ASKI

Analysis of

Sensitivity and

Kernel

Inversion

User Manual

ASKI – version 1.2

Aug 2016
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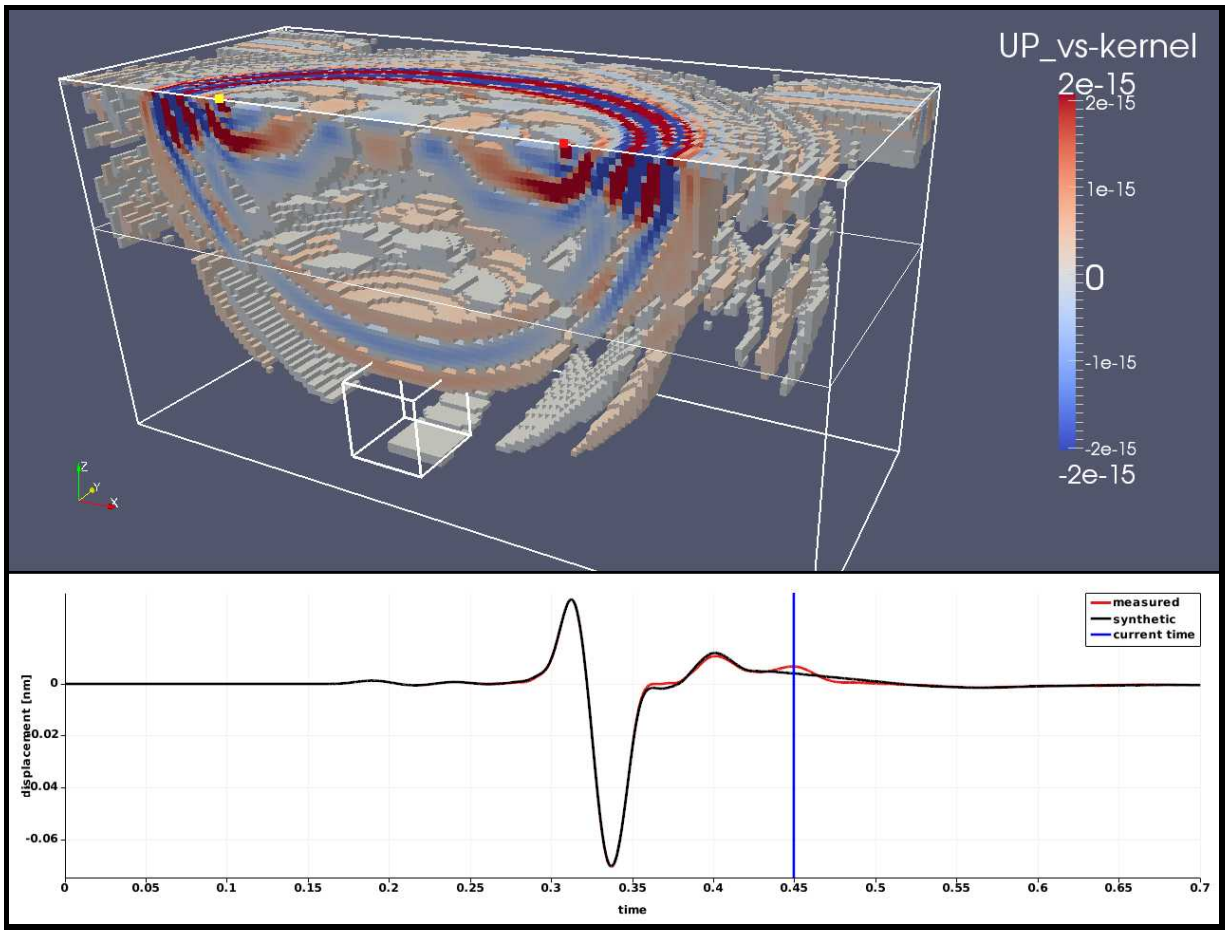

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If you use ASKI for your own research, please cite our paper [SFL16]:

F. Schumacher, W. Friederich and S. Lamara,
"A flexible, extendable, modular and computationally efficient approach to scattering-integral-based seismic full waveform inversion",
Geophysical Journal International, (February, 2016) 204 (2): 1100-1119
http://dx.doi.org/10.1093/gji/ggv505

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/ASKI or to improve this documentation by incorporating your experiences with 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). When you have developed new ASKI components or have modified existing once, please extend / modify the ASKI documentation accoringly.

Furthermore, I am aware of the poor LaTeXcoding 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 LaTeXsource files and all related components of this document are available via https://github.com/seismology-RUB/ASKI , subdirectory doc/ASKI_manual/ of the repository.

Florian Schumacher, Aug 2016

Contents

What is ASKI?

ASKI is a modularized software package written by the main authors Florian Schumacher and Wolfgang Friederich (Ruhr-University Bochum, Germany). It offers sensitivity and regularization analysis tools for seismic datasets as well as a scattering-integral-type full waveform inversion (FWI) concept based on waveform sensitivity kernels (i.e. Fréchet derivatives of seismic waveform data functionals) derived from Born scattering theory, having Gauss-Newton convergence properties. This inversion concept is presented in our paper [SFL16] and in Florian's doctoral dissertation [Sch14].

ASKI does not implement an intrinsic code for simulation of seismic wave propagation in order to solve the seismic forward problem, but instead provides generalized interfaces to different external wave propagation codes. At the moment, the 1D semi-analytical code Gemini [FD95] and the 3D spectral element code SPECFEM3D [TKL08] are supported in *both*, Cartesian and spherical framework. Additionally ASKI supports the 3D nodal discontinuous Galerkin code NEXD [Lam15b] and we plan to implement support for the Finite Difference code SOFI [Boh02] in the future. Please do not hesitate to add your own forward code (refer to the ASKI developers manual in `devel/doc/ASKI_developers_manual/`). If you encounter any problems or have suggestions to improve this process, we are happy to hear from you.

The resulting very modular concept of ASKI allows us to keep the spatial description of the inverted models completely independent of the spatial description of the model used for solving the forward problem. This way, the overall inverse problem can be approached and regularized more physically compared with using the forward grid for inversion, too. The normally very fine spatial discretization of the model domain is employed by the forward solver. This discretization is usually weigh too fine to be used directly for inversion since usually seismic data can only resolve much coarser structures and the resolving power the data possesses also varies throughout the model domain. The separation concept of ASKI *naturally* alows to choose the spatial model resolution heterogeneously and *anew* in each iteration of FWI.

Instead of using time-dependent values of ground motion (i.e. samples of time-serieses of seismic data), ASKI uses freqency-dependent complex values of ground displacement, recorded at certain receivers excited by certain seismic sources. This, mainly, has reasons of computational feasibility. For time-domain forward methods, we implement an on-the-fly Fourier Transform in order to provide the required spectral waveforms.

Using sensitivity kernels K, data residuals δd_i are connected to model uptdate values δm_j by an integral relation $\delta d_i = \int_{\text{Earth}} \delta\vec{m} \cdot \vec{K}_i$. In order to build a linear system, the model update $\delta\vec{m}$ is assumed to be constant throughout small scattering volumes Ω_j, where $\Omega = \dot{\bigcup}_j \Omega_j$. These volumes constitute the cells of the volumetric inversion grid and the sensitivity matrix contains entries of preintegrated kernels $\int_{\Omega_j} K_i$ (and model update values δm_j are associated with cells Ω_j for a particular elastic parameter).

The sensitivity kernels K are computed from forward wavefields and strains produced on a set

of points in space, which is dependent on the particular forward method. This set of points is refered to in ASKI as *wavefield points*. The wavefields are written to file, by the respective forward method, which may require large disk space. Providing methods for constructing quadrature rules for arbitrary point sets contained in arbitrary (hexahedral or tetrahedral) volumes, ASKI computes integration weights for integration of functions given on the wavefield points (particularly kernels) over the volumetric cells of the inversion grid. The inversion grid takes care of the localization of wavefield points inside the inversion grid cells and, if requested, the transformation of cells to a hexahedral (or tetrahedral) standard cell for the computation of the integration weights. Hence, exotic combinations of wavefield points (i.e. forward methods), integration weight types and inversion grid types might not be possible (e.g. using the SPECFEM-internal inversion grid built by the spectral elements along with wavefield points from another forward method).

The pre-integrated kernel values are also written to files, which may be flexibly read in (e.g. reading in kernels of specific data subsets only) by the sets of independent ASKI executables conducting any sensitivity analysis or interation steps in the iterative full waveform inversion. Those tools work on the sensitivity matrix, which in the FWI is used in a linear system of equations which relates data residua δd_i to a model improvement δm. In the course of the iterative full waveform inversion, it is naturally possible by ASKI to gradually increase the frequency content of the inverted data and to choose smaller inversion grid cells in each iteration, i.e. increasing the spatial resolution dependent on frequency.

How to get started

How to use this manual

Only chapter 0 (page 13) is intended to be read through, presenting recipes (todo lists/algorithms) for different workflows that can be conducted by software package ASKI. For this reason, that chapter is held as compact as possible and may itself be regarded as "the manual", with the appending chapters only containing more specific detail on processes or objects which chapter 0 refers to. After all, the very modular character of ASKI requires documentation which itself is modular.

In other words: just start reading the respective section of chapter 0, which you are interested in and whenever you feel the need for more detail follow the respective references. This way, we try to focus the user on necessary information and successfully guide through the lot of details contained in this document.

When you conduct a specific ASKI operation for the first time, we recommend you to first fully read through the respective guiding list and the referred basic steps before you start running any programs. This way you will get an impression of the requirements for your operation.

All chapters appending chapter 0 are not intended to be read through section by section but may well serve the user as a reference. Especially section 3.1 (page 63) can provide the experienced user with additional executables that conduct some more features which are not referenced somewhere in the document.

Please preserve your experience!

If you struggled with the existing ASKI documentation (user manual, comments in code, doxygen, developers manual) because it was inconsistent, incomplete or simply wrong and you invested time to find out how it works, *please let future generations of users and developers benefit from your gained knowledge!* Everybody knows that documenting code and writing manuals consumes a lot of time, but correct documentation is essential for everyone using and developing software, and I'm sure you know that from your own experience. So, please invest a bit more time in correcting/extending the ASKI documentation (where applicable: user manual, comments in code, doxygen, developers manual) and at best modify the respective source files and issue a pull request on gitHub. In any case let us know about it (via https://github.com/seismology-RUB or http://www.rub.de/aski)! Otherwise your knowledge is lost forever (you might even lose your knowledge yourself after some while, so please write it down).

Thank you! (on behalf of everybody)

Installing ASKI

- Clone the latest version of the master branch of the ASKI gitHub repository to some directory (exemplarily called /your/programs/) on your local computer by executing
  `git clone --depth 1 --branch master https://github.com/seismology-RUB/ASKI`
  (in one line, of course) from local path /your/programs/ . This will create subdirectory /your/programs/ASKI containing the code and documentation of the current release of the ASKI main package.

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

  Webpage http://www.rub.de/aski might provide additional information for you, just have a look.

- Follow the directions in file ASKI/README.md for configuration and compilation of the ASKI ececutables.

Throughout the ASKI documentation, "ASKI installation directory" refers to directory ASKI/, i.e. /your/programs/ASKI, where you have cloned/extracted the git repository to.

Toy example: synthetic waveform inversion

In order to get familiar with applying ASKI for full waveform inversion, you might consider to download and reproduce the synthetic inversion presented in Florian's dissertation [Sch14] (chapter 5.1) as well as in our GJI paper [SFL16] (section 4.1), see section 0.4 (page 18).

ASKI versions

ASKI's release version numbering does not follow any standard of version numbering. Since releases were not very frequent so far and the source code was not publically available under version control, it was considered sufficient to have only a simple numbering for the purpose of distinguishing release versions. In case that developments and releases become more frequent in the future, the ASKI developers might consider to follow some standard for future release version numbering.

ASKI 0.3

ASKI's first release version was numbered 0.3, with 0 indicating a pre-release that was not very well tested at that point and 3 being the third version of internal development when porting from another internal versioning repository.

ASKI 1.0

After some while of intensive testing and application of ASKI to synthetic and real-world cases, as well as development of a lot of ASKI tools, version 1.0 was released as the first ready-to-use version of ASKI.

ASKI 1.1

In general, version 1.1 should be compatible with 1.0 in terms of file formats and general use of the software. The main reason for this release was the fix of a pointer problem with gfortran. Compared with the previous release, some more tools are available (addSpikeCheckerToKim, createSpectralFilters, create_ASKI_evstat_filters.py) and forward-code-specific definition of complex frequencies is available (e.g. for use with Gemini). Some bugs were fixed.

ASKI 1.2

Version 1.2 is just an intermediate version number and denotes the status of the code when moving the development repository permanently to git and providing the current working ready-to-use version of ASKI by the master branch of repository https://github.com/seismology-RUB/ASKI.

Significant changes to version 1.1:

- There is an additional subdirectory devel/ containing developer tools and developer documentation.
- The source files of the ASKI user manual as well as a compiled pdf of the manual are provided now in subdirectory doc/
- Inversion grids of type chunksInversionGrid now provide base cell refinement capabilities (at the moment a random "toy" method is implmemented for illustration, but serious refinement method can now be implemented easily into module chunksInversionGrid.
- New/renamed/removed tools:

  chunksInvgrid2vtk for special vtk files related to chunks and refined cells

  createShoreLines (Fortran executable) and create_shore_lines.py (Python program utilizing the f2py interface generator) for generating shore line vtk files from native binary GSHHS shore line data files

  Executable createMeasuredData was renamed in transformMeasuredData

  Python script create_ASKI_evstat_filters.py is removed (functionality not required anymore)

The gitHub master branch

After porting ASKI to https://github.com/seismology-RUB/ASKI in August 2016, the current version of its master branch should serve as a stable version to use, along with the current versions of the forward code packages supported by ASKI.

Chapter 0

ASKI workflows

This chapter is intended to guide you, dependent on what workflow you want to follow, through all necessary steps to achieve your goals. Make sure that you have read section entitled "How to get started".

If you don't know about ASKI yet, we recommend you to quickly read through the previous section entitled "What is ASKI?", which explains some basic terminology in ASKI and the concepts it is based on.

The sections below address possible operations you can conduct with ASKI. For every operation, we only refer to the necessary basic steps (by $\rightarrow$), which are described in chapter 1 (page 25).
Make sure to have a complete read-through before hastily doing anything!

Good Luck!

0.1 Full Waveform Inversion using pre-integrated spectral Waveform Sensitivity Kernels

Iterative inversion scheme which uses waveform sensitivity kernels to gain model updates form data residua.

You should have already installed ASKI, see section entitled "How to get started". In addition to ASKI, you will need to install a supported software which solves the forward problem → 1.10 (page 42).

Before The First Iteration Step

- Create a main parameter file (e.g. in the parent directory of your specific inversion directory, or where you collect main parameter files for all your inversion projects) → 1.1 (page 25). You will need this file as an input argument to almost all programs/scripts.
  Set MAIN_PATH_INVERSION to a correct value. The directory does not need to exist yet, if not, then it will be created.
  You should keep the default values of ITERATION_STEP_PATH and PARFILE_ITERATION_STEP unless you know what you are doing. If you wish to use different values for the complete inversion process, it makes senese to adjust them now.
  All other parameters can be adjusted later.

- Create a directory structure for the expected number of iteration steps of your inversion → 1.3 (page 25)

- Make yourself familiar with the form of data used in ASKI → 1.4 (page 26).
  Set APPLY_EVENT_FILTER, APPLY_STATION_FILTER, PATH_MEASURED_DATA, PATH_EVENT_FILTER, PATH_STATION_FILTER, FILE_EVENT_LIST, and FILE_STATION_LIST, as well as MEASURED_DATA_FREQUENCY_STEP, MEASURED_DATA_NUMBER_OF_FREQ and MEASURED_DATA_INDEX_OF_FREQ in your main parameter file, before preparing your data in the required form → 1.5 (page 27), as well as any filters → 1.6 (page 27).

- Set FORWARD_METHOD in your main parameter file to the value of your choice. If you want to use different methods in the course of inverting one dataset (e.g. starting with a 1D method, continuing with a 3D method), then it may make sense to create a different directory structure for each method and using the final model of one method as the starting model for the next method.

- Choose a model parametrization by setting MODEL_PARAMETRIZATION in the main parameter file to a value of your choice (which is supported by your forward method).

Before Each Iteration Step (including the first one)

- Set CURRENT_ITERATION_STEP in your main parameter file to the correct value. When continuing your inversion with a different method, you may also keep the current iteration step index (in order for you not to get confused) and leave subdirectories of your MAIN_PATH_INVERSION empty (or delete them after creation if they are not needed): e.g. an inversion with one method could start with iteration step 4 (and respective subdirectory), if you have already conducted 3 iteration steps with other methods.

- Define the inversion grid of the current iteration → 1.7 (page 28).
- Set all parameters in the specific iteration step parameter file to correct values → 1.2 (page 25), including the correct reference to your inversion grid. Refer to the documentation of your forward method on how to set filenames `FILE_WAVEFIELD_POINTS` and `FILE_KERNEL_REFERENCE_MODEL` (as the handling of these file are method dependent).
- Dependent on your method and model parametrization, take care about communicating the current model (inverted in the previous iteration) to your forward method → 1.9 (page 42). Before the first iteration, however, you need to define some starting model → 1.8 (page 41).

Conducting An Iteration Step

- Compute forward wavefields and Green tensor components w.r.t. the current model by your method. Refer to the respective documentation of your method.
  After that, you may prepare the synthetic data in the way `ASKI` expects it (see sections 1.4 (page 26) and 2.6 (page 56)). Refer to the documentation of your method on how to do it.
- Set `TYPE_INTEGRATION_WEIGHTS` in the iteration specific parameter file → 1.11 (page 43). You should keep the default values of `FILE_INTEGRATION_WEIGHTS`, unless you know what you are doing (can be any name, will be created, but is referred to, afterwards. You could compute different types of weights and store them in different files, this way).
- Initiate basic requirements for all programs and scripts → 1.13 (page 44).
- Define data and model space, where the paths are mainly important for now → 1.12 (page 43).
- Compute sensitivity kernels for your specific set of paths and your set of model parameters → 1.14 (page 45).
  If desired, you may have a look at your kernels → 1.16 (page 46).
- Choose a specific data and model space. You may well play around with different subsets of data or smoothing (next step) in the course of inverting for different models → 1.12 (page 43).
- Finally compute the inverted model by solving the kernel system → 1.18 (page 46), possibly varying the regularization constraints.
- After deciding whether or not to do another iteration of full waveform inversion and choosing a model for the next iteration → 1.19 (page 47), repeat all operations beginning with “Before Each Iteration Step (including the first one)”.

