited to the devel branch on 3 September 2015, or are about to be commited 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

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 default
```

1.5 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 SPECFEM3D_Cartesian git master by 2015 Nov 7, extended by the two modifications described above in section 1.4:

1. install SPECFEM3D_Cartesian on your system and make it run, gain experience in using it (below, the installation path is refered to as SPECFEM3D/).
2. Copy file ASKI_1.0/SPECFEM3D_Cartesian_for_ASKI/specfem3D_for_ASKI.f90 to SPECFEM3D/src/specfem3D/
3. Replace file SPECFEM3D/src/generate_databases/model_external_values.f90 by ASKI_1.0/SPECFEM3D_Cartesian_for_ASKI/model_external_values.f90
4. Append content of file ASKI_1.0/SPECFEM3D_Cartesian_for_ASKI/parallel_ASKI.f90 to file SPECFEM3D/src/shared/parallel.f90

5. Append content of file ASKI_1.0/SPECFEM3D_Cartesian_for_ASKI/specfem3D_par_ASKI.f90 to file SPECFEM3D/src/specfem3D/specfem3D_par.f90

6. In SPECFEM3D/src/specfem3D/rules.mk : add the following line into the definition of specfem3D_OBJECTS (e.g. before line with $(EMPTY_MACRO))
   [tab_character]$O/specfem3D_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 SPECFEM3D/src/specfem3D/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 SPECFEM3D/src/specfem3D/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 SPECFEM3D/src/specfem3D/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 SPECFEM3D/setup/constants.h (or wherever your file constants.h is located).

11. Recompile all SPECFEM3D binaries, possibly by issuing make in directory SPECFEM3D/

12. In order to produce ASKI output in SPECFEM3D simulations, copy file ASKI_1.0/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), refer to documentation or examples on how to use it.

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 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 extendet by .main, see 9.2. 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, 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 throughoutly use USE_SOURCES_RECVS_Z = .true. in SPECFEM3D/setup/constants.h.

- When using the provided SPECFEM3D version SPECFEM3D_Cartesian_git_master_2015-11-07_extended_for_ASKI.tar.gz, or using file model_external_values.f90 as provided by package SPECFEM3D_Cartesian_for_ASKI_1.0.tar.gz, the functionality controled 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 funktionality into model_external_values.f90.

- 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 for details on how to import the current model of an inverision (the 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 9.

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 for details on how to import the current model of an inverision (the 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_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 so far there is no support to do "displ" simulations (i.e. producing kernel displacement output) with preventing the python script from setting `ASKI_DECONVOLVE_STF = .true.`. This does not allow, e.g. to directly use a Ricker wavelet for simulations of type "displ". You will always need to provide your source wavelet as event filters in `ASKI` (produce such a filter e.g. using the executable `createSpecfem3dFilters` → 8 (page 12)).

(**TODO IN THE FUTURE:** Allow for using Ricker wavelet for simulations of type "displ")

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.

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.

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 `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 (= 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`!

5 Importing external models into `SPECFEM3D` , 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 `SPECFEM3D`, using a special implementation of the `SPECFEM3D` 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 modesl 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 `SPECFEM3D_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 nott 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_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 $z_{node} = z_{max} - depth_{node}$).

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. amust 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/m^3] 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.
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.

(**TODO IN THE FUTURE:** Provide here a list of arguments with more detailed descriptions)

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

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 transformSpecfem3dCartesianMeasuredData.
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.

(**TODO IN THE FUTURE:** Provide here a list of arguments with more detailed descriptions)

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!

8 Create `ASKI` filter file from source time function

(**TODO IN THE FUTURE:** move this executable to the `ASKI` main package, providing general functionality of producing filter files for standard filters or arbitrary source-time-function input files, having a proper user interface)

You can produce a filter file, which is conform to `ASKI` from a time-domain trace file (e.g. the output txt file `plot_source_time_function.txt`) using the **experimental** executable `createSpecfem3dFilters`. **Do not just execute `createSpecfem3dFilters` without argument, it will print *no* usage message!**

This experimental executable must be prepared by you for your specific time and frequency discretization. It expects a txt file called "ricker.txt" in the directory from where you execute the program, containing two columns (e.g. first column time, second column amplitude of stf). *The first column is entirely ignored!* The file is read in completely from first line (first time sample) to last line (last time sample). This solely defines the number of time samples `nt` used by the program.

You must edit the source file `ASKI_1.0/SPECFEM3D_Cartesian_for_ASKI/createSpecfem3dFilters.f90` in the upper part and set the values of `df`, `nf` and `ifreq` according to the desired frequency discretization of the output filter file. You must set the value of `dt` according to the time step on which the input stf file "ricker.txt" is based. *This time step is not inferred from the first column of the input stf file (which is entirely ignored, as said above).* Set `nt1` which defines the time sample index of the start time of the source wavelet: `nt1*dt` defines this time (i.e. if you want the source wavelet to be interpreted as starting at time $t = 0$, the set `nt1 = 0`, for negative starting time, set `nt1` to the respective negative time-sample index). `nt2` defines the time index of the end time of the input source wavelet and *must be set consistently, such that* `nt = nt2 - nt1 + 1`, this is parameter is not inferred from `nt1` and the length of the input source wavelet.

The output is a file called "ricker_spec.txt", written to the directory from where you execute the program. *Existing files will be overwritten!*

9 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 `SPECFEM3D` if used

along with an ASKI extended SPECFEM3D installation. If in such an installation 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.

9.1 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 10)). 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)).

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 10).

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).

9.2 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 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 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 external model, if MODEL = external in Par_file and any external model is defined as described above in section 9.1 ! 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_Cartesian_for_ASKI/specfem3D_par_ASKI.f90 with which all output files of the current simulation will be taged, and it will be used to check consistency of the files (could be a timestamp, eventID, station name, component etc).

9.3 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 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.

9.4 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*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`)
   NOT TO BE USED WITH SPECFEM3D Cartesian!
   ASKI internal, but SPECFEM independent more elaborate spherical inverison 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 >= - 0.5*ASKI_wx and x <= 0.5*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 assinged to values! Set to 0. if no rotation should be applied.
- scartInversionGrid only supports ASKI_rot_Z and uses a different definintion 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

[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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