Using SPECFEM3D_Cartesian-2.1 for ASKI - Analysis of Sensitivity and Kernel Inversion, version 0.3

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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.
Please do not hesitate to improve this documentation by incorporating your experiences with SPECFEM3D for ASKI and your personal experience of getting used to it.

Furthermore, my moderate experience with LaTeXmay well give rise to improving the document style, hence the readability of the manual as a whole, as well as the coding style of the .tex file.

The LaTeXsource files and all related components of this document are contained in the SPECFEM3D_Cartesian-2.1 for ASKI 0.3 package, available via http://www.rub.de/ASKI

Florian Schumacher, 2013

Guide Through This Manual

We assume that you have sufficient knowledge of how to run the regular SPECFEM3D_Cartesian code.

For details on how to extend the regularly installed SPECFEM3D_Cartesian-2.1 code to produce output for ASKI , please read section 8.

Before you start using the code to produce output for ASKI , please consider the general comments in section 1.

If you are going to use the automated python script run_specfem3dCartesianForASKI_simulations.py then please start reading section 3.

If you want to conduct one single simulation producing some output for `ASKI` , please start reading section 2.

Section 7 is intened 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 General Stuff 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 7.1. Use the main ASKI output file of some arbitrary ASKI output, e.g. the kernel displacement output of the first source.
- As there is a fixed order assumed of ASKI wavefield points (by procs and local element numbering), the computation of many kernels (e.g. for many seismic 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).
- there is (probably?!) no proper support for multiple sources in case of producing output for ASKI .
- Green tensor simulations are done using value ALT in the station definition as the FORCESOLUTION depth value, in order to allow receivers to be located not only on the surface. It, hence, may be sensible to throughoutly use USE_SOURCES_RECVS_Z = .true. in SPECFEM3D/src/shared/constants.h.
- As the coordinates of wavefield points (and, hence, inversion grid coordinates) SPECFEM3D for ASKI uses:
  First coordinate = X, second coordinate = Y, third coordinate = Z.
- ...

2 One Single Simulation

As usual, you need to do (external or internal) meshing for the appropriate (current) background model. See section 4 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 7.

After that, you are ready to run the code. As there is no ASKI dependent change of SPECFEM3D components which are sensitive to compiling, you do not need to recompile the SPECFEM3D code every time you run a SPECFEM3D simulation for ASKI .

3 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 4 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 conducts the specified kernel simulations (as described inside the script on the top) by iteratively running SPECFEM3D simulations, using appropriate settings of the parameter files for each iteration.
You need to edit the first lines of the script (above definition of class simulation) 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 iteratively conducts SPECFEM3D simulations.
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.

3.1 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.

- 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, you need to manually set all parameters concerning the inversion grid, i.e. ASKI_type_inversion_grid, ASKI_(cw)(xyz), ASKI_rot_(XYZ)

3.2 Manually Setting FORCESOLUTION

The python script *always* automatically sets “latitude:”, “longitude:”, “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 “hdur:” is set to “0.”. So, if you wish to do a data simulation for single force sources, using a different “hdur:” value, you should conduct those in a separate run of the python script.

3.3 Manually Setting CMTSOLUTION

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

3.4 Manually Setting `STATIONS`

The standard SPECFEM3D STATIONS file should contain the definition of stations as in the ASKI file file_stations_list, in consistend SPECFEM3D notation, i.e. coordinate columns being lat (= Y, third column of STATIONS and fourth column of file_stations_list) and lon (= X, fourth column of STATIONS and third column of file_stations_list) and elev (= Z, sixth column of STATIONS and fifth column of file_stations_list).

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

4 Importing the currently inverted model for next iteration step

Exported .kim files (as produced by ASKI program exportKim) may be read used as a model by SPECFEM3D for ASKI, as explained in the following:

The model values defined by the kernel inverted model will be *superimposed* onto the SPECFEM3D default model values as defined by e.g. Cubit, using a special implementation of the SPECFEM3D module model_external_values.

Set MODEL = external in Par_file. Then directory DATA must contain a file named model_external_ASKI which must contain 3 lines:

line 1 *interpolation type:*
The first line may be of the following formats:

- shepard_standard meaning that a standard inverse distance interpolation, respecting for direction of neighbours, after Shepard is used to interpolate model values from the inversion grid cell centers onto the new SPECFEM3D GLL points. The radii of the inversion grid cells are used to decide whether a GLL point is in range of an inversion grid cell or not.
- shepard_factor_radius FACTOR whereby FACTOR is a factor to be applied to the inversion grid cell radii before applying the same interpolation method as in case shepard_standard.

line 2 *model file type:*
only kim_export supported by now, meaning that the file given in line 3 must be an exported .kim file as produced by ASKI program exportKim.

line 3 *name of model file:*
name of model file of type as defined in line 2, which is expected to be in directory DATA

5 Preparing Synthetic Data as Expected by `ASKI`

Use binary createSpecfem3dSyntheticData. Calling createSpecfem3dSyntheticData -h will print a help message how to use it.

It is assumed that a copy of the OUTPUT_FILES folder (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 3), 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.