0.2 Toy Example Using SPECFEM3D_Cartesian as a forward solver

Please refer to section 0.4 (page 18).

0.3 Toy Example Using SPECFEM3D_GLOBE as a forward solver

This section describes a very short example of computing a spherical waveform kernel for just one event-station pair using the setting of example "regional_Greece_small" from the SPECFEM3D_GLOBE 7.0.0 release package (example uses 4 CPU cores only).

The kernel files of this example package were computed with ASKI version 1.0, which however should be reproducable also with higher versions of ASKI since the changes to version 1.2 do not effect the computations or compatibility of the output files. It may, however, occur that numbers might not be reproduced in a numerically exact way, which is also likely to happen when a different compiler (version) is used.

You should have already installed the ASKI main package, see section entitled "How to get started".

Then download the example package ASKI_example_spherical_small.tar.gz which is attached to release v1.0 of gitHub repository https://github.com/seismology-RUB/ASKI (198 MB, probably go to https://github.com/seismology-RUB/ASKI/releases/tag/v1.0). The wavefield files in this example package were produced by version 1.0 of the extension package SPECFEM3D_GLOBE for ASKI (https://github.com/seismology-RUB/SPECFEM3D_GLOBE_for_ASKI/releases/tag/v1.0), but you should be able to re-produce them as well with version 1.2 of the extension package (https://github.com/seismology-RUB/SPECFEM3D_GLOBE_for_ASKI/releases/tag/v1.2).

Please note that this example is not documented as detailed as the Cartesian cross-borehole example → 0.4 (page 18). Even if you do not intent to use the forward code SPECFEM3D_Cartesian, you are still advised to have a look at the Cartesian cross-borehole example (or get to know ASKI otherwise), in order to practice the operations of the main ASKI package and, thus, learn about how to conduct any steps *after* the forward problem is solved, in particular how to compute kernels. Otherwise, refer to the general FWI workflow until the point of kernel computation → 0.1 (page 14) in order to re-produce the kernels provided in this example package.

Most importantly, you must change the value of MAIN_PATH_INVERSION in file ASKI_example_spherical_small/main_parfile to "your_base_path/" in order for all the example directory to work. If you do not want to overwrite the existing output, alternatively you should create a separate inversion directory from scratch → 1.3 (page 25) and leave ASKI_example_spherical_small/ as a reference only.

0.4 Cross Borehole Example

This section describes the synthetic cross borehole example presented in Florian's dissertation [Sch14] (chapter 5.1) as well as in our GJI paper [SFL16] (section 4.1). It is an example of lull waveform inversion using pre-integrated spectral waveform sensitivity kernels (as described in the first recipe 0.1 (page 14) of this chapter.

The example files referred to in the following, were computed with ASKI version 1.0, which however should not pose any problem since the changes from version 1.0 to 1.2 do not effect the computations or compatibility of any output files. It may, however, occur that numbers might not be reproduced in a numerically exact way, which is also likely to happen when a different compiler (version) is used.

You should have already installed ASKI, see section entitled "How to get started".

Then download the example package ASKI_inversion_cross_borehole.tar.gz which is attached to release v1.0 of gitHub repository https://github.com/seismology-RUB/ASKI (566 MB, probably go to https://github.com/seismology-RUB/ASKI/releases/tag/v1.0). In this package, all files of the first 2 iterations (plus illustrating extras) are provided. In order to keep the download small, wavefield output is not provided for iterations 3 to 12. You should be able to reproduce the wavefields immendiately for any iteration step from the provided inverted models without reproducing all preceeding iterations. The pre-integrated sensitivity kernel files are only provided for iterations 1 to 3. Kernel files for the other iterations can be downloaded by interested users seperately as package ASKI_inversion_cross_borehole_sensitivity_kernels_iter04-iter12.tar.gz (907 MB, same location https://github.com/seismology-RUB/ASKI/releases/tag/v1.0).

Most importantly, you must change the value of MAIN_PATH_INVERSION in file ASKI_inversion_cross_borehole/main_parfile_cross_borehole to "your_base_path/" in order for all the example directory to work. If you do not want to overwrite the existing output, alternatively you should create a separate inversion directory from scratch → 1.3 (page 25) and leave ASKI_inversion_cross_borehole/ as a reference only.

This example was generated using SPECFEM3D_Cartesian 3.0 for ASKI version 1.0. (https://github.com/seismology-RUB/SPECFEM3D_Cartesian_for_ASKI/releases/tag/v1.0). Even if you intend to use a different forward method, you can still practice the operations of the main ASKI package and, thus, learn about how to conduct any steps in the full waveform inversion *after* the forward problem is solved. Just read the description of the contained files in ASKI_inversion_cross_borehole/README.

If you want to reproduce also the forward wavefields from SPECFEM3D_Cartesian 3.0, you need to install it, of course → 1.10 (page 42).

0.5 Time-Domain Sensitivity Kernels

This section describes, how to compute time-domain waveform sensitivity kernels for a specific set of sources receivers with respect to a certain background earth model as an operation seperate of any other ASKI operations. The kernels in time-domain are much more intuitive to look at for human beings, than the standard frequency-domain sensitivity kernels. You may, as well, compute time-domain sensitivity kernels from the kernels produced in any iteration step of a full waveform inversion (page 14). For this purpose, apply the steps "Transforming to Time-Domain Sensitivity Kernels" (below) after you computed the spectral kernels in you iteration step, as the time-domain waveform kernels are produced by an inverse Fourier transform from the standard frequency-domain waveform sensitivity kernels on which ASKI is based.

Please do not get confused by the general terminology of *inversion* and *iteration*, etc. Technically you will be conducting an incomplete first iteration step of a full waveform inversion, using all the program infrastructure which is also used for a full waveform inversion.

You should have already installed ASKI, see section entitled "How to get started". In addition to ASKI, you will need to install a supported software which solves the forward problem → 1.10 (page 42).

Preceding Considerations

- Create a main parameter file (e.g. in the parent directory of your specific inversion directory, or where you collect main parameter files for all your inversion projects or analyses) → 1.1 (page 25). You will need this file as an input argument to almost all programs/scripts.
  Set MAIN_PATH_INVERSION to a correct value. The directory does not need to exist yet, if not, then it will be created.
  Set ITERATION_STEP_PATH and PARFILE_ITERATION_STEP to desired values, or leave the default values, if present.
  All other parameters can be adjusted later.

- Create a directory structure for only one iteration step → 1.3 (page 25)

- Even if you do not have any measured data, it might still be beneficial for you to make yourself (roughly) familiar with the form of data used in ASKI → 1.4 (page 26).
  In your main parameter file, set the following values:

  – Set FILE_EVENT_LIST and FILE_STATION_LIST to define the sources and receivers which are involved in the paths that you would like to compute the kernels for.

  – Dependent on the (length of the) time series you want to deal with, define the frequency discretization of the spectral kernels that will be produced first. This must be done by MEASURED_DATA_FREQUENCY_STEP, MEASURED_DATA_NUMBER_OF_FREQ and MEASURED_DATA_INDEX_OF_FREQ.

  In general, for the pure kernel computation you do not need any measured data. So, here you do not need to prepare data in the ASKI required form.

- Set APPLY_EVENT_FILTER, APPLY_STATION_FILTER (and if required PATH_EVENT_FILTER and PATH_STATION_FILTER) in your main parameter file. In case the forward wavefields were calculated w.r.t. an impulse source time function (or the

source-time function was deconvolved), you should apply filters → 1.6 (page 27) that taper down the amplitude spectrum before the maximum frequency used. Otherwise, the inverse Fourier transform below can create artefacts.

- Set FORWARD_METHOD in your main parameter file to the value of your choice.
- Choose a model parametrization by setting MODEL_PARAMETRIZATION in the main parameter file to a value of your choice (which is supported by your forward method).
- Set CURRENT_ITERATION_STEP in your main parameter file to value 1, as you are technically starting to conduct the first (and only) iteration step of a full waveform inversion.
- It is highly recommended to set DEFAULT_VTK_FILE_FORMAT to BINARY in the main parameter file, since a lot of vtk files might be generated (one for every time step). Using the binary format significantly reduces storage.
- Define the inversion grid → 1.7 (page 28), which controls the spacial volumetric discretization (resolution) of the computed sensitivity kernels. In case of just computing (time) kernels to look at, it is not crucial to regard this resolution as the resolution of some inverted model, as no inversion will be conducted on the inversion grid. Since there might be a lot of vtk files generated (one for every time step), it is highly recommended to set
  VTK_GEOMETRY_TYPE = CELL_CENTERS in the inversion grid parameter file (if your type of inversion grid supports that functionality). This significantly reduces the amount of geometry information written to the vtk files, hence their size.
- Set all parameters in the specific iteration step parameter file to correct values → 1.2 (page 25), including the correct reference to the inversion grid. Set ITERATION_STEP_NUMBER_OF_FREQ and ITERATION_STEP_INDEX_OF_FREQ to the *same* values as the MEASURED_DATA_NUMBER_OF_FREQ and MEASURED_DATA_INDEX_OF_FREQ in the main parameter file! Refer to the documentation of your forward method on how to set filenames FILE_WAVEFIELD_POINTS and FILE_KERNEL_REFERENCE_MODEL (as the handling of these file are method dependent).
- Dependent on your method and model parametrization, define your background model with respect to which the kernels will be computed. If you have some inverted model file, use → 1.9 (page 42). For defining a starting model, see → 1.8 (page 41).

Computing Spectral Waveform Sensitivity Kernels

- Compute forward wavefields and Green tensor components w.r.t. the current model by your method. Refer to the respective documentation of your method.
  After that, you may prepare the synthetic data in the way ASKI expects it (see sections 1.4 (page 26) and 2.6 (page 56)). Refer to the documentation of your method on how to do it.
- Set TYPE_INTEGRATION_WEIGHTS in the iteration specific parameter file → 1.11 (page 43). If you intend to compute the time kernels on wavefield points only, you will technically never use the integration weights, but nevertheless they need to be correctly created (in that case use a simple type of weights like 5 or 0). You should keep the default values of FILE_INTEGRATION_WEIGHTS, unless you know what you are doing (can be any name, will be created, but is referred to, afterwards. You could compute different types of weights and store them in different files, this way).

- Initiate basic requirements for all programs and scripts → 1.13 (page 44).
- If you have many paths, you may define a data and model space concentrating on defining paths → 1.12 (page 43). If you have only one path or just a few, it is possible (and propably also convenient) to just continue to the computation of the kernels.
- Compute the standard frequency-domain sensitivity kernels for your specific set of paths (or the one or few paths, one after another). In case you want to transform to time-domain kernels *on wavefield points* (and not pre-integrated kernels on inversion grid), use option `-wp` → 1.14 (page 45)
  If desired, you may have a look at the standard frequency-domain kernels → 1.16 (page 46).

Transforming to Time-Domain Sensitivity Kernels

- Transform the standard frequency-domain waveform kernels to time domain. In case you want to get time-domain kernels *on wavefield points*, (and not pre-integrated kernels on inversion grid), you must use option `-wp` (in this case, you already should have used `-wp` to compute spectral kernels) → 1.15 (page 45).
  Make sure that the wavefield spectra have a sufficiently small amplitude spectrum at high frequencies, in order for the inverse Fourier Transform to work satisfactorily. Otherwise use filters.
- Plot the time kernels → 1.17 (page 46).

0.6 Analysis of Acquisition Geometry using Kernel Focussing

THIS SECTION IS WORK IN PROGRESS!

The general concept of Backus-Gilbert-based focussing of sensitivity kernels on a defined focussing region in the model space is published in [Sch14], Chapter 7.1. On the basis of this way of finding linear combinations of data which are sensitive only to changes in a model subspace, the dataset can be analysed w.r.t. finding event-station paths (and components / frequencies) which optimally illuminate the model subspace.

Executable `focusSpectralKernels` → 3.1.14 (page 75) produces the coefficients of the linear combination of data required for the analysis. However, this section does not yet give a detailed list of steps how to conduct such an analysis.

- step 1
- step 2
- ...

0.7 Full Waveform Inversion - Focused Waveform Sensitivity Kernels

THIS SECTION IS WORK IN PROGRESS!

The general concept of Backus-Gilbert-based focussing of sensitivity kernels on a defined focussing region in the model space is published in [Sch14], Chapter 7.1. On the basis of this way of finding linear combinations of data which are sensitive only to changes in a model subspace, different disjoint subdivisions of the model space can be chosen, finding the finest subdivision that is resolved by the data (i.e. where focussing of sensitivity on each subdivision cell is still successfull). This gives the finest model space that the data can resolve. Also this gives a set of "new" data consisting of linear combinations of the original data, for which each of this new data is sensitive only to a certain spot in the model space. Doing inversion steps of full waveform inversion with the focussed kernels and the focussed data, the hope is to overall conduct a waveform inversion at the maximum resolving power of the data. This can also be seen as a sophisticated form of regularizing the overall inverse problem.

Such a "focussed waveform inversion" still remains an idea and was not yet approached to be implemented in `ASKI`. Please don't hesitate to implement and test this concept.

todo list:

- step 1
- step 2
- ...

Chapter 1

Basic Steps

Important:
This chapter is *not* intended to be read through item by item (as a manual)! If you are new to ASKI and accidently looked up this chapter in the hope to find what you're looking for, you are strongly advised to quickly read section "How to get started" at the beginning of this document, explaining how to use this manual.

In general, in this chapter we provide only basic information. For more detail on specific steps or objects, we always refer to the respective sections below in this document.

1.1 Create Main Parameter File

The simplest way to create a specific main parameter file for your operation is to modify / adjust a copy of the template file `template/main_parfile_template`.

Refer to the commented documentation in `main_parfile_template` or to sections 2.1 (page 49) and 2.1.1 (page 50).

1.2 Iteration Step Parameter Files

Having created a directory environment for your operation, as described in section 1.3 (page 25), there should automatically have been created template parameter files in each directory of an iteration step, having filenames as defined by parameter `PARFILE_ITERATION_STEP` in the main parameter file.

Refer to the commented documentation in those template files or to sections 2.1 (page 49) and 2.1.2 (page 53).

1.3 Create Directory Environment

Call python script `create_ASKI_dir.py`

```
USAGE: please give 2 arguments:
[1] main parmeter file of inversion
[2] number of iteration steps
```

```
EXAMPLE:
create_ASKI_dir.py ./main_parfile_Aegean1 10
```

Put your main parameter file (see 1.1 (page 25)) as the first, and the expected number of iteration steps as the second argument.
You can always *recall this script at any later time* with a larger number of iteration steps. All existing directories *will not be affected*, only additional non-existing objects will be created. Recalling this script with a smaller number of steps will not delete anything.

1.4 Data in ASKI

One certain data sample in ASKI is characterized by a seismic *source*, a *component* of a seismic *station* (receiver), and a *frequency*, as well as if it is *real* or *imaginary* part of the complex spectral values. It has the value of displacement of the ground in the unit of meters.

Events and Stations

The events file (2.2 (page 55)) and stations file (2.3 (page 55)) constitute a collection of *all* events (stations) which will be involved *in any way* in your ASKI operation.
All programs/scripts will refer to a specific event (station) by its event-ID (station-name).

Station Components

All programs/scripts will refer to a specific station component by the following abbreviatory names.
Dependent on the coordinate system in which the stations are defined (Cartesian or spherical, which is defined by the first line of the station list file), the supported names of station components may have a different meaning:

Cartesian stations

CX: Cartesian X-coordinate (first Cartesian coordinate)

CY: Cartesian Y-coordinate (second Cartesian coordinate)

CZ: Cartesian Z-coordinate (third Cartesian coordinate)

N: same as −CX

S: same as CX

E: same as CY

W: same as −CY

UP: same as CZ

DOWN: same as −CZ

Spherical stations

`CX`: Cartesian `X`-coordinate with `X`-axis through equator and $0°$-meridian

`CY`: Cartesian `Y`-coordinate with `Y`-axis through equator and $90°$E-meridian

`CZ`: Cartesian `Z`-coordinate with `Z`-axis through north pole

`N`: local north

`S`: local south

`E`: local east

`W`: local west

`UP`: local up

`DOWN`: local down

Frequency Discretization

In `ASKI`, frequencies are given by a frequency step Δf[Hz] and by a set of integer valued frequency indices.

For specific frequency index $k \in \mathbb{N}$, the corresponding real-valued frequency f_k [Hz] computes as $f_k = k \cdot \Delta f$. E.g. $\Delta f = 10$ Hz and frequency indices $k = 2,\ 3,\ 5,\ 7,\ 10$ define the set of discrete frequencies $f_k = 20.0,\ 30.0,\ 50.0,\ 70.0,\ 100.0$ [Hz].

Some forward methods (at the moment only Gemini) implicitely use *complex* frequencies, which are related to the above definition of real-valued frequencies $f_k = k \cdot \Delta f$. Gemini, e.g., adds to these real-valued frequencies a constant imaginary part $\sigma = -5\Delta f/2\pi$, thus implicitely using the complex frequencies $f_k = k \cdot \Delta f + i \cdot \sigma$, where i is the imaginary unit.

1.5 Prepare Measured Data

For measured data given in some basic data formats like Seismic Unix and time-series given as textfiles per trace, the executable `transformMeasuredData` → 3.1.28 (page 90) converts the time-domain data to the special frequency-domain form required by `ASKI`. Executing `transformMeasuredData` (without arguments), will print a short help message how to use it.

Otherwise you might well prepare measured data files on your own as required by `ASKI`, see sections 1.4 (page 26) and 2.4 (page 56).

1.6 Prepare Frequency-Domain Filters

In `ASKI`, synthetic wavefields (for synthetic data and sensitivity kernels) are preferred to be modelled as impulse responses, i.e. w.r.t. an impulsive Dirac source-time-function, and filtered afterwards in the frequency domain (by multiplication of wavefield spectra and spectral filter) before being compared to measured data. Therefore, `ASKI` uses spectral filters, independently associated with each seismic source and each station component. This

way, independent source-time-functions for each event, as well as independent instrument responses for each station component can be modelled. Whether or not to use event-associated filters or station-associated filters at all, is controlled in the main parameter file via flags `APPLY_EVENT_FILTER, APPLY_STATION_FILTER` → 2.1.1 (page 51).

Executable `createSpectralFilters` → 3.1.11 (page 69) provides means to generate event filters from time-domain wavelets (i.e. specific source-time-functions) or as Butterworth filters. Executing `createSpectralFilters` (without arguments) will print a short help message how to use it. For now, there is no possibility to generate station filters by this executable, since it is assumed that instrument responses were already deconvolved from the data.

If you need station filters, or require filters that cannot be generated by `createSpectralFilters`, you would have to generate filter files by yourself in the required format, see section 2.5 (page 56). Even if you want to use the same filter for each event (station component), you would need to create a filter file for each event (station component), e.g. by copy-paste-rename operations.

At the moment, `ASKI` does *not* support to have an independent filter for each event-station path (i.e. for each seismogram seperately).

1.7 Define an Inversion Grid

There are different types of `ASKI` inversion grids suitable for different geometries, forward methods, hence, applications.

All inversion grids are defined by setting parameters `TYPE_INVERSION_GRID` and `PARFILE_INVERSION_GRID` in the parameter file of the current iteration step.

In the following, we present the supported inversion grid types and explain the particular parameters in the respective inversion grid parameter file.

1.7.1 `chunksInversionGrid`

The chunks inversion grid consists of 1, 2, 3 or 6 chunks of a cubed sphere (for the order and positioning of the chunks, see fig. 1.3). The chunk width is always 90 degrees, except for 1-chunk grids where smaller chunks are allowed. The inversion grid base cells are equi-angularly distributed, resulting in cells which are more or less evenly distributed in size (by contrast to the schunk inversion grid, where the lateral projections of the cells onto the tangential plane have an equi-distant distribution on the plane).
2-chunk grids consist of two neighbouring 90-degree chunks, 3-chunk grids of three chunks which are ALL neighbours of each other (i.e. essentially half of the Earth).
Inside the chunks, the inversion grid cells are constructed on the basis of regularly distributed base cells in the fashion of the schunk inversion grid (or scart inversion grid), having a certain number of refinement blocks in depth inside which a fixed regular (equi-angular) lateral resolution and fixed depth resolution can be chosen. Thereafter, by certain mechanisms the base cells can be locally refined, i.e. subdivided into a specific distribution of subcells. *At the moment, only an experimental random refinement is implemented for illustration* (see fig. 1.2), in the future, cell refinements based e.g. on the ray coverage of the data could be implemented.

The inversion grid is defined via a paramter file, a template of which is file `template/chunksInversionGrid_parfile_template` (the template file defines the inversion

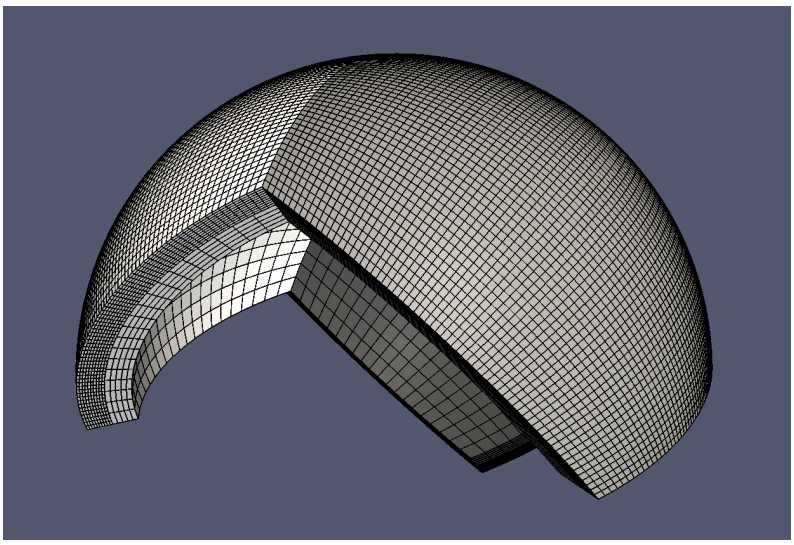

Figure 1.1: Example of a chunks inversion grid (with 3 chunks in global projection)

grid shown in fig. 1.1). The meaning of the keywords in the parameter file defining an inversion grid of type `chunksInversionGrid` are as follows:

CHUNKS_INVGRID_GEOM_NCHUNK

Number of chunks (1, 2, 3, or 6).

CHUNKS_INVGRID_GEOM_RMAX

Maximum radius (upper boundary of the chunk(s)) [must be the same unit in which wavefield points are given, usually be in km]

CHUNKS_INVGRID_GEOM_CLAT, CHUNKS_INVGRID_GEOM_CLON

Center of cubed-sphere chunk in degrees.

CHUNKS_INVGRID_GEOM_WLAT, CHUNKS_INVGRID_GEOM_WLON

Assuming `ROT = 0`.
Width of cubed-sphere chunk in degrees (must be 90.0 for NCHUNK > 1).

CHUNKS_INVGRID_GEOM_ROT

Rotation of chunk around local vertical counterclockwise in degrees.

CHUNKS_INVGRID_BASE_NREF_BLOCKS

Number of blocks of layers within which lateral cell width remains comstant.
(compare `scartInversionGrid` 1.7.3 (page 35): definition and usage of `NREF_BLOCKS`, `NLAY`, `THICKNESS`, `NX`, `NY`)

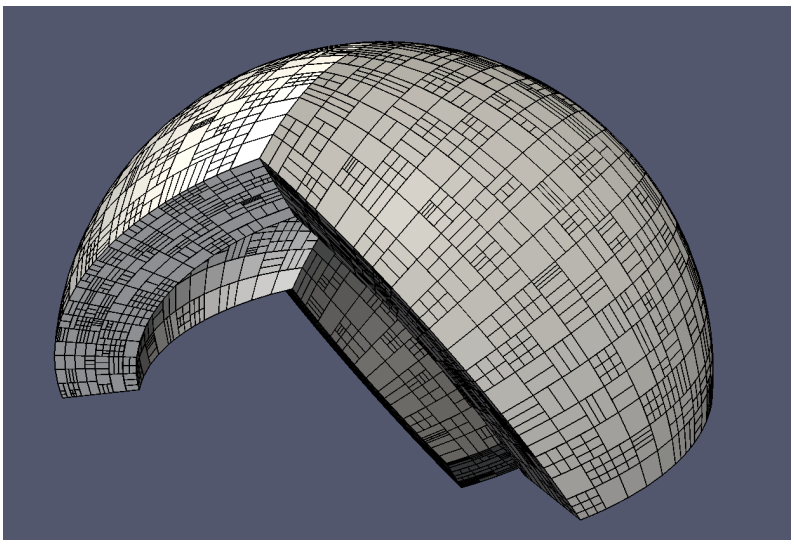

Figure 1.2: Example of a chunks inversion grid (with 3 chunks in global projection) with randomly refined base cells:

```
CHUNKS_INVGRID_CREF_METHOD = EXPERIMENTAL_RANDOM_SUBDIVISION
CHUNKS_INVGRID_CREF_PARAMETERS = 0 10
CHUNKS_INVGRID_BASE_NREF_BLOCKS = 2
CHUNKS_INVGRID_BASE_NLAY = 4 3
CHUNKS_INVGRID_BASE_THICKNESS = 180. 250.
CHUNKS_INVGRID_BASE_NLAT = 18 12
CHUNKS_INVGRID_BASE_NLON = 18 12
```

CHUNKS_INVGRID_BASE_NLAY

Number of layers within each block (integer array).
(compare `scartInversionGrid` 1.7.3 (page 35): definition and usage of `NREF_BLOCKS`, `NLAY`, `THICKNESS`, `NX`, `NY`)

CHUNKS_INVGRID_BASE_THICKNESS

Thickness of layers in each block in km (real array).
(compare `scartInversionGrid` 1.7.3 (page 35): definition and usage of `NREF_BLOCKS`, `NLAY`, `THICKNESS`, `NX`, `NY`)

CHUNKS_INVGRID_BASE_NLAT, CHUNKS_INVGRID_BASE_NLON

Number of cells in latitude/longitude direction for each layer block.
(compare `scartInversionGrid` 1.7.3 (page 35): definition and usage of `NREF_BLOCKS`, `NLAY`, `THICKNESS`, `NX`, `NY`)

CHUNKS_INVGRID_CREF_METHOD, CHUNKS_INVGRID_CREF_PARAMETERS

Definition of individual base cell refinement. If only base cells should be used, and no base cell refinement should be done at all, set `CHUNKS_INVGRID_CREF_METHOD = NONE` (in this case, `CHUNKS_INVGRID_CREF_PARAMETERS` has no meaning).

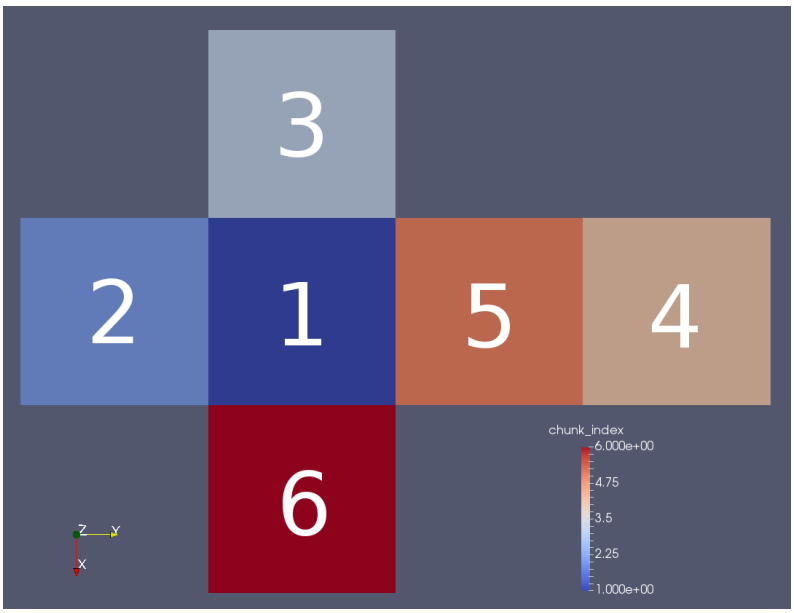

Figure 1.3: distribution of chunks of the chunksInversionGrid in `LOCAL_FLAT` projection

At the moment, only the following experimental method is supported (for illustration and testing):
`CHUNKS_INVGRID_CREF_METHOD = EXPERIMENTAL_RANDOM_SUBDIVISION` , requiring two integer values given by `CHUNKS_INVGRID_CREF_PARAMETERS` (if real values are given, they are rounded down by `int()`):
first value: input value seed for function `srand(seed)` (you can reproduce random results, using the same seed value)
second value: upper bound of subcells by which any base cell can be subdivided (number of subcells cannot exceed this number). *Note*: if subcells are subdivided themselves, these subsubcells add to this number, but their parent cell (original subcell) will *not* be seen as an external inversion grid cell. This means, that the actual number of subcells of a base cell that are used as cells of the inversion grid can be smaller than *second value*.
By the simple (and old-school) pseudo-random generator `rand`, a cell will be divided by 2, 3 or 4 in every dimension (also subcells will themselves be subdivided until upper limit is reached).

Ideas for future development:
Give here the absolute paths of the station and event list files, as well as a data model space info file containing the paths. According to the thereby defined ray coverage, the base cells could be locally refined in a recursive manner (each cell could e.g. be halfened in each dimension of space recursively if a certain criterion is met). The refinement criteria could be dependent on a maximum global depth and a threashold value could handle the number of rays which a cell must be intersected with before it is refined, etc.

`CHUNKS_INVGRID_FILE`

Filename of binary inversion grid file (relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH/`) to which a newly created inversion grid will be written and from which the inversion grid will be read if it exists and if not recreating the inversion grid.

VTK_PROJECTION

VTK_PROJECTION is one of:

'GLOBAL': center of chunk(s) in CLAT, CLON, with applied CHUNKS_INVGRID_GEOM_ROT

'LOCAL_CURV': center of chunk in x=y=0, NO CHUNKS_INVGRID_GEOM_ROT applied, but with curvature

'LOCAL_FLAT': center of chunk in x=y=0, NO CHUNKS_INVGRID_GEOM_ROT, NO curvature, i.e. projection of each depth onto the tangential x-y-plane

'LOCAL_NORTH_CURV': same as 'LOCAL_CURV', but WITH CHUNKS_INVGRID_GEOM_ROT applied, i.e. x really points to south

'LOCAL_NORTH_FLAT': same as 'LOCAL_FLAT', but WITH CHUNKS_INVGRID_GEOM_ROT applied, i.e. x really points to south

VTK_GEOMETRY_TYPE

Select the geometry type. VTK_GEOMETRY_TYPE is one of:

'CELLS': data on inversion grids will be written on the volumetric inversion grid CELLS (hexahedral) to vtk files (as UNSTRUCTURED_GRID datasets) → intuitive volumetric view

'CELL_CENTERS': data on inversion grids will be written on the cell center POINTS to vtk files (as POLYDATA datasets) → smaller files, better to apply filters in ParaView

SCALE_VTK_COORDS, VTK_COORDS_SCALING_FACTOR

Scale vtk geometry coordinates by factor VTK_COORDS_SCALING_FACTOR, if SCALE_VTK_COORDS = .True. this may be helpful if coordinate values (e.g. in m) get so large that they cause problems in paraview.

1.7.2 schunkInversionGrid

The spherical chunk inversion grid is derived from a simple planar cartesian grid by projection of each grid plane onto a spherical shell, assuming that the cartesian grid plane touches the spherical shell at its center. Since cells have uniform size in the planar cartesian grid plane, cells on the spherical shell become successively smaller with distance from the center of the spherical chunk. Radially, the inversion grid may consist of several layer blocks each of which may have its own cell size.
To describe points in the spherical chunk, we either use LOCAL cartesian coordinates with the center of the chunk at x=y=0 and z=r, or GLOBAL cartesian coordinates with z pointing towards the north pole, x pointing towards the equator at lon=0 and y pointing towards the equator at lon=90.
The center of the chunk may be shifted to any place on the sphere and, in addition, may be rotated counterclockwise around its local vertical.

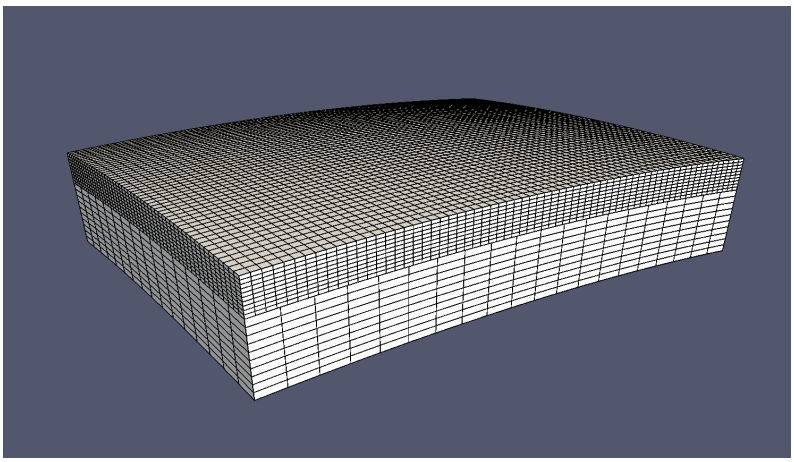

Figure 1.4: Example of a simple chunk inversion grid (global projection, note the slight curvature of the small chunk)

The inversion grid is defined via a paramter file, a template of which is file `template/schunkInversionGrid_parfile_template` (the template file defines the inversion grid shown in the above figure). The meaning of the keywords in the parameter file defining an inversion grid of type `schunkInversionGrid` are as follows:

SCHUNK_INVGRID_CLAT,SCHUNK_INVGRID_CLON

Geographic latitude/longitude of center of spherical chunk in degrees.

SCHUNK_INVGRID_RMAX

Maximum radius (upper boundary of spherical chunk) in km.

SCHUNK_INVGRID_WLAT, SCHUNK_INVGRID_WLON

Assuming `ROT = 0`.
Width of spherical chunk parallel to longitude/latitude in degrees.

SCHUNK_INVGRID_ROT

Rotation of chunk around local vertical counterclockwise in degrees.

SCHUNK_INVGRID_NREF_BLOCKS

Number of blocks of layers within which lateral cell width remains constant.
(compare `scartInversionGrid` 1.7.3 (page 35): definition and usage of `NREF_BLOCKS`, `NLAY`, `THICKNESS`, `NX`, `NY`)

SCHUNK_INVGRID_NLAY

Number of layers within each block (integer array).
(compare scartInversionGrid 1.7.3 (page 35): definition and usage of NREF_BLOCKS, NLAY, THICKNESS, NX, NY)

SCHUNK_INVGRID_THICKNESS

Thickness of layers in each block in km (real array).
(compare scartInversionGrid 1.7.3 (page 35): definition and usage of NREF_BLOCKS, NLAY, THICKNESS, NX, NY)

SCHUNK_INVGRID_NLAT, SCHUNK_INVGRID_NLON

Number of cells in latitude/longitude direction for each layer block.
(compare scartInversionGrid 1.7.3 (page 35): definition and usage of NREF_BLOCKS, NLAY, THICKNESS, NX, NY)

VTK_PROJECTION

VTK_PROJECTION is one of:

'GLOBAL': center of chunk in CLAT, CLON, with applied SCHUNK_INVGRID_ROT

'LOCAL_CURV': center of chunk in x=y=0, NO SCHUNK_INVGRID_ROT applied, but with curvature

'LOCAL_FLAT': center of chunk in x=y=0, NO SCHUNK_INVGRID_ROT applied, NO curvature, i.e. projection of each depth onto the tangential x-y-plane

'LOCAL_NORTH_CURV': same as 'LOCAL_CURV', but WITH SCHUNK_INVGRID_ROT applied, i.e. x really points to south

'LOCAL_NORTH_FLAT': same as 'LOCAL_FLAT', but WITH SCHUNK_INVGRID_ROT applied, i.e. x really points to south

VTK_GEOMETRY_TYPE

Select the geometry type. VTK_GEOMETRY_TYPE is one of:

'CELLS': data on inversion grids will be written on the volumetric inversion grid CELLS (hexahedral) to vtk files (as UNSTRUCTURED_GRID datasets) → intuitive volumetric view

'CELL_CENTERS': data on inversion grids will be written on the cell center POINTS to vtk files (as POLYDATA datasets) → smaller files, better to apply filters in ParaView

SCALE_VTK_COORDS, VTK_COORDS_SCALING_FACTOR

Scale all VTK point coordinates by an additional factor, if `SCALE_VTK_COORDS = .false.`, then `VTK_COORDS_SCALING_FACTOR` is ignored.

1.7.3 scartInversionGrid

A `S`imple `CART`esian inversion grid covers a Cartesian cuboid which can be shifted to a certain location in Cartesian space and may be rotated about the local vertical axis. Its cells are distributed in layers. Each layer has a certain thickness and a regularly distributed number of inversion grid cells along each lateral direction of the cuboid.