The option -data allows you to also transform synthetically created "real" data (e.g. for a pure synthetic inversion) to the required form. Also in this case it is assumed that a copy of the OUTPUT_FILES folders can be found at paths as choosen by the automated python script, i.e. the base filename of the measured data for the respective event with extension _OUTPUT_FILES. The "real" data then is written in the required form to the measured data files with base filenames as defined in the iteration step info database.

6 Preparing synthetically computed "measured" data as expected by ASKI

You can produce ASKI files for measured data in the required form from SPECFEM3D for ASKI "data" simulations (e.g. produced by automated python script, 3). This functionality may be used for synthetic tests, in which you must produce data for some perturbed earth model, which is treated as measured data.

Use binary createSpecfem3dMeasuredData. Calling createSpecfem3dMeasuredData -h will print a help message how to use it.

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 at 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.

7 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.

7.1 ASKI output

COMPUTE_ASKI_OUTPUT, OVERWRITE_ASKI_OUTPUT

Parameter COMPUTE_ASKI_OUTPUT controls if any ASKI functionality is applied by SPECFEM3D and output files (i.e. kernel green tensor kernel displacement files) are produced. If true, OVERWRITE_ASKI_OUTPUT controls if those files shall be overwritten if existend or not. If false and files exist, the SPECFEM3D solver will terminate raising an error message.

ASKI_outfile, ASKI_output_ID

ASKI_outfile defines the absolute base file name of ASKI output files. ASKI_output_ID is a character string of maximum lenght as defined by parameter length_ASKI_output_

ID in file specfem3D_par_ASKI.f90 with which all output files of a certain run will be taged, and it will be used to check consistency of the files (could be a timestamp, eventID, station name, component etc).

7.2 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) before (i.e. 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.

7.3 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 = ccsInversionGrid)
   NOT TO BE USED WITH SPECFEM3D Cartesian! **NOT SUPPORTED YET**
   ASKI internal, but SPECFEM independent 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 CUBIT, 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 ....)

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 not used.
- 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).

8 Extend SPECFEM3D_Cartesian-2.1 to produce output for ASKI

This section explains how to use the SPECFEM3D_Cartesian software http://geodynamics.org/cig/software/specfem3d 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 than the SPECFEM3D_Cartesian code, except that it needs a bit more memory and disc space. You should, therefore, have sufficient knowledge of

how to run the regular SPECFEM3D_Cartesian software. Furthermore, you need an installation of ASKI (obviously).

8.1 Download and Dependencies

The extension package SPECFEM3D_Cartesian-2.1 for ASKI can be downloaded from http://www.rub.de/ASKI.
It assumes a running version of SPECFEM3D_Cartesian on your system which must be capable of a certain functionality. If the currently availabe release version of SPECFEM3D_Cartesian does not have this functionality, you can download http://www.rub.de/ASKI. This is a basic extract from the SPECFEM3D_Cartesian svn-repository (svn-revision by 9 june 2013, SPECFEM3D version 2.1) which has been debugged and slightly modified such that it is capable of the required functionality. Important functionality is listed in the following, whereby the code references are related to the previously mentioned modified svn revision:

- in case of USE_FORCE_POINT_SOURCE = .true. in Par_file the sources should be interpolated inside the source array and not just set to the closest GLL point (compare src/specfem3D/locate_source.f90, comments FS FS)
  This, however, is not a strict necessity, you can also use SPECFEM3D_Cartesian codes which do not do this.

- in case of USE_FORCE_POINT_SOURCE = .true. and USE_RICKER_TIME_FUNCTION = .false. in Par_file, the regular Heaviside source time function (function comp_source_time_function) must be used (compare src/specfem3D/compute_add_sources_viscoelastic.f90, src/specfem3D/setup_sources_receivers.f90 comments FS FS)

- using external models (MODEL = external in Par_file), subroutine model_external_values must be passed the default model values on enter (compare src/generate_databases/get_model.f90, comments FS FS)

- the general user interface of the SPECFEM3D_Cartesian code (i.e. definition of source mechanisms and receivers, models, output files etc.) must be compatible with SPECFEM3D_Cartesian version 2.1 by june 2013.

8.2 Installation

Extract the files of the extension package SPECFEM3D_Cartesian-2.1 for ASKI into a subdirectory of your ASKI installation path, in the following refered to as SPECFEM_for_ASKI. I.e. the directory SPECFEM_for_ASKI is contained in directory ASKI .
Install a SPECFEM3D_Cartesian code on your system which meets the requirements as in subsection 8.1, in the following the SPECFEM3D_Cartesian installation path is refered to as SPECFEM3D.

- Follow the 9 items in the "Installation" section of file ASKI/SPECFEM_for_ASKI/README, whereby the first one should already be completed.

- Adjust variables SHELL, BLAS, LAPACK etc. in SPECFEM_for_ASKI/Makefile in the same way as you did in ASKI/Makefile for the installation of ASKI . The same environment variables are assumed here, too.

- Run `make clean` and `make all` in `ASKI/SPECFEM_for_ASKI`.
- Set `USE_SOURCES_RECVS_Z = .true.` in `SPECFEM3D/src/shared/constants.h` (or wherever your `constants.h` is).
- Recompile your `SPECFEM3D_Cartesian` code by running `make clean` and `make all` in `SPECFEM3D`.

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