Please consult the documentation of your forward method (1.10 (page 42)) if it supports inversion grids of type `scartInversionGrid`.
All coordinates, e.g. of events and stations or wavefield points, are interpreted by this type of inversion grid as `X` (first coordinate), `Y` (second coordinate), `Z` (third coordinate). Their units (e.g. meters or kilometers) are not assumed by the inversion grid and are essentially defined by the wavefield points, hence, they might be method dependent and must be overall consistend.
Every type of integration weights is supported by this type of inversion grid, except weights of type `6` (external integration weights).

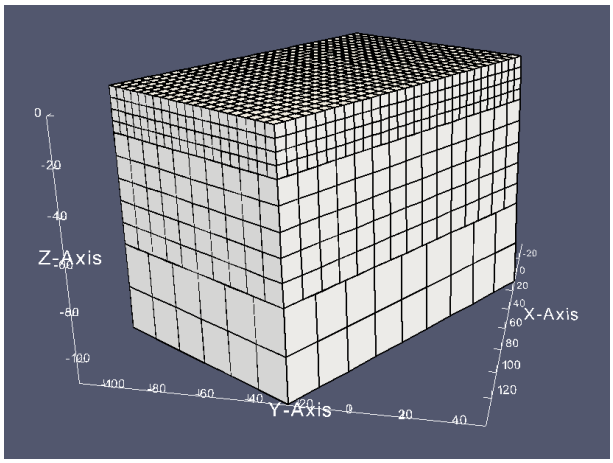

Figure 1.5: Example of a simple Cartesian inversion grid

The shape of the cuboid, as well as the distribution of inversion grid cells, are defined via a paramter file, a template of which is file `template/scartInversionGrid_parfile_template`. In the following, the particular parameters are explained, with the example values always refering to the inversion grid as displayed in figure 1.5 (page 35).

SCART_INVGRID_CX

`X`-coordinate of center of cuboid (real number)
Example:
`SCART_INVGRID_CX = 50.0`

SCART_INVGRID_CY

`Y`-coordinate of center of cuboid (real number)

Example:
SCART_INVGRID_CY = -30.0

SCART_INVGRID_ZMAX

Maximum Z-coordinate of cuboid (real number), i.e. Z-coordinate of the "surface" of the inversion grid
Example:
SCART_INVGRID_ZMAX = 0.0

SCART_INVGRID_WX

Width of cuboid in X-direction (real number)
Example:
SCART_INVGRID_WX = 100.0

SCART_INVGRID_WY

Width of cuboid in Y-direction (real number)
Example:
SCART_INVGRID_WY = 150.0

SCART_INVGRID_ROT

Angle in degrees of anti-clockwise rotation about the local Z-axis through the lateral center of the cuboid (real number)
Example:
SCART_INVGRID_ROT = 60.0

SCART_INVGRID_NREF_BLOCKS, SCART_INVGRID_NLAY, SCART_INVGRID_THICKNESS

For an arbitrary number of SCART_INVGRID_NREF_BLOCKS blocks of layers, the vectors SCART_INVGRID_NLAY (integer values) and SCART_INVGRID_THICKNESS (real values), both of length SCART_INVGRID_NREF_BLOCKS, define the Z-direction refinement of each block, whereby SCART_INVGRID_NLAY(i) defines the number of layers in block i, and SCART_INVGRID_THICKNESS(i) defines the thickness of all layers contained in block i.
Hence, the overall Z-direction coverage of the inversion grid is defined by SCART_INVGRID_ZMAX (which is the coordinate of the top of the first layer in the first refinement block) and SCART_INVGRID_ZMAX - SUM_i(THICKNESS(i) * NLAY(i)) (coordinate of the bottom of the last layer in last refinement block).
Example:
SCART_INVGRID_NREF_BLOCKS = 3
SCART_INVGRID_NLAY = 4 5 2
SCART_INVGRID_THICKNESS = 5.0 10.0 20.0

SCART_INVGRID_NX

Vector (of length SCART_INVGRID_NREF_BLOCKS) of integer values, defining number of inversion grid cells in X-direction, one value for each refinement block
Example:
```
SCART_INVGRID_NX = 20 10 6
```

SCART_INVGRID_NY

Vector (of length SCART_INVGRID_NREF_BLOCKS) of integer values, defining number of inversion grid cells in Y-direction, one value for each refinement block
Example:
```
SCART_INVGRID_NX = 30 15 9
```

USE_LOCAL_INVGRID_COORDS_FOR_VTK

Logical value to indicate whether to use local inversion grid coordinates for vtk geometry, i.e. no rotation by SCART_INVGRID_ROT and no shift by SCART_INVGRID_CX, SCART_INVGRID_CY, SCART_INVGRID_ZMAX (cuboid centered in X=Y=0 and ZMAX=0)
Example:
```
USE_LOCAL_INVGRID_COORDS_FOR_VTK = .false.
```

VTK_GEOMETRY_TYPE

Select the geometry type. VTK_GEOMETRY_TYPE is one of:

> 'CELLS': data on inversion grids will be written on the volumetric inversion grid CELLS (hexahedral) to vtk files (as UNSTRUCTURED_GRID datasets) → intuitive volumetric view
>
> 'CELL_CENTERS': data on inversion grids will be written on the cell center POINTS to vtk files (as POLYDATA datasets) → smaller files, better to apply filters in ParaView

SCALE_VTK_COORDS, VTK_COORDS_SCALING_FACTOR

Scale vtk geometry coordinates by factor VTK_COORDS_SCALING_FACTOR (real number), if SCALE_VTK_COORDS = .true.. This may be helpful if coordinate values (e.g. in meters) get so large that they cause problems when plotting in paraview.
Example:
```
SCALE_VTK_COORDS = .false.
VTK_COORDS_SCALING_FACTOR = 1.0
```

1.7.4 ecartInversionGrid

EXPERIMENTAL FEATURE: *so far, this type of inversion grid works for tetrahedral cells only, since support for hexahedreal cells is not completed throughout (neighbour detection not yet implemented, no localization of wavefield points / computation of integration weights implemented, no computation of cell volume). However, even for tetrahedra the automatic detection*

of neighbours did not work properly in some test cases (compare `ASKI` *developers manual, "To do" section)! The neighbours are only required for model smoothing in case of regularizing the Kernel system of equations by smoothing conditions (and possibly for importing inverted models in the forward code, depends on the forward method in use). If you need neighbours, please check them by executable* `invgrid2vtk` *along with option* `-all_nb`*. Execute* `invgrid2vtk` *(without arguments)* → 3.1.17 (page 77) *for further details on how to use it. Otherwise, kernel computation and pre-integration of kernels onto the inversion grid, as well as plotting etc., should work properly! Alternatively you may implement an alternative smoothing method that does not require neighbours (compare the suggestions in the* `ASKI` *developers manual, "To do" section).*

An External `CART`esian inversion grid is defined by several text files containing the definintion of nodes (i.e. essentially the corner points, or rather the control nodes of the inversion grid cells) and the definition of cells by refering to the nodes. At the moment, 4-node tetrahedral cells are fully supported, and 8-node hexahedral cells are partly supported. Those files may be produced by any meshing tool. In case you are interested to export meshes your own way, section 2.9 (page 59) defines the required file formats.
`ASKI` provides the `python` module `cubit2ASKIecartInversionGrid.py` which can be used with the meshing software `Cubit` in a `python` script by first importing the module:

```
import cubit2ASKIecartInversionGrid
```

and at the very end of your meshing process calling:

```
cubit.cmd('compress all')
cubit2ASKIecartInversionGrid.export2ASKI('EXPORT_PATH')
```

whereby you may replace `EXPORT_PATH` by some location where the output files will be written.

Please consult the documentation of your forward method (1.10 (page 42)) if it supports inversion grids of type `ecartInversionGrid`.
All coordinates, e.g. of events and stations or wavefield points, are interpreted by this type of inversion grid as `X` (first coordinate), `Y` (second coordinate), `Z` (third coordinate). Their units (e.g. meters or kilometers) are not assumed by the inversion grid and are essentially defined by the wavefield points, hence, they might be method dependent and must be overall consistend.
Every type of integration weights is supported by this type of inversion grid, except weights of type `6` (external integration weights).

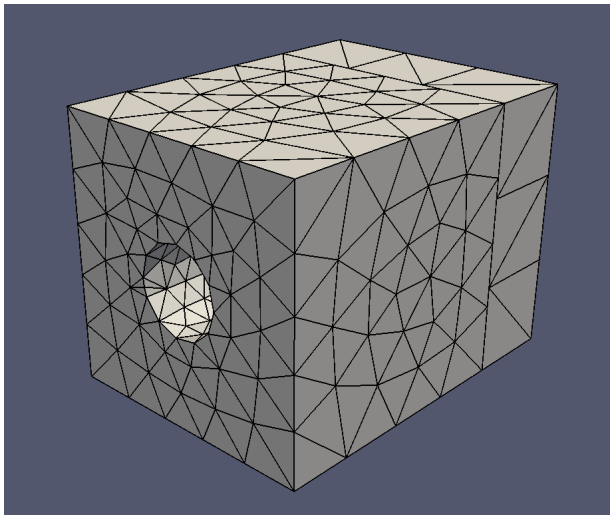

Figure 1.6: Example of an external Cartesian inversion grid created by Cubit

The nodes and cell files, e.g. produced by `Cubit`, are referred to in a parameter file, a tem-

plate of which is file `template/ecartInversionGrid_parfile_template`. In the following, the particular parameters are explained. An example inversion grid of this type is displayed in figure 1.6 (page 38).

ECART_INVGRID_USE_NODES_COMMON

Logical value to indicate whether to use one common nodes coordinates file for all cell types (only use parameter `ECART_INVGRID_FILE_NODES` below), or to use an individual nodes coordinates file for each cell type (use parameters files `ECART_INVGRID_FILE_NODES_TET4`, `ECART_INVGRID_FILE_NODES_HEX8`, ... below).
When using module `cubit2ASKIecartInversionGrid` you should set:
`ECART_INVGRID_USE_NODES_COMMON = .True.`

ECART_INVGRID_FILE_NODES_COMMON

File name relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH/` of nodes coordinates file to be commonly used for definition of cells of all types in case of `ECART_INVGRID_USE_NODES_COMMON = .True.`
When using module `cubit2ASKIecartInversionGrid` you should set:
`ECART_INVGRID_FILE_NODES_COMMON = node_coordinates`

ECART_INVGRID_FILE_NODES_TET4

File name relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH/` of nodes coordinates file to be used for definition of tet4-type cells in case of `ECART_INVGRID_USE_NODES_COMMON = .False.`

ECART_INVGRID_FILE_NODES_HEX8

File name relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH/` of nodes coordinates file to be used for definition of hex8-type cells in case of `ECART_INVGRID_USE_NODES_COMMON = .False.`

ECART_INVGRID_FILE_CELLS_TET4

File name relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH/` of cell connectivity file for definition of tet4-type cells.
When using module `cubit2ASKIecartInversionGrid` you should set:
`ECART_INVGRID_FILE_CELLS_TET4 = cell_connectivity_tet4`

ECART_INVGRID_FILE_CELLS_HEX8

File name relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH/` of cell connectivity file for definition of hex8-type cells.

When using module cubit2ASKIecartInversionGrid you should set:
ECART_INVGRID_FILE_CELLS_HEX8 = cell_connectivity_hex8

ECART_INVGRID_FILE_NEIGHBOURS

File name relative to MAIN_PATH_INVERSION/ITERATION_STEP_PATH/ of cell neighbours file. If not present, this file will be created when first using the inversion grid. If present, its content defines the neighbour structure of the inversion grid cells. If, however, the inversion grid is to be recreated (e.g. when calling initBasics -recr, see section 1.13 (page 44)), this file is recreated.

ECART_INVGRID_FILE_NEIGHBOURS_IS_BINARY

Logical value to indicate whether ECART_INVGRID_FILE_NEIGHBOURS should be binary or not.

VTK_GEOMETRY_TYPE

Select the geometry type. VTK_GEOMETRY_TYPE is one of:

'CELLS': data on inversion grids will be written on the volumetric inversion grid CELLS (hexahedral) to vtk files (as UNSTRUCTURED_GRID datasets) → intuitive volumetric view

'CELL_CENTERS': data on inversion grids will be written on the cell center POINTS to vtk files (as POLYDATA datasets) → smaller files, better to apply filters in ParaView

SCALE_VTK_COORDS, VTK_COORDS_SCALING_FACTOR

Scale vtk geometry coordinates by factor VTK_COORDS_SCALING_FACTOR (real number), if SCALE_VTK_COORDS = .true.. This may be helpful if coordinate values (e.g. in meters) get so large that they cause problems when plotting in paraview.
Example:
SCALE_VTK_COORDS = .false.
VTK_COORDS_SCALING_FACTOR = 1.0

1.7.5 specfem3dInversionGrid

An inversion grid of type specfem3dInversionGrid is method dependent and is to be used with METHOD = SPECFEM3D only. Whole spectral elements are used as inversion grid cells and all GLL points inside such an element as the wavefield points. All information regarding the element geometry, including information on neighbour cells and the values of the jacobian for every wavefield point contained in an element are read from files which are produced by SPECFEM3D methods.

Every type of integration weights is supported by this type of inversion grid, including weights of type 6 (external integration weights, i.e. the very integration weights that already SPECFEM3D uses to integrate over spectral elements).

Please refer to the documentation of your SPECFEM3D forward method (1.10 (page 42)) on how to generate any files required for using an inversion grid of type specfem3dInversionGrid.

As with all other types of inversion grids, a parameter file defines any details of the grid, a template of which is file template/specfem3dInversionGrid_parfile_template. In the following, the particular parameters are explained.

SPECFEM3D_ASKI_MAIN_FILE

File name relative to MAIN_PATH_INVERSION/ITERATION_STEP_PATH/ of file from SPECFEM3D containing all information about the inversion grid (any .main output file)
Example:
```
SPECFEM3D_ASKI_MAIN_FILE = kernel_displacements/kernel_displ_
S001.main
```

VTK_GEOMETRY_TYPE

Select the geometry type. VTK_GEOMETRY_TYPE is one of:

'CELLS': data on inversion grids will be written on the volumetric inversion grid CELLS (hexahedral) to vtk files (as UNSTRUCTURED_GRID datasets) → intuitive volumetric view

'CELL_CENTERS': data on inversion grids will be written on the cell center POINTS to vtk files (as POLYDATA datasets) → smaller files, better to apply filters in ParaView

SCALE_VTK_COORDS, VTK_COORDS_SCALING_FACTOR

Scale vtk geometry coordinates by factor VTK_COORDS_SCALING_FACTOR (real number), if SCALE_VTK_COORDS = .true.. This may be helpful if coordinate values (e.g. in meters) get so large that they cause problems when plotting in paraview.
Example:
```
SCALE_VTK_COORDS = .false.
VTK_COORDS_SCALING_FACTOR = 1.0
```

SPECFEM3D_R_EARTH_KM

In case of using SPECFEM3D_GLOBE, define here the maximum radius [km] of the sphere, by which Earth is approximated (only used to interpret "depth" and "altitude" of events and stations when plotting to vtk files; ignored for SPECFEM3D_Cartesian applications).
Example:
```
SPECFEM3D_R_EARTH_KM = 6371.0
```

1.8 Define a Starting Model

There are two possibilities to define an earth model for the forward wave propagation in your first iteration:

On the one hand you may use any (standard) earth model provided by the forward method you are using, if appropriate.

If this is not possible, or the models provided do not meet your needs, you may use executable `createStartmodelKim` along with the inversion grid of your first iteration (which you should have already defined) to produce an inverted model file containing some simple model on this inversion grid. Executing `createStartmodelKim` (without arguments) will print a short help message how to use the program → 3.1.12 (page 72). Afterwards you may export the produced model file to your forward method as explained in section 1.9 (page 42). Template files of starting model descriptions may be found in `template/`.

1.9 Export Inverted Model

The executable `exportKim` exports an inverted model file ("kim" stands for "K"ernel "I"nverted "M"odel) along with the respective inversion grid specifications to a text file, which may be used to communicate such a model to a forward method or postprocess the model values in any way. Executing `exportKim` (without argument) will print a short help message how to use it → 3.1.13 (page 74).

1.10 Solving the Forward Problem

In the following, all wave propagation codes which are supported by `ASKI` are listed. Refer to the given documentation on any details regarding the interaction of the forward codes with `ASKI`.

Gemini II

`Gemini II` (by [FD95]) is supported in this release version, for Cartesian as well as spherical setting. The `Gemini` routines producing spectral output for `ASKI`, however, might not yet be available. We hope to be able to provide them in due time. Until now, please contact us via `http://www.rub.de/aski` if you want to use `Gemini II` as a forward solver for `ASKI`.

SPECFEM3D_Cartesian

The Cartesian spectral element code `SPECFEM3D_Cartesian` (by [TKL08]), version `3.0` is fully supported by this `ASKI` release version, cf. [Sch15]. A copy of the code (extended for use with `ASKI`), as well as the code package `SPECFEM3D_Cartesian_for_ASKI` and documentation is available via `https://github.com/seismology-RUB/SPECFEM3D_Cartesian_for_ASKI` (follow the directions in file `README.md` and the provided manual).

SPECFEM3D_GLOBE

The global spectral element code `SPECFEM3D_GLOBE` (by [TKL08]), version `7.0.0`, is fully supported by this `ASKI` release version, cf. [Sch16]. A copy of the code (extended for use with

ASKI), as well as the code package SPECFEM3D_GLOBE_for_ASKI and documentation is available via https://github.com/seismology-RUB/SPECFEM3D_GLOBE_for_ASKI (follow the directions in file README.md and the provided manual).

NEXD

The nodal discontinous Galerkin code NEXD (by [Lam15b]) is fully supported by this ASKI release version. NEXD, including ASKI support, will be available under terms of the GPL in the near future via http://www.rub.de/nexd.

1.11 Choose Integration Weights

In order to numerically integrate the sensitivity kernels, which are computed on the wavefield points, over the inversion grid cells by a weightet summation of values, there are different types of integration weights provided, following different rules of integration.

The integer values of the type have the following meaning:

0 → all weights are the same, weight = 1/number_of_points_in_box, i.e. no integration(!), just building the average sensitivity value (e.g. convenient for comparison of sensitivities computed with different methods on different forward grids)

1 → Scattered Data Integration, as in [Lev99], polynomial degree 1

2 → Scattered Data Integration, as in [Lev99], polynomial degree 2, i.e. approximation order 3 (?)

3 → Scattered Data Integration, as in [Lev99], polynomial degree 3, i.e. approximation order 4 (?)

4 → for each cell, compute the highest possible order of Scattered Data Iintegration integration after [Lev99] (trying types 3,2,1 (in that order) until computation was successful)

5 → average of function values, multiplied with volume of box (i.e. $\sim$ linear integration)

6 → external integration weights, to be used along with a suitable inversion grid (e.g. of type specfem3dInversionGrid, see section 1.7.5 (page 40))

A detailed description of some of the integration weights, especially the weights after [Lev99] can be found in section 3.3 (page 92).

1.12 Create a Data and Model Space

In order to choose a set of data samples which to invert and a set of model values which to invert for, you need to define a data space and a model space. Essentially, if you have m data samples, the space in which the data live is just $\mathbb{R}^m$ (analogously, for n model values, the model lives in $\mathbb{R}^n$). You only need to define which data sample (model value) refers to which dimension (i.e. entry in vector) of the data space (model space), respectively.

The $m \times n$ sensitivity kernel matrix will then connect a vector of model updates from model space in $\mathbb{R}^n$ to your specific data vector from $\mathbb{R}^m$.

In the following, it is described how data samples and model values are characterized in this software package and how you can choose specific subsets to be used.

1.12.1 How Data Samples are Characterized

Since `ASKI` derives a model update in an iteration of FWI by frequency-domain sensitivity equations, the data needs to be provided frequency domain, too.
A data sample is uniquely characterized by a seismic *source*, a *component* of a seismic *station*, and a *frequency*, as well as whether it is the *real* or *imaginary* part of the complex spectral values. Refer to 1.4 (page 26) for details on data in `ASKI`.

1.12.2 How Model Values are Characterized

A model value is uniquely characterized by a parameter name (must be a valid parameter name of the model parametrization as defined by `MODEL_PARAMETRIZATION` 2.1.1 (page 50)) and an inversion grid cell index in valid range.

1.12.3 How to Define Data and Model Space: Choosing a Set of Data Samples and Model Values

Create a text file as described in section 2.8 (page 57), e.g. by adjusting the provided template files in `template/`.

1.13 Initiate Basic Requirements

Use the executable `initBasics`. Executing `initBasics` (without arguments) will print a short help message how to use it → 3.1.15 (page 76).

It first checks if all parameters needed are present in the parameter files and then creates all basic requirements for `ASKI` operations:
It reads in required files like event list and station list files, the wavefield points and the kernel reference model.
Furthermore, it creates the inversion grid (possibly storing some inversion grid files, dependent on the type of grid), localizes the wavefield points inside it and computes the integration weights, which are written to file. Once those files exist, `initBasics` and all other programs will always read the integration weights (and possibly (part of) the inversion grid) from file, *regardless* of what the parameter files say! So if at some you point want to use different integration weights or a different inversion grid, you will have to either delete the respective file(s) and rerun `initBasics`, or run `initBasics -recr` in order to recreate them.

Also a lot of `.vtk` files with statistics are produced having base filename `FILEBASE_BASIC_STATS` as defined in the parameter file of the current iteration step. Those files mainly regard the inversion grid, the wavefield points and the integration weights, where the respective filenames are extended (by something with ".vtk"). It is *highly recommended* to call

`initBasics -recr` in order to assure that all those `.vtk` files are produced and to actually have a look at them before continuing any `ASKI` operation!

If you use a spherical setting, you might find it useful for your plots to generate `.vtk` files containing shore lines in the specific `VTK_PROJECTION` of the inversion grid in use → 1.20 (page 47).

1.14 Compute Spectral Waveform Sensitivity Kernels

The kernels are computed by combining green tensor component(s) and forward wavefield for a given event-station pair (called "path" below. By default, the kernels are integrated over the inverison grid cells. I.e. there is one sensitivity kernel file for a specific event-station path. This file contains sensitivity values of the requested station components for the requested model parameters of your model parametrization, with the values living on the inverison grid cells. Alternatively, kernels can be computed on the wavefield points, without pre-integration (for inspection only, cannot be used for waveform inversion in that case).

Use executable `computeKernels`. Executing `computeKernels` (without arguments) will print a short help message how to use it → 3.1.8 (page 67). It makes sense, to only compute kernel files for those event-station paths that you are going to use (defined by your data-model-space file).

You can define the set of event-station paths, station components and model parameters for which sensitivities should be computed in two ways:

way 1 compute a kernel for only one event-station path, defined by eventID and station name using options `-evid`, `-stname`, `-comp`, `-param`

way 2 input a data-model-space file (as defined by 1.12 (page 43)) by option `-dmspace`, defining all event-station paths and respective station components and model parameters for which kernels should be computed; optionally define range of path index by `-ipath1`, `-ipath2`

Setting option `-wp` will compute plain kernel values on wavefield points (no pre-integration onto inversion grid). *This option will produce separate files, so you can compute both, kernels on wavefield points and on inversion grid.*

1.15 Transform to Time-Domain Sensitivity Kernels

The time kernels are computed from the standard frequency-domain kernels (which were computed path-wise) by applying an inverse Fourier transform.

Use executable `spec2timeKernels`. Executing `spec2timeKernels` (without arguments) will print a short help message how to use it → 3.1.26 (page 88).

The set of event-station paths, station components and model parameters for which time kernels should be produced are defined in the same "two ways" (by the same options) as computing spectral waveform kernels → 1.14 (page 45).

Additionally, you need to define the time discretization of the produced time kernel by options `-dt`, `-nt1`, `-nt2`, `-t0`.

1.16 Plot Spectral Waveform Sensitivity Kernels

One way to plot a specific sensitivity Kernel in frequency domain, i.e. the sensitivity spectra for a specific event-station path, is to procuce vtk files using executable `kernel2vtk`. Executing `kernel2vtk` will print a short help message how to use it → 3.1.19 (page 79).

Please note, that the output `.vtk` files (one for every frequency) might get large, dependent on the resolution of the inversion grid, since the geometry information of the inversion grid cells is contained in each `.vtk` file. If the files become too large for you, you might consider setting `DEFAULT_VTK_FILE_FORMAT = BINARY` in your main parameter file.

1.17 Plot Time Sensitivity Kernels

One way to plot a specific sensitivity Kernel in time domain, is to procuce vtk files using executable `timeKernel2vtk`. Executing `timeKernel2vtk` (without arguments) will print a short help message how to use it → 3.1.27 (page 89).

Please note, that the output `.vtk` files (one for every time step) might get large, dependent on the resolution of the inversion grid, since the geometry information of the inversion grid cells is contained in each `.vtk` file. If the files become too large for you, you might consider setting `DEFAULT_VTK_FILE_FORMAT = BINARY` in your main parameter file. For a lot of time steps, the `.vtk` file format is actually not optimally chosen by `ASKI`, since the complete geometry information is contained in every time-step file (a lot of redundant information is written to hard disc).

1.18 Solve Kernel System

At the moment, there are 3 executable programs implemented which solve the kernel linear system.

- `solveKernelSystem` is a serial program which sets up the kernel matrix, reads in synthetic and measured data, adds regularization condutions to the system if requested (smoothing, damping) and solves the system based on `LAPACK` libraries.
  Executing `solveKernelSystem` (without arguments) will print a short help message how to use it → 3.1.24 (page 84).

- `solveParKernelSystem` does essentially the same as `solveKernelSystem`, but uses parallelized `ScaLAPACK` libraries to solve the (regularized) kernel linear system. You must compile executable `solveParKernelSystem` separately (`make all` does not compile it, make sure you have `ScaLAPACK` libraries installed and linked in the `Makefile`). Executing `solveParKernelSystem` (without arguments) will print a short help message how to use it → 3.1.25 (page 86). This executable requires an additional parameter file, see template file `templated/solveParKernelSystem_parfile_template`.

- `solveCglsrKernelSystem` sets up the (regularized) kernel linear system, as the above excecutables do, but the uses a conjugate gradient algorithm to solve the kernel linear system in a least-squares sense → 3.1.23 (page 81). This executable requires an

additional parameter file, see template file
`templated/solveCglsKernelSystem_parfile_template`.
Executing `solveCglsKernelSystem` (without arguments) will print a short help message how to use it → 3.1.23 (page 81).

1.19 Investigate State of Convergence of Waveform Inversion

These kinds of operations probalby still need further development in `ASKI`.

Whenever solving the linear system of kernel equations in an interation step of full waveform inversion (see above section 1.18 (page 46)), the current linear misfit is printed to output files or on screen, i.e. the the sum of residual squares of the linear system of equations. Also the current misfit between synthetics and measured data can be computed by executable `computeMisfit` → 3.1.9 (page 68). However, comparing these two during variation of the regularization parameters does not give sensible information on which regularization to choose. The development of the non-linear misfit, i.e. comparing synthetic data based on the new models with the measured data, can only be observed after solving the forward problem for each of the models to choose from. There is not yet an automated way implemented in `ASKI` that does this. Evaluating the non-linear misfit, i.e. conducting suitable forward calculations, would have to be done by hand for the selected models resulting from the selected regularization parameters.

If you would like to do traditional resolution tests, executable `computeDataFromKernelSystem` → 3.1.5 (page 66) computes the "measured" data d in the equation $d - s = K(m1 - mref)$ for any given model m1. This can be used for traditional linear computation of checkerboard data by forward multiplication of the sensitivity matrix with an artificial model vector containing checker anomalies. A model containing checker or spike-like anomalies can be produced by the preliminary hard-coded executable `addSpikeCheckerToKim` → 3.1.1 (page 63).

1.20 Generate Shore Line Vtk Files

`ASKI` provides two implementational realizations for creating shore line `.vtk` files from GSHHS data provided in native binary format. The current version of this widely used geographical dataset is available via `https://www.ngdc.noaa.gov/mgg/shorelines/data/gshhg/latest/`. You should download the dataset in form of native binary files (probably package named like `gshhg-bin-?.?.?.zip`).

The files `gshhs_c.b`, `gshhs_l.b`, `gshhs_i.b`, `gshhs_h.b`, `gshhs_f.b` (different resolutions), can be used as an input for the following executables.

1.20.1 excutable purely written in Fortran

The executable `createShoreLines` → 3.1.10 (page 68) is purely written in Fortran and is by default compiled when you compile the `ASKI` binaries.

1.20.2 python program based on Fortran-to-python interface generator `f2py`

The python program `create_shore_lines.py` → 3.2.2 (page 92) is based on the Fortran-to-python interface generator `f2py` and requires an additional module to be compiled manually before you are able to use it.

Make sure your system has installed the `f2py` interface generator.

Go to the `ASKI` installation directory `ASKI_1.1/`. In `Makefile`, adjust the `f2py_COMPILER` and `BLAS_F2PY`, if necessary. Excecute
`make shore_lines_module_for_python`

The additional module `create_shore_lines_f2py.so` should have been created in directory `ASKI_1.1/py` which is neede by python program `create_shore_lines.py`.

1.21 Path-Specific Approach to an Iteration of Waveform Inversion

`ASKI` supports a "path-specific" approach to an iteration of full waveform inversion, which is enabled by flag `USE_PATH_SPECIFIC_MODELS` in the iteration step parameter file → 2.1.2 (page 53).

This approach was applied by [Lam15a] in his first iteration of full waveform inversion using the 1D code Gemini as a forward solver. Due to the complex structure of the investigated region (Aegean), it was infeasible to choose a single 1D background model for solving the total forward problem. Therefore, an individual 1D background model was chosen for each event-station path which explained the particular seismogram of that path very well.

This path-specific concept requires to account for different kernel reference models and to introduce a correction term in the linear system of kernel equations in order to invert for a global 3D model. Any required functionality is implemented in `ASKI` and was successfully applied. We refer to [Lam15a] and [SFL16] on a more detailed description of the concept.

The required quantity of the correction term, called synthetic correction, can be computed in `ASKI` by executable `computeCorrectionSyntheticData` → 3.1.4 (page 65).

Chapter 2

Files

Important:
This chapter is *not* intended to be read through item by item (as a manual)! If you are new to ASKI and accidently looked up this chapter in the hope to find what you're looking for, you are strongly advised to quickly read section "How to get started" at the beginning of this document, explaining how to use this manual.

This chapter collects documentation on file formats involved in ASKI.

2.1 Parameter Files

Parameter files are simple text files.

The following type of lines are ignored:

- comment lines, i.e. lines STARTING with an arbitrary number of blanks followed by a "#" character
- empty lines and lines containing blanks only
- lines not containing any "=" character

How to specify one parameter:

- valid lines have the form "keyword = value" (blanks leading or following "keyword", "=", or "value" are ignored)
- in a valid line, all characters in front of "=" (without leading and appending blanks) are interpreted as the keyword, allowing for blank characters within the keyword (e.g. for lines " key word = value ", the string "key word" is used as the keyword)
- all characters behind "=" (without leading and appending blanks) are interpreted as the value string from which the value is read, which in particular means that "#" comments at the end of a line (such as " keyword = value # comment ") are *not* allowed!

By convention, specify *paths* (i.e. directory names, which will be concatenated with a filename of a file in that directory) always ending on "/" and specify *filenames* always *without* leading "/".

2.1.1 Main Parameter File

Here, shortly all keywords required in the main parameter file for your specific program operation, are described.

FORWARD_METHOD

GEMINI

SPECFEM3D → SPECFEM3D_Cartesian and SPECFEM3D_GLOBE

NEXD

For details on the methods and references to their documentation, refer to section 1.10

MODEL_PARAMETRIZATION

isoLameSI → isotropic Lamé parameters and density in SI units: ρ (rho) [kg/m^3], λ (lambda) [Pa], μ (mu) [Pa]

isoVelocitySI → isotropic seismic velocities and density in SI units: ρ (rho) [kg/m^3], v_p (vp) [m/s], v_s (vs) [m/s]

isoVelocity1000 → isotropic seismic velocities and density in units involving a factor of 1000: ρ (rho) [g/cm^3], v_p (vp) [km/s], v_s (vs) [km/s]

No other parameterization supported yet.

PARAMETER_CORRELATION_MODE

Any model parameters can be correlated to others which are not inverted for. So far supported correlation modes:

NONE → no parameter correlation will be done whatsoever

CORRELATE_KERNELS → will add correlated kernel values of other parameters to the kernels of those parameters which are inverted for (experimental feature, not yet generally applicable in practice, please refer to ASKI developers manual for things "to do" in order to properly support this feature).

PARAMETER_CORRELATION_FILE

File (relative to MAIN_PATH_INVERSION) containing the definition of the correlation and the correlation coefficients. The given filename is ignored in case of PARAMETER_CORRELATION_MODE = NONE.

MAIN_PATH_INVERSION

All subpaths for filenames are considered relative to this main path. This directory is thought to contain all your relevant output and (temporary) data.
Example: `MAIN_PATH_INVERSION = /data/inversions/Aegean1/`

CURRENT_ITERATION_STEP

Example: `CURRENT_ITERATION_STEP = 3`

ITERATION_STEP_PATH

Relative to main path, defining name of subdirectory of `MAIN_PATH_INVERSION` which contains all relevant (meta)data of an inversion step. A three-digit integer (= `CURRENT_ITERATION_STEP`) and "/" will be appended to `ITERATION_STEP_PATH` (i.e. "001/", "002/", ...) defining the first, second ... iteration step directory.
Example (default): `ITERATION_STEP_PATH = iteration_step_`

PARFILE_ITERATION_STEP

File name of iteration step specific parameter file, relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH` Example: `PARFILE_ITERATION_STEP = iter_parfile`

PATH_MEASURED_DATA, APPLY_EVENT_FILTER, PATH_EVENT_FILTER, APPLY_STATION_FILTER, PATH_STATION_FILTER

Paths and flags related to the measured data. The paths are *absolute*, i.e. can be everywhere, e.g. close to where you have stored/processed your (time domain) data, or in directory `MAIN_PATH_INVERSION`, etc. ...

If you do not wish to use any filtering per events, you can switch to
`APPLY_EVENT_FILTER = .false.`,
if you do not wish to use any fitering per stations, you can switch to
`APPLY_STATION_FILTER = .false.`.
In these cases, the respective filter files are not expected to exist and the respective filter paths are ignored.

The naming convention of the files in the respective directories is:
`FILE_MEASURED_DATA`: `data_EVENTID_STATIONNAME_COMP`,
`FILE_EVENT_FILTER`: `filter_EVENTID`,
`FILE_STATION_FILTER`: `filter_STATIONNAME_COMP`,
where station filters are dependet on component and `STATIONNAME` and `EVENTID` are defined in `FILE_STATION_LIST` and `FILE_EVENT_LIST` file, and `COMP` is a valid component (for valid components see 1.4)
Example:

```
PATH_MEASURED_DATA = /mydata/your_name_of_inversion/ASKI_data/
PATH_EVENT_FILTER = /mydata/your_name_of_inversion/ASKI_event_
filter/
PATH_STATION_FILTER = /mydata/your_name_of_inversion/ASKI_
```

station_filter/

FILE_EVENT_LIST

Absolute filename where ASKI finds a text file defining a set of events in the required format (2.2)
Example: FILE_EVENT_LIST = /mydata/your_name_of_inversion/ASKI_events

FILE_STATION_LIST

Absolute filename where ASKI finds a text file defining a set of stations in the required format (2.3)
Example: FILE_STATION_LIST = /mydata/your_name_of_inversion/ASKI_stations

MEASURED_DATA_FREQUENCY_STEP,MEASURED_DATA_NUMBER_OF_FREQ, MEASURED_DATA_INDEX_OF_FREQ

Discretized frequency window of measured data (same expected in event_filter/station_filter!) given by a frequency step FREQUENCY_STEP [Hz] and a vector of frequency indices INDEX_OF_FREQ (of length NUMBER_OF_FREQ), where for specific frequency index i the corresponding frequency f_i [Hz] computes to $f_i = i \cdot$ FREQUENCY_STEP
Example:
MEASURED_FREQUENCY_STEP = 10.
MEASURED_NUMBER_OF_FREQ = 5
MEASURED_INDEX_OF_FREQ = 2 3 5 7 10
which corresponds to the 5 frequencies $20, 30, 50, 70, 100$ Hz

UNIT_FACTOR_MEASURED_DATA

Indicate the unit factor of the measured data. The definition of the factor is:
Multiplication of the measured data (displacement) with this factor gives values in the SI unit of meters [m].
Example: If you use seismic time-domain data for ASKI in the unit of nano meters [nm], then UNIT_FACTOR_MEASURED_DATA must be set to 1.0e-9 , because the data values in nano meters [nm] must be divided by $1.0 \cdot 10^9$ in order to get meters [m]. If you use seismic displacement data in the SI unit of meters, then UNIT_FACTOR_MEASURED_DATA must be set to 1.0.

DEFAULT_VTK_FILE_FORMAT

Either BINARY or ASCII defining the default type of vtk files which will be produced in the course of running the programs.

2.1.2 Parameter File for Specific Iteration Step

Here, shortly all keywords required in a parameter file for a specific iteration step, i.e. MAIN_PATH_INVERSION/ITERATION_STEP_PATH/PARFILE_ITERATION_STEP , are described.

These parameter files are created automatically by script py/create_ASKI_dir.py. Alternatively, you can look at the template file template/iter_parfile_template.

USE_PATH_SPECIFIC_MODELS

Set the flag to .true. if you intend to use the ASKI functionality of path specific kernel reference models (usually only for the very first iteration and a 1D method, as described in section 1.21 (page 48)). For a regular iteration, i.e. using one global kernel reference model (for all paths, i.e. kernels) set this flag to .false..

ITERATION_STEP_NUMBER_OF_FREQ, ITERATION_STEP_INDEX_OF_FREQ

Frequency discretization of this iteration step, must be a subset of global frequency discretization for this inversion defined as defined by 2.1.1.
ITERATION_STEP_NUMBER_OF_FREQ must be smaller or equal to MEASURED_DATA_NUMBER_OF_FREQ and vector
ITERATION_STEP_INDEX_OF_FREQ (of length ITERATION_STEP_NUMBER_OF_FREQ) must only contain indices contained in MEASURED_DATA_INDEX_OF_FREQ.
All indices here are assumed in accordance with the global frequency step MEASURED_DATA_FREQUENCY_STEP.

TYPE_INVERSION_GRID, PARFILE_INVERSION_GRID

Type of inversion grid (as supported, cf. 1.7) and corresponding filename of parameter file defining this inversion grid, relative to
MAIN_PATH_INVERSION/ITERATION_STEP_PATH/

TYPE_INTEGRATION_WEIGHTS

Type of integration weights (integer number), cf. 1.11 for supported values.

FILE_INTEGRATION_WEIGHTS

Filename of the integration weights file, which will be created and used, relative to MAIN_PATH_INVERSION.

FILE_WAVEFIELD_POINTS

Filename of the wavefield points file, relative to MAIN_PATH_INVERSION, which is in general created by the method you are using. Just refer here to this file.

FILE_KERNEL_REFERENCE_MODEL

Dependent on the method you are using, these filenames may be handled individually. Please refer to the respective documentation of the methods for recommendations how to use these parameters, or which naming to choose.

FILEBASE_BASIC_STATS

Base filename of vtk stats output files (related to inversion grid, wavefield points, integration weights, events, stations), relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH`.

PATH_OUTPUT_FILES

Folder relative to which some sensitivity analysis and inversion programs may write their output (relatively small output like models, coefficients etc., NO wavefields/kernels etc.!), relative to `MAIN_PATH_INVERSION/ITERATION_STEP_PATH`. Make sure the path ends on "/".

PATH_KERNEL_DISPLACEMENTS

Subdirectory of current iteration step path `MAIN_PATH_INVERSION/ITERATION_STEP_PATH` which contains the kernel displacement files. Make sure the path ends on "/".

PATH_KERNEL_GREEN_TENSORS

Subdirectory of current iteration step path `MAIN_PATH_INVERSION/ITERATION_STEP_PATH` which contains the kernel green tensor files. Make sure the path ends on "/".

PATH_SENSITIVITY_KERNELS

Subdirectory of current iteration step path `MAIN_PATH_INVERSION/ITERATION_STEP_PATH` which contains the velocity kernel files. Make sure the path ends on "/".

PATH_SYNTHETIC_DATA

Subdirectory of current iteration step path `MAIN_PATH_INVERSION/ITERATION_STEP_PATH` which contains the files with synthetic data. Make sure the path ends on "/".

PATH_KERNEL_REFERENCE_MODELS

This path and any contained files are only relevant for `USE_PATH_SPECIFIC_MODELS = .true.`! Subdirectory of current iteration step path `MAIN_PATH_INVERSION/ITERATION_STEP_PATH` in which path-specific kernel reference models are expected. The reference model files are assumed to have names like `krm_EVENTID_STATIONNAME`. Make sure the path ends on "/".

2.2 Event List File

Please find the template event list file `template/file_event_list_template`.

- first line contains single character “C” or “S”, defining the coordinate system (“C”artesian or “S”pherical) with respect to which the given event coordinates lat,lon are interpreted
- each following non-empty line of the file is interpreted as a definition of one event and must contain the following space-separated values:

eventid	13 character name, (e.g. `2006.10.2977` or `061113_141238`) should *not* contain whitespace!
origintime	characters of form `yyyymmdd_hhmmss_nnnnnnnnn` or `yyyymmdd_hhmmss` (i.e. with or without nano-seconds), e.g. `20130320_170012` or `20130320_170002_718000000`
lat	latitude in degrees, `-90 <= lat <= 90` (“S”) or first coordinate in wavefield points / inversion grid - frame (“C”) → read the section on inversion grid definitions (1.7)
lon	longitude in degrees, `0 <= lon <= 360` (“S”) or second coordinate in wavefield points / inversion grid -frame (“C”) (read 1.7)
depth	source depth in km (“S”), or third coordinate in wavefield points / inversion grid -frame (“C”) (read 1.7)
mag	factor on source mechanism
typ	source type: 0 = force, 1 = moment tensor, -1: not specified
mom/frce	either 3 values (force vector) or 6 values (moment tensor)

2.3 Station List File

Please find the template station list file `template/file_station_list_template`.

- first line contains single character “C” or “S”, defining the coordinate system (“C”artesian or “S”pherical) with respect to which the given event coordinates lat,lon are interpreted
- each following non-empty line of the file is interpreted as a definition of one station and must contain the following space-separated values:

station_name	5 character name, which should *neither* contain whitespace *nor* underscors “_”!
network_code	6 character network code
lat	latitude in degrees, `-90 <= lat <= 90` (“S”) or first coordinate in wavefield points / inversion grid - frame (“C”) → read the manual on inversion grid definitions (1.7)
lon	longitude in degrees, `0 <= lon <= 360` (“S”) or second coordinate in wavefield points / inversion grid -frame (“C”) (read 1.7)
elevation	altitude of station (“S”), or third coordinate in wavefield points / inversion grid - frame (“C”) (read 1.7)

2.4 Measured Data Files

All measured data files are expected to be located in the directory PATH_MEASURED_DATA as defined in the main parameter file.

One measured data file contains all data values for one specific station component and a specific event. Its filename is by convention data_EVENTID_STATIONNAME_COMP

The files are text files containing 1 column of MEASURED_DATA_NUMBER_OF_FREQ complex numbers, which can be understood by FORTRAN read command, i.e. of form (real_part , imag_part) .

Line i contains the measured data value for the i^{th} frequency, as defined by vector of indices MEASURED_DATA_INDEX_OF_FREQ and frequency step MEASURED_DATA_FREQUENCY_STEP.
In particular, this means that *all* measured data files must contain the *same* frequency discretization, given by parameters MEASURED_DATA_INDEX_OF_FREQ, MEASURED_DATA_FREQUENCY_STEP of the main parameter file.

2.5 Event (Station) Filter Files

All event (or station) filter files are expected to be located in the directory PATH_EVENT_FILTER (or PATH_STATION_FILTER), respectively. Both paths savely be set to the same directory.

A filter file contains all spectral filter values associated with a specific event (or station component). The file names are by convention filter_EVENTID (or filter_STATIONNAME_COMP), respectively.

In the same way as measured data files, the filter files are text files containing 1 column of MEASURED_DATA_NUMBER_OF_FREQ complex numbers, which can be understood by FORTRAN read command, i.e. of form (real_part , imag_part) .

Line i contains the filter value for the i^{th} frequency, as defined by vector of indices MEASURED_DATA_INDEX_OF_FREQ and frequency step MEASURED_DATA_FREQUENCY_STEP.
In particular, this means that *all* filter files must contain the *same* frequency discretization, given by parameters MEASURED_DATA_INDEX_OF_FREQ, MEASURED_DATA_FREQUENCY_STEP of the main parameter file.

2.6 Synthetic Data Files

All synthetic data files are expected to be in the directory PATH_SYNTHETIC_DATA as defined in the parameter file of the current iteration step.

One synthetic data file contains the complete synthetic data values for one specific combination of event, station and station component. Its filename is by convention synthetics_EVENTID_STATIONNAME_COMP

The files are text files containing 1 column of ITERATION_STEP_NUMBER_OF_FREQ complex numbers, which can be understood by FORTRAN read command, i.e. of form (real_part , imag_part) .

Line i contains the synthetic data value for the i^{th} frequency, as defined by vector of indices ITERATION_STEP_INDEX_OF_FREQ and frequency step MEASURED_DATA_FREQUENCY_STEP.

2.7 Vtk Files

For visualization of basic objects of the inversion, such as the inversion grid, the wavefield points, the integration weights etc., as well as some inversion results and models, ASKI uses vtk files in the old "legacy" format.

These files contain *both*, geometry information and data values on geometric objects. The format can be either ASCII or BINARY, controlled by flag DEFAULT_VTK_FILE_FORMAT in main parfile.
General information on the file format may be found under www.vtk.org/VTK/img/file-formats.pdf

ASKI uses separate software modules for writing vtk based on wavefield points, or inversion grids or event-station path lines (or event, station coordinates).

2.8 Data and Model Space File

Files in which a data and model space is defined have the following form. *It might be very instructive to also have a look at the provided example template files* template/data_model_space_info_template_*.

The blocks described in the subsections below should be put into a text file, one after another, in arbitrary order, i.e. it does not matter which block comes first (DATA SAMPLE or MODEL VALUES). It is also supported to provide only one of the blocks, if the other one is not required for some application.

There can be arbitrary commentary in front of a block, between blocks and after the blocks. However, any line starting with DATA SAMPLES or MODEL VALUES is interpreted as the starting line of the respective block. Inside the blocks, ther must not be unexpected lines!

2.8.1 Model Values Block

line: MODEL VALUES
this line defines that the model values block (definition of the model values) starts here.

line: INVERSION_GRID_CELLS value
where value is either ALL (all inversion grid cells are taken) or SPECIFIC (specific definition of set of invgrid cells following below)

line: PARAMETERS value
where value is either ALL (all inversion grid cells are taken) or SPECIFIC (specific definition of model parameters for each invgrid cell, following below. Only allowed if INVERSION_GRID_CELLS SPECIFIC).

If PARAMETERS ALL, line: nparam param_1 ... param_n
defines the parameters used for all inversion grid cells (assuming MODEL_PARAMETRIZATION defined in main parameter file).

If INVERSION_GRID_CELLS SPECIFIC, the following line must contain the number of cells ncell which should be taken, followed by ncell blocks of lines, each defining an inversion grid cell. In case of PARAMETERS ALL, these blocks consist of a single line line containing an inversion grid cell index. In case of PARAMETERS SPECIFIC, these blocks consist of two lines: one line containing an inversion grid cell index and an additional second line of the form
nparam param_1 ... param_n
defining the parameters to be used for this specific inversion grid cell (assuming MODEL_PARAMETRIZATION defined in main parameter file).

2.8.2 Data Samples Block

line DATA SAMPLES
this line defines that the data samples block starts (definition of data samples) here.

line of form: WEIGHTING value, where value is one of is one of NONE, BY_PATH, BY_FREQUENCY, BY_PATH_AND_FREQUENCY (by defining such weights, you might account for event clustering or huge differences in magnitudes of the events)
In case of NONE, all data weights are internally set to 1.0 (i.e. no actual weighting is performed). Values BY_PATH and BY_PATH_AND_FREQUENCY are only allowed in case of PATH SPECIFIC, in which case the pairs evid staname in a specific path definition (below) is expected to be followed by one number > 0.0 and ≤ 1.0 (the weight). The frequency dependent weighting values (in cases BY_FREQUENCY, BY_PATH_AND_FREQUENCY) are defined in a separate line following the lines of form nfreq ifreq_1 ... ifreq_n (for either case of FREQUENCIES ALL or FREQUENCIES SPECIFIC). This separate lines have themselves the form nfreq w_1 ... w_n defining nfreq weights in range > 0.0 and ≤ 1.0. In case BY_PATH_AND_FREQUENCY, both weights (for path and frequency) are *multiplied* for each data sample.

line of form: PATHS value, where value is either ALL (all paths for a given set of event and station indices are used), or SPECIFIC (a specific definition of paths as a series of event and station index pairs follows below)

If PATHS ALL, the next two lines are of form nev iev_1 ... iev_n and nstat istat_1 ... istat_n, defining the set of event and station indices, which form (by all combinations) the used paths.

line of form: COMPONENTS value, where value is either ALL (for all paths, the same components are used) or SPECIFIC (only allowed if PATHS SPECIFIC, for each path a specific set of components may be defined)

If COMPONENTS ALL, the next line is of form ncomp comp_1 ... comp_n defining the component indices for all paths.

line of form: FREQUENCIES value, where value is either ALL (for all paths, the same frequency indices are used) or SPECIFIC (only allowed if PATHS SPECIFIC, for each path a specific set of frequency indices may be defined)

If FREQUENCIES ALL, the next line is of form nfreq ifreq_1 ... ifreq_n defining the frequency indices for all paths.

line of form: IMRE value, where value is either ALL (for all paths, the same set of imaginary/real parts are used) or SPECIFIC (only allowed if PATHS SPECIFIC, for each path a specific set of imaginary/real parts may be defined)

If IMRE ALL, the next line is of form nimre imre_1 ... imre_n defining imaginary (i.e. imre_i = im) or real parts (imre_i = re) for all paths.

If PATHS SPECIFIC, the following line must contain the number npaths of paths which should be used, followed by npahts blocks of lines, each defining the path and the data samples for that path.
These blocks constist of at least one line containing the event /station index pair iev istat. For each keyword COMPONENTS, FREQUENCIES and IMRE – if SPECIFIC – one line is added to such a block of lines, in the same form as the line following keyword ALL (see above), defining the specific components, frequencies or set of imaginary/real parts for each of the specific paths.

2.9 ecartInversionGrid Files

2.9.1 Nodes Coordinates Files

These files contain a collection of points in space, given in Cartesian X-, Y-, Z-coordinates. They must be text files and have the following format.

The first line contains a single integer value, indicating the number of lines to come (i.e. the number of points).
Each following line contains 3 floating point numbers (separated by white space) defining Cartesian X-, Y-, Z-coordinates of a point.

2.9.2 Cell Connectivity Files

These files contain the definition of cells, based on points as defined in the nodes coordinates files. They must be text files and have the following format.

The first line contains a single integer value, indicating the number of lines to come (i.e. the number of cells).
Each following line contains n integer numbers (separated by white space, n = 4 in case of tet4-type cells, n = 8 in case of hex8-type cells), which define the control nodes of the cell and correspond to the point indices in the respective nodes coordinates file, whereby the lowest point index is 1, corresponding to the second line (first point) in the nodes coordinates file.

The order of the point indices in a line is assumed to correspond to the vtk cell conventions! In case one of the cell connectivity files not existing, or their first line containing value 0, no cells of the respective type will be created.

2.9.3 Cell Neighbours File

The terminology “lines” below refers to the case of this file not being binary, but a text file. In case of this file being binary, the file content is expected value by value as on the rows of the text file. It will be opened by FORTRAN code with attribute access='stream' (i.e. expecting the values as a simple byte stream) and expects integer values of kind=4.

The first line contains the total number of inversion grid cells ncell.
The next ncell lines (one for each cell in order of the cell index) are of the form:
nnb icell_1 ... icell_nnb

whereby `nnb` is the number of neighbours of the respective cell (must be `0` if no neighbours) followed by `nnb` cell indices `icell_1 ... icell_nnb`, defining the neighbour cells, if there are any neighbours.

2.10 GSHHS native binary shore line files

The files that are meant here, are GSHHG files containing shore line data in native binary format. The files can be downloaded e.g. via `https://www.ngdc.noaa.gov/mgg/shorelines/data/gshhg/latest/`, choosing the package probably named like `gshhg-bin-?.?.?.zip`, extracting the shore line files `gshhs_c.b`, `gshhs_l.b`, `gshhs_i.b`, `gshhs_h.b`, `gshhs_f.b`.

`ASKI` expects the files to contain 4-byte integers in big-endian. The file is written sequentially, information of one the shore line polygons one after another.

For each polygon, there is a header consisting of 11 4-byte signed integers. The first entry of the header is the polygon index (in consecutive numbering, starting from 0). The second entry of the header gives the number of points contained in the polygon (the point information follows after the header). All other header information are ignored by `ASKI`.

After reading a polygon header, `ASKI` reads the expected number of points for that polygon (as given by second entry of header). Each point is a pair of two 4-byte signed integers representing longitude and latitude (in that order) in the unit of micro-degrees.

This native binary format GSSHS shore line files is documented, e.g. at the end of file `https://www.ngdc.noaa.gov/mgg/shorelines/data/gshhg/latest/readme.txt`):

```
   struct GSHHG {  /* Global Self-consistent Hierarchical High-resolution Shorelines */
         int id;         /* Unique polygon id number, starting at 0 */
         int n;          /* Number of points in this polygon */
         int flag;       /* = level + version << 8 + greenwich << 16 + source << 24 + river << 25 */
         /* flag contains 5 items, as follows:
          * low byte:    level = flag & 255: Values: 1 land, 2 lake, 3 island_in_lake,
                                                     4 pond_in_island_in_lake
          * 2nd byte:    version = (flag >> 8) & 255: Values: Should be 12 for GSHHG release 12
                                                              (i.e., version 2.2)
          * 3rd byte:    greenwich = (flag >> 16) & 1: Values: Greenwich is 1 if Greenwich is crossed
          * 4th byte:    source = (flag >> 24) & 1: Values: 0 = CIA WDBII, 1 = WVS
          * 4th byte:    river = (flag >> 25) & 1: Values: 0 = not set, 1 = river-lake and level = 2
          */
         int west, east, south, north;   /* min/max extent in micro-degrees */
         int area;       /* Area of polygon in 1/10 km^2 */
         int area_full;  /* Area of original full-resolution polygon in 1/10 km^2 */
         int container;  /* Id of container polygon that encloses this polygon (-1 if none) */
         int ancestor;   /* Id of ancestor polygon in the full resolution set that was the source of
                                                                        this polygon (-1 if none) */
};

Following each header structure is n structures of coordinates:

struct GSHHG_POINT { /* Each lon, lat pair is stored in micro-degrees in 4-byte signed integer format */
 int32_t x;
 int32_t y;
};

Some useful information:

A) To avoid headaches the binary files were written to be big-endian.
   If you use the GMT supplement gshhg it will check for endian-ness and if needed will
   byte swab the data automatically. If not then you will need to deal with this yourself.

B) In addition to GSHHS we also distribute the files with political boundaries and
   river lines.  These derive from the WDBII data set.
```

C) As to the best of our knowledge, the GSHHG data are geodetic longitude, latitude
locations on the WGS-84 ellipsoid. This is certainly true of the WVS data (the coastlines).
Lakes, riverlakes (and river lines and political borders) came from the WDBII data set
which may have been on WGS072. The difference in ellipsoid is way less then the data
uncertainties. Offsets have been noted between GSHHG and modern GPS positions.

D) Originally, the gshhs_dp tool was used on the full resolution data to produce the lower
resolution versions. However, the Douglas-Peucker algorithm often produce polygons with
self-intersections as well as create segments that intersect other polygons. These problems
have been corrected in the GSHHG lower resolutions over the years. If you use gshhs_dp to
generate your own lower-resolution data set you should expect these problems.

E) The shapefiles release was made by formatting the GSHHG data using the extended GMT/GIS
metadata understood by OGR, then using ogr2ogr to build the shapefiles. Each resolution
is stored in its own subdirectory (e.g., f, h, i, l, c) and each level (1-4) appears in
its own shapefile. Thus, GSHHS_h_L3.shp contains islands in lakes for the high res
data. Because of GIS limitations some polygons that straddle the Dateline (including
Antarctica) have been split into two parts (east and west).

F) The netcdf-formatted coastlines distributed with GMT derives directly from GSHHG; however
the polygons have been broken into segments within tiles. These files are not meant
to be used by users other than via GMT tools (pscoast, grdlandmask, etc).

Chapter 3

Programs, Scripts and Modules

Important:
This chapter is *not* intended to be read through item by item (as a manual)! If you are new to `ASKI` and accidently looked up this chapter in the hope to find what you're looking for, you are strongly advised to quickly read section "How to get started" at the beginning of this document, explaining how to use this manual.

This chapter collects scripts, binary programs or modular program components contained in the `ASKI` package. It is not refered to any code, here, but give details on application by the user or background knowledge.

3.1 Executable Fortran Programs

The commands are executed in the form:

command [-options]...[positional arguments]

Commands with several positional arguments have to be executed with positional arguments in correct order (the order given in the subsections "Positional arguments").

In front of positional arguments, there can be options, for which the order is not relevant since they are indicated by some keyword starting with "-". The name "option" should, however, not be taken literally, since some of these arguments might be required and are therefore called "Mandatory options". Others, that are actually optional, are referred to as "Optional options" below.

Calling an executable without arguments will print a very short help message on how to use it.

3.1.1 `addSpikeCheckerToKim`

This is a hard-coded preliminary tool! Do not expect to see a help message when executing `addSpikeCheckerToKim` *without arguments, execution of the source code will start immediately!*

This excecutable adds checkerboard or spike-like anomalies to a given `.kim` model file. All specifcations about the current inversion grid and any filenames must be given in a *hard-coded*

way by modifying the source file `f90/addSpikeCheckerToKim.f90` accordingly. Some documenting commentary is given there.

This executable is intended to serve the experienced user and must be compiled separately by `make addSpikeCheckerToKim`

3.1.2 chunksInvgrid2Vtk

Create special `.vtk` file(s) of a `chunksInversiongrid`-type inversion grid. Use this executable complementary to `invgrid2vtk` → 3.1.17 (page 77), especially if the inversion grid has base cell refinement or multiple chunks.

Mandatory options

`-igpar invgrid_parfile` `invgrid_parfile` is `PARFILE_INVERSION_GRID` as in `ASKI` iteration step parameter file (assuming inversion grid type `chunksInversionGrid` here!).

`-igpath invgrid_path` `invgrid_path` is treated as current iteration step path, used for inversion grid to write/read own files.

Optional options

`-o outbase` `outbase` is output base name (default is `inversion_grid`)

`-base` If set, produce a `.vtk` file containing the inversion grid's base cells only; assigned cell data: base cell indices. In case of no base cell refinement: output is equal to `invgrid2vtk` output file (inversion grid consists of base cells only).

`-base_ichk` If set, produce a `.vtk` file containing the inversion grid's base cells only; assigned cell data: chunk indices. This is only interesting for multi-chunk inversion grids (otherwise: constant data equal to 1).

`-ichunk` If set, produce a `.vtk` file containing the inversion grid cells; assigned cell data: chunk indices. In case of no base cell refinement, output is equal to `-base_ichk`.

`-subs "ibc_1 ... ibc_n"` Given a vector of `n` base cell indices `ibc_1`,...,`ibc_n`, for each indicated base cell a `.vtk` file will be written containing the subcells of that base cell (with assigned data: cell indices). If a base cell is not refined, output file will contain base cell only. Output file extension will contain base cell index. *In the future*: may be helpful to also accept ranges like "20:40". Must not be set simultaneously along with `-all_subs`.

`-all_subs` Same as `-subs` but for *all* base cell indices. Must not be set simultaneously along with `-subs`.

-overwr If set, existing output files will be overwritten.

-bin If set, the output vtk files will be binary, otherwise they will be ascii.

-recr If set, the existing inversion grid file(s) (if any existing, and if type creates any) will be recreated with current invgrid parfile specifications. If not set (default), an existing inversion grid will be read in only, *without any effect of potential changes in the parfile!*

3.1.3 combineInvertedModels

Compute linear combination `coef1 * kim1 + coef2 * kim2` of two models on inversion grid `kim1`, `kim2`.

Positional arguments

kim1_file `.kim` file of the first model `kim1`.

kim2_file `.kim` file of the second model `kim2`.

kim_outfile Output file basename (will be extended by `.kim`) of resulting combined model.

main_parfile Main parameter file of inversion.

Optional options

-c1 coef1 If set, it defines the first coefficient `coef1` by which the first model is multiplied in the linear combination. If not set, the default value `coef1 = 1.0` is used.

-c2 coef2 If set, it defines the second coefficient `coef2` by which the second model is multiplied in the linear combination. If not set, the default value `coef2 = 1.0` is used.

-rel If set, the program computes relative to `kim1`, i.e.
`(coef1*kim1 + coef2*kim2) / kim1`

3.1.4 computeCorrectionSyntheticData

Computes additional files in iteration-step-specific subdirectory `SYNTHETIC_DATA` which are named as `corr_EVENTID_STATIONNAME_COMPONENT`. These files contain the quantities c_i^0 (as defined in our GJI paper eq. (26)), which are corrections to synthetic data due to change from path to global reference model.

Positional arguments

dmsi_file Data-model-space-info file

main_parfile Main parameter file of inversion.

3.1.5 computeDataFromKernelSystem

Computes the 'measured' data d in the equation d-s(-sc) = K (m1 - mref) for given model m1.

Can be used for (old-fashioned) linear computation of checkerboard data by forward multiplication of the sensitivity matrix with an artificial model vector containing checker anomalies.

Positional arguments

dmsi_file Data-model-space-info file

kim_file kernel-inverted-model file which contains model m1.

outdir_data Output directory where the new 'measured' data files are written to.

main_parfile Main parameter file of inversion.

3.1.6 computeFocussedMisfit

Compute focussed misfit of a dataset applying the focussing coefficients produced by executable `focusSpectralKernels`.

Positional arguments

dmspace_file Data model space input file which defines data and model space.

foc_coef_file Output text file containing the focussing coefficients, as written by program `focusSpectralKernels`

main_parfile Main parameter file of inversion.

3.1.7 computeKernelCoverage

Summate the absolute values of the column vectors of a given kernel matrix (for a given number `nwin` of frequency windows).

Positional arguments

`dmspace_file` Data-model-space-info file to set up the kernel linear system.

`vtk_outfile_base` Base name for output files (vtk output is produced on inversion grid only).

`main_parfile` Main parameter file of inversion.

Mandatory options

`-jf1` Vector of starting indices of `nwin` frequency windows. It must have the same length `nwin` as `-jf2` and `jf1 <= jf2` for all windows.

`-jf2` Vector of end indices of `nwin` frequency windows. It must have the same length `nwin` as `-jf1` and `jf1 <= jf2` for all windows.

Optional options

`-overwr` If set, the output files will be overwritten (if existing). By default, nothing is overwritten.

3.1.8 `computeKernels`

This executable computes (and pre-integrates) spectral sensitivity kernels. There are two possibele ways to define a set of spectral kernels that are computed:

(way 1): compute kernel for only one path, defined by eventID and station name using options `-evid`, `-staname`, `-comp` and `-param`

(way 2): use flag `-dmspsce` in connection with optional range definition of the path index (flags `-ipath1` `-ipath2`)
in order to define a subset of the paths contained in the given data-model-space description. If the upper (lower) limit of the path range is not defined (i.e. `-ipath1` (`-ipath2`) not set), the maximum (minimum) possible value is used. Then, all kernels for the defined range of paths in the given data-model-space description are computed.

Positional arguments

`main_parfile` Main parameter file of inversion.

Mandatory options

`-evid event_id` Defines the event id of the one path (must belong to an event in main event list). (way 1)

-staname station_name Defines the station name of the one path (must belong to a station in main station list). (way 1)

-comp "comp_1 ... comp_n" Vector of station components for which the kernel should be computed. For valid components see 1.4 (page 26). (way 1)

-param "param_1 ... param_n" Vector of parameter names for which the kernel should be computed. Only valid parameter names of the chosen model parametrization are accepted. (way 1)

-dmspace dmspace_file Data model space input file to define a set of paths. (way 2)

Optional options

-ipath1 path1 `path1` is the first index of the path loop. By default, `path1 = 1` (way 2)

-ipath2 path2 `path2` is the last index of the path loop. By default, `path2 = max_number_of_paths` as to data-model-space description. (way 2)

-wp If set, then plain kernel values on *wavefield points* are produced. Otherwise (if not set), pre-integrated kernels on inversion grid cells are computed

3.1.9 computeMisfit

Reads in measured and synthetic data characterized by data model space info file and computes the data misfit.

Positional arguments

dmspace_file Data model space info file which defines data and model space.

main_parfile Main parameter file of inversion.

Optional options

-jf "jf1..jfn" Vector of `nf` frequency indices. Additionally to the misfit of the whole dataset defined by `dmspace_file`, the misfit is computed for data subsets restricted to these individual frequencies.

3.1.10 createShoreLines

This application creates a `.vtk` file containing shore lines trimmed to the domain of the currently used inversion grid and transformed to the currently used `VTK_PROJECTION`.

Positional arguments

filename_GSHHS_bin Name of GSHHS file in native binary format, containing the shore line data. Such files can be downloaded via `https://www.ngdc.noaa.gov/mgg/shorelines/data/gshhg/latest/`. you should download the dataset in form of native binary files (probably package named like `gshhg-bin-?.?.?.zip`) and choose here a file of specific resolution e.g. `gshhs_c.b`, `gshhs_l.b`, `gshhs_i.b`, `gshhs_h.b`, `gshhs_f.b`. If you are interested in the file format of GSHHS native binary files, as expected by `ASKI`, see 2.10 (page 60).

outfile_base Absolute output file base (will be concatenated by "`.vtk`" for vtk output). *Existing output files will be overwritten!*

main_parfile Main parameter file of inversion.

3.1.11 createSpectralFilters

Generate spectral filter files as used in `ASKI` from source wavelets or as Butterworth high-/low-/bandpass filters (de)convolved by other wavelets or spectral filters.

The filter coefficients are computed in the frequency discretization of the "measured data" as defined in the main parameter file. The files are directly written to the designated paths specified in the main parameter file, having the correct filenames. This exectuable *ignores* the flags `APPLY_EVENT_FILTER, APPLY_STATION_FILTER` in the main parameter file!

In order for the executable to work, only the measured-data frequency discretiation, the filter paths and the filenames of event and station file are used from the main parameter file. All other entries need to have sensible values (for consistency checks), which however are not used. Furthermore, the station and event file need to be defined correctly. Any other (iteration-specific) information is not required by the executable.

In case a forward method (such as e.g. Gemini) in general uses complex frequencies with an imaginary part > 0, the complex filter values as well must be computed at these complex frequencies. This executable automatically takes care of that dependent on which forward method is set by keyword `FORWARD_METHOD` in the main parameter file. Only the main parameter file is used by this executable and must be set correctly, the iteration step specific parameter file is not used by this executable.

Option `stationf` is not yet supported by this executable. "station filters" somehow relate to instrument responses, which so far are assumed to be already deconvolved from the data before inverting it by `ASKI`. Setting the station filters to the respective (inverse) instrument responses, one could invert raw data by `ASKI`.

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

`-eventf event_filter_parfile` By setting option `-eventf`, event filters are generated. Argument `event_filter_parfile` is the filename of a parameter file as provided by `template/createSpectralFilters_parfile_event-filter_template` . The content of this parameter file is described below. At least one of options `-eventf`, `-stationf` must be set; they can both be set at the same time.

`-stationf station_filter_parfile` *This option is not yet supported and cannot actually be used!*
Once implemented, by setting option `-stationf` station filters can be generated. Argument `station_filter_parfile` will be the filename of a parameter file as provided by `template/createSpectralFilters_parfile_eventstation-filter_template` . The content of this parameter file will be described below. At least one of options `-eventf`, `-stationf` must be set; they can both be set at the same time.

The parameter file for option `-eventf`

In the following, the required keywords of the parameter file for option `-eventf` are described (documenting commentary is also contained in the template parfile `template/createSpectralFilters_parfile_event-filter_template`).

`CREATE_FILTERS_BY_SOURCE_WAVELET, CREATE_FILTERS_BY_SPECTRAL_BUTTERWORTH`
These logical flags decide if the event filters should be created by a source wavelet (defined by other keywords below), or by a spectral butterworth low-/high-/bandpass filter (defined by other keywords below). *Exactly* one of these two flags must be `.true.`, the other must be `.false.`

`NUMBER_OF_EVENTS, EVENT_IDS`
Define those event ID's for which an event filter file should be generated (filter will be the *same* for all events, if you need different filters for different events, you need to re-run this executable appropriately). There are two valid formats of the value of keyworkd `EVENT_IDS`:

`EVENT_IDS = ALL` (all event ID's will be used and the value of `NUMBER_OF_EVENTS` is ignored)

`EVENT_IDS = source01 source02 source204` (white-space-separated vector of valid event ID's, `NUMBER_OF_EVENTS` gives the number of values in the vector)

`CONVOLVE_WITH_OTHER_WAVELET, MULTIPLY_BY_OTHER_SPECTRAL_FILTER`
Decide whether the resulting spectral event filters should be *convolved* by some other wavelet of multiplied by some other spectral filter (defined below by other keywords). This functionality is sensible to use, e.g. if you want to create a butterworth filter which should be convolved with some finite source moment-rate function. Note, that the resulting event filters should describe the *source* contribution to the filter that brings the synthetic displacement wavefield to the measured data. Hence, the functionality of `CONVOLVE_WITH_OTHER_WAVELET` or `MULTIPLY_BY_OTHER_SPECTRAL_FILTER` should *not* be used to deconvolve the Gaussian that was used to generate synthetics in some iteration step, since the resulting event filters are not intended to be modified throughout an inversion. However, if you know what you're do-

ing, you are (of course) welcome to "abuse" this functionality for your own purposes. The logical flags CONVOLVE_WITH_OTHER_WAVELET and MULTIPLY_BY_OTHER_SPECTRAL_FILTER can both be .true. (in that case accounting for both contributions).

STF_FILE, STF_COLUMN_OF_TRACE, STF_DT, STF_NSTEP
Define by STF_FILE the *absolute* filename of the source time function text file which should be used to generate the filters in case of CREATE_FILTERS_BY_SOURCE_WAVELET = .true. . The integer value STF_COLUMN_OF_TRACE defines the column of the file that is used as the wavelet trace. For instance, if the file contains the time as first column and amplitude values as second column, set STF_COLUMN_OF_TRACE = 2 . If only one column with amplitude values is contained in the files, set STF_COLUMN_OF_TRACE = 1, etc. All other columns are ignored! STF_DT and STF_NSTEP define the time discretization by which the selected column will be interpreted. The first sample is interpreted to have time 0.0 . This should not pose a problem, since program transformMeasuredData makes the very same assumption and all forward methods should produce their spectral synthetics in the same way (as displacement wavefields w.r.t. a Dirac impuls at time 0.0 and with the Fourier transform starting with the first time-sample at time 0.0).

BTW_LOW_PASS_APPLY, BTW_LOW_PASS_ORDER, BTW_LOW_PASS_FC
Decide whether a low-pass butterworth filter should be applied (logical BTW_LOW_PASS_APPLY) and define order (integer BTW_LOW_PASS_ORDER) and corner frequency (real BTW_LOW_PASS_FC). If BTW_LOW_PASS_APPLY = .false., then any values given for BTW_LOW_PASS_ORDER and BTW_LOW_PASS_FC are ignored.

If you want to define a Butterworth band-pass filter, please define *both*, a suitable low-pass *and* a suitable high-pass filter. If above CREATE_FILTERS_BY_SPECTRAL_BUTTERWORTH = .true. , at least one of BTW_LOW_PASS_APPLY or BTW_HIGH_PASS_APPLY must be set to .true.

BTW_HIGH_PASS_APPLY, BTW_HIGH_PASS_ORDER, BTW_HIGH_PASS_FC
Decide whether a high-pass butterworth filter should be applied (logical BTW_HIGH_PASS_APPLY) and define order (integer BTW_HIGH_PASS_ORDER) and corner frequency (real BTW_HIGH_PASS_FC). If BTW_HIGH_PASS_APPLY = .false., then any values given for BTW_HIGH_PASS_ORDER and BTW_HIGH_PASS_FC are ignored.

If you want to define a Butterworth band-pass filter, please define *both*, a suitable low-pass *and* a suitable high-pass filter. If above CREATE_FILTERS_BY_SPECTRAL_BUTTERWORTH = .true. , at least one of BTW_LOW_PASS_APPLY or BTW_HIGH_PASS_APPLY must be set to .true.

CONV_WAVEL_FILE, CONV_WAVEL_COLUMN_OF_TRACE, CONV_WAVEL_DT, CONV_WAVEL_NSTEP
Define by CONV_WAVEL_FILE the *absolute* filename of the wavelet text file which should be used for convolution in case of CONVOLVE_WITH_OTHER_WAVELET = .true. . The integer value CONV_WAVEL_COLUMN_OF_TRACE defines the column of the file that is used as the wavelet trace. For instance, if the file contains the time as first column and amplitude values as second column, set CONV_WAVEL__COLUMN_OF_TRACE = 2 . If only one column with amplitude values is contained in the files, set CONV_WAVEL__COLUMN_OF_TRACE = 1, etc. All other columns are ignored! CONV_WAVEL_DT and CONV_WAVEL_NSTEP define the time discretization by which the selected column will be interpreted. The first sample is interpreted to have time 0.0 . This should not pose a problem, since executable transformMeasuredData makes the very same assumption and all forward methods should produce their spectral synthetics in the same way (as displacement wavefields w.r.t. a Dirac impuls at time 0.0 and with the Fourier transform starting with the first time-sample at time 0.0).

DECONVOLVE_WAVEL_INSTEAD
Logical flag DECONVOLVE_WAVEL_INSTEAD controls whether instead of *con*volving with the wavelet, it should be *de*convolved.

CONV_SPEC_FILE
CONV_SPEC_FILE gives the *absolute* file name of a text file in the format of a filter file, containing the spectral filter which is in the end to be multiplied onto the event filters. The file must contain MEASURED_DATA_NUMBER_OF_FREQ many rows, each of which corresponds to the frequency as defined by MEASURED_DATA_INDEX_OF_FREQ and MEASURED_DATA_FREQUENCY_STEP (in the ASKI main parameter file) and on each row a complex value must define the filter coefficient as understood by Fortran, i.e. in the format:
`( real_part , imag_part )`

DECONVOLVE_SPEC_INSTEAD
Logical flag DECONVOLVE_SPEC_INSTEAD controls whether instead of multiplying with the spectrum (i.e. convolving with the filter), it should be *divided* by it (i.e. *de*convolvolving the filter)

The parameter file for option `-stationf`

Option stationf is not yet supported by this executable.

3.1.12 createStartmodelKim

Create a file of type kernel_inverted_model (.kim) containing pre-defined values on the inversion grid. Can be used to create a start model for the full waveform inversion process.

Mandatory options

-igtype invgrid_type invgrid_type is TYPE_INVERSION_GRID as in ASKI iteration step parameter file.

-igpar invgrid_parfile invgrid_parfile is PARFILE_INVERSION_GRID as in ASKI iteration step parameter file.

-igpath invgrid_path invgrid_path is treated as current iteration step path, used for inversion grid to write/read own files.

-mpmtrz model_pmtr model_pmtrz is the model parametrization of the model which is to be created (must be consistent with content of model_file, see -mfile).

-mtype model_type model_type is a string defining the type of model_file and the interpolation type:
'1D_linear':
linear interpolation of values between coordinates given in 1D model file.
'3D _structured':
trilinear interpolation of values between coordinates given in 3D structured model file.

1D model file must have the following format

line 1: `nval ncol`

`nval` = number of model values /interpolation coordinates to come

`ncol` = number of columns to read from file, `ncol=1+N`, where `N` is number of parameters

line 2: `icoord param1 ... paramN`

`icoord` = index of inversion grid / wavefield point coordinate for which the interpolation should be applied (either 1,2 or 3)

`param1 ... paramN` = N parameter names associated with the values in the columns below

lines 3 ...`nval`+2: `coord val1 ... valN`

these following `nval` lines contain the interpolation coordinate and N model values for the respective parameters, as defined by line 2. The values '`coord`' are assumed to be be strictly monotonical(!) and can be either increasing or decreasing. You may choose this monotonicity at your will dependent on the coordinate for which the interpolation should be done (which, dependent on your inversion grid type may be depth or positive z-value...)

3D model file must have the following format:

line 1: `nx ny nz`

`nx`, `ny` and `nz` are the number of model points in X-, Y- and Z-direction

line 2: `minX minY minZ`

`minX, minY` and `minZ` are the smallest coordinates in the model

line 3: `maxX maxY maxZ`

`maxX, maxY` and `maxZ` are the highest coordinates in the mode

`nval`, the total number of vaules in the model is given by `nval = nx*ny*nz`

line 4: `param1 ... paramN`

`param1 ... paramN`, N parameter names associated with the values in the columns below

line 5+: `nval` model values

The model values have to be sorted like:

```
DO i=minX,maxX+1
    DO j=minY,maxY+1
        DO k=minZ,maxZ+1
            READ model value
```

END DO

END DO

END DO

-mfile model_file `model_file` is the model input file of type defined by `model_type`.

Optional options

-o outbase `outbase` is output base name (default is `start_model`).

-bin If set, the output vtk files will be binary, otherwise they will be ascii.

3.1.13 exportKim

Program exportKim produces a text file (option `-otxt`) containing information of cell centers and radii (radius $\simeq$ some approximate average spatial expansion of the cell from the cell center) of all inversion grid cells and all cell neighbours, as well as model values and respective invgrid cell indices for each model parameter, as contained in a given kernelInvertedModel file. This text file may be used by any forward method to define the simulation model for the next iteration step, or by any tool handling final models.
The format of the produced text file is as follows:
The first 3 lines contain:

```
model_parametrization
number_of_parameters name_param_1 ... name_param_n
number_of_invgrid_cells
```

The next `number_of_invgrid_cells` lines contain for each inversion grid cell:

```
c1 c2 c3 r nnb inb1 ... inbn
```

where `c1,c2,c3` are the 3 coordinates of the cell center (in wavefield point coords), `r` is the cell radius (i.e. rough expansion of cell), `nnb` is the number of cell neighbours and `inb1,...,inbn` are their nnb cell indices (if `nnb>0`, otherwise line ends on `nnb=0`). Then `number_of_parameters` blocks are following in the file, each having the following format:

```
name_param
nval
cell_indx
model_values
```

where `name_param` is the name of the parameter to which the following model values belong, `nval` is the number of model values following, `cell_indx` is a vector of `nval` cell indices to which the model values belong (space separated on one line) and `model_values` is an vector of the actual `nval` model values (space separated on one line).

Additionally (or alternatively) the program converts the .kim file to vtk files (option `-ovtk`).
The two options `-otxt` , `-ovtk` can be used independently of each other.

Positional arguments

`main_parfile` Main parameter file of inversion.

Mandatory options

`-kim kernel_inverted_mode_file` `kernel_inverted_mode_file` is the binary file containing the inverted model, which is to be exported.

`-otxt outfile_txt` `outfile_txt` is the text output file to which inversion grid and model information will be written. At least one of `-otxt`, `-ovtk` must be set.

`-ovtk outfile_vtk` `outfile_vtk` is the output file base to which standard vtk files of the .kim file will be written. At least one of `-otxt`, `-ovtk` must be set.

3.1.14 `focusSpectralKernels`

Compute Backus-Gilbert focussing of sensitivity kernels on a defined focussing region in the model space.

The concept of this kernel focussing is published in [Sch14], Chapter 7.1.

It might get problematic in spherical settings to use focussing regions (refined by mandatory options `c1min`, `c1max`, `c2min`, ...) which overlap the zero meridian or include the poles. Furthermore, a region defined by minimum/maximum of latitude/longitude/depth (or Cartesian X/Y/Z) might not meet your requirements. In this respect, this executable could be improved, since basically any subset of the model space can be focussed on.

Positional arguments

`dmspace_file` Data model space indo file which defines the rows and columns of the kernel matrix.

`outfile_base` Base name of output files *relative* to iteration step output directory (used for all files, with suitable extensions).

`main_parfile` Main parameter file of inversion.

Mandatory options

`-c1min c1min_value` Minimum first coordinate of focussing subvolume. In case of a Cartesian inversion grid, "first coordinate" means Cartesian X, in case of spherical inversion grids it means latitude in degrees (value between -90 and 90).

`-c1max c1max_value` Maximum first coordinate of focussing subvolume. In case of a Cartesian inversion grid, "first coordinate" means Cartesian X, in case of spherical inversion grids it means latitude in degrees (value between -90 and 90).

`-c2min c2min_value` Minimum second coordinate of focussing subvolume. In case of a Cartesian inversion grid, "second coordinate" means Cartesian Y, in case of spherical inversion grids it means longitude in degrees (value between 0 and 360).

`-c2max c2max_value` Maximum second coordinate of focussing subvolume. In case of a Cartesian inversion grid, "second coordinate" means Cartesian Y, in case of spherical inversion grids it means longitude in degrees (value between 0 and 360).

`-c3min c3min_value` Minimum third coordinate of focussing subvolume. In case of a Cartesian inversion grid, "third coordinate" means Cartesian Z, in case of spherical inversion grids it means depth in km.

`-c3max c3max_value` Maximum third coordinate of focussing subvolume. In case of a Cartesian inversion grid, "third coordinate" means Cartesian Z, in case of spherical inversion grids it means depth in km.

`-param "param_1 ... param_n"` List of model parameters which will be focussed on, e.g. `"vp vs"` .

3.1.15 `initBasics`

Initiating and testing all basic requirements for ASKI programs (parameter files, event and station list, inversion grid, wavefield points, integration weights, reference model).

Positional arguments

`main_parfile` Main parameter file of inversion.

Optional options

`-recr` If set, existing files will be recreated with current parfile specifications (overwrites existing files will be read in and not newly created). Affected files are:

- `inversion_grid` and `integration_weigts` and all related `.vtk` files (including `wavefield_points.vtk` files)

- `stations.vtk`, `events.vtk`

- kernel reference model files (on wavefield points, and as interpolation on inversion grid)

IF NOT SET (default), EXISTING FILES (especially `inversion_grid`, `integration_weights`) WILL BE READ IN ONLY, POSSIBLY WITHOUT ANY EFFECT OF POTENTIAL CHANGES IN PARFILES! So, if you change the specification of inversion grid, or integration weights (or stations, events which is only relevant for `station.vtk` `events.vtk`), after having already created the respective files, you should set `-recr`.

3.1.16 `investigateDataResiduals`

Gets some statistics about the data residuals of a given data (sub)set.

Positional arguments

`dmsi_file` Data-model-space-info file

`outdir_stats_files` Output directory where residual files per path and component will written.

`main_parfile` Main parameter file of inversion.

Optional options

`-ovtk outfile_vtk` `outfile_vtk` of output vtk files. If not set, no vtk files will be produced. (Default = dataset)

3.1.17 `invgrid2vtk`

Create vtk file(s) of the given inversion grid (useful to look at, to see if the specifications are correct).

Mandatory options

`-igtype invgrid_type` `invgrid_type` is `TYPE_INVERSION_GRID` as in `ASKI` iteration step parameter file.

`-igpar invgrid_parfile` `invgrid_parfile` is `PARFILE_INVERSION_GRID` as in `ASKI` iteration step parameter file.

`-igpath invgrid_path` `invgrid_path` is treated as current iteration step path, used for inversion grid to write/read own files.

Optional options

-o outbase `outbase` is output base name (default is `inversion_grid`)

-overwr If set, existing output files will be overwritten.

-nb "idx_1 ... idx_n" Vector of `n` cell indices, indicating a set of cells the neighbours of which will be written as vtk files. IN THE FUTURE: may be helpful to also accept ranges like "20:40". Must not be set simultaneously along with `-all_nb`.

-all_nb Indicating to use all cell indices to write neighbours for. Must not be set simultaneously along with `-nb`.

-bin If set, the output vtk files will be binary, otherwise they will be ascii.

-recr If set, the existing inversion grid file(s) (if any existing, and if type creates any) will be recreated with current invgrid parfile specifications. If not set (default), existing inversion grid will be read in only, *possibly without any effect of potential changes in the parfile!*

3.1.18 kdispl2vtk

Extract kernel displacement spectra to vtk files for certain wavefield and strain components and frequencies.

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

-evid event_id Defines the event ID of the kernel displacement object (must belong to an event in main event list).

-ifreq "idx_1 ... idx_n" Vector of `n` frequency indices at which the wavefield output is extracted and vtk files are generated. Exactly one of options `-ifreq` , `-all_ifreq` must be set.

-all_ifreq If set, for all frequency indices of the current iteration wavefield output is extracted and vtk files are generated. Exactly one of options `-ifreq` , `-all_ifreq` must be set.

-ucomp "comp_1 ... comp_n" Vector of n wavefield components for which the wavefield output is extracted and vtk files are generated. Wavefield components are denoted by ux, uy, uz (meaning underived x, y, z components of the wavefield) and exx, eyy, ezz, eyz, exz, exy (meaning strain components). Exactly one of options -ucomp, -all_ucomp must be set.

-all_ucomp If set, for all underived wavefield components ux, uy, uz and strains exx, eyy, ezz, eyz, exz, exy wavefield output is extracted and vtk files are generated. Exactly one of options -ucomp, -all_ucomp must be set.

3.1.19 kernel2vtk

Program kernel2vtk writes the pre-integrated spectral sensitivity kernels as vtk files for specific paths, parameters, components and frequencies.

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

-evid event_id Defines the event id of the one path. (must belong to an event in main event list)

-staname station_name Defines the station name of the one path. (must belong to a station in main station list)

-comp "comp_1 ... comp_n" Vector of station components for which vtk files should be generated. For valid components see 1.4 (page 26).

-param "param_1 ... param_n" Vector of parameter names for which vtk files should be generated. Only valid parameter names of the chosen model parametrization are accepted.

-ifreq "idx_1 ... idx_n" Vector of n frequency indices for which vtk files should be generated. Exactly one of options -ifreq , -all_ifreq must be set.

-all_ifreq If set, for all frequency indices of current iteration vtk files will be generated. Must not be set simultaneously along with -ifreq. Exactly one of options -ifreq , -all_ifreq must be set.

Optional options

-wp If set, then the original kernels on the wavefield points are produced (recalculated!) INSTEAD of the pre-integrated ones on the inversion grid.

3.1.20 kgt2vtk

Extract kernel green tensor spectra to vtk files for certain wavefield and strain components and frequencies.

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

-staname station_name Defines the station name of the kernel green tensor object (must belong to a station in main station list).

-scomp "scomp_1 ... scomp_n" Vector of `n` station components of station `station_name` for which wavefield output is extracted and vtk files are generated. For valid components see 1.4 (page 26).

-ifreq "idx_1 ... idx_n" Vector of `n` frequency indices at which the wavefield output is extracted and vtk files are generated. Exactly one of options `-ifreq`, `-all_ifreq` must be set.

-all_ifreq If set, for all frequency indices of the current iteration wavefield output is extracted and vtk files are generated. Exactly one of options `-ifreq`, `-all_ifreq` must be set.

-ucomp "comp_1 ... comp_n" Vector of `n` wavefield components for which the wavefield output is extracted and vtk files are generated. Wavefield components are denoted by `ux`, `uy`, `uz` (meaning underived `x`, `y`, `z` components of the wavefield) and `exx`, `eyy`, `ezz`, `eyz`, `exz`, `exy` (meaning strain components). Exactly one of options `-ucomp`, `-all_ucomp` must be set.

-all_ucomp If set, for all underived wavefield components `ux`, `uy`, `uz` and strains `exx`, `eyy`, `ezz`, `eyz`, `exz`, `exy` wavefield output is extracted and vtk files are generated. Exactly one of options `-ucomp`, `-all_ucomp` must be set.

3.1.21 krm2kim

Interpolate kernel reference model onto inversion grid and produce a `.kim` file of it.

Positional arguments

`outfile_base` Basename of output model files – will additionally be written as vtk.

`main_parfile` Main parameter file of inversion.

Optional options

`-krm kernel_reference_mode_file` If set, then instead of using the kernel reference model file defined by the iteration step parfile, the given file `kernel_reference_mode_file` is used to read in the kernel reference model.

3.1.22 `paths2vtk`

Plots all paths contained in the data space definition as vtk lines.

Positional arguments

`dmsi_file` Data-model-space-info file

`outfile` Output file (basename) of the vtk file(s).

`main_parfile` Main parameter file of inversion.

3.1.23 `solveCglsKernelSystem`

Solves linear system of sensitivity kernel equations in parallel by a conjugate-gradient method. The algorithm applied here is the ”CGLS1” from paper [BES98].

By default, the conjugate-gradient algorithm uses single precision. In case the program crashes due to what looks like precision problems (dividing by 0, getting values “NaN” etc.), you may try to switch to double precision (change the respective line in the very beginning of code file `f90/solveCglsKernelSystem.f90` and recompile `solveCglsKernelSystem`).

This executable is parallelized using `MPI`. Hence, it should be called like
`mpirun -np 8 solveCglsKernelSystem` (with respective arguments)
The executable uses the maximum number of parallel slots being available in the `MPI` environment, in the above example this would be 8.

There is a mechanism implemented that allows you to terminate the algorithm at any time without just killing the process, but with the current solution of the CG algorithm actually being written out as if the termination criteria of the alorithm were met. This can be useful, e.g. if you notice that the algorithm actually has converged, but the termination criteria were defined in an unsuitable way, or if the convergence is very slow and you want to continue the process later by restarting the executable with passing the intermediate solution to option `-startsol`. This kind of save termination of the algorithm is executed if the existence of a file with filename `outfile_base_TERMINATE.txt` is detected. So you can manually create a file with this

name, i.e. output file base as defined by positional argument `outfile_base`, plus extension `_TERMINATE.txt` (case sensitive). This file can be empty, e.g. use command `touch` to create it.

If there is an error that some values become `NaN` , you should try to use double precision variables for vectors and scalars in the CG algorithm. This might be helpful if the kernel matrix contains values which are so low that certain summations become not representable in single prercision. In order to use double precision, you need to set
`CUSTOM_REAL = SIZE_DOUBLE`
at the very beginning of the declarations in source file `solveCglsKernelSystem.f90` . In this case, more memory will be required. For single precision, use `SIZE_REAL` there instead (default setting).

Positional arguments

`dmsi_file` Data-model-space-info file which defines data and model space.

`outfile_base` Base name of output files (will be used for all files, with suitable extensions) – output model will additionally be written as vtk.

`CG_parfile` Parameter file defining details related to the conjugate gradient algorithm used to solve the linear system. A description of its content can be found at the end of this subsection and a template is provided:
`template/solveCglsKernelSystem_parfile_template`

`main_parfile` Main parameter file of inversion.

Optional options

`-regscal type_regul_scaling` `type_regul_scaling` is the type of scaling of regularization constraints, at the moment only `absmax_per_param`, `overall_factor`, `absmax_per_param`, `param_factors` and `none` are supported. Option `-regscal` can only be requested when adding damping or smoothing conditions by options `-smooth` or `-damp`.

`-smoothing scaling_values` If set, smoothing conditions are applied. `scaling_values` is a vector of scaling values consistent with `-regscal`:
`absmax_per_param`, `overall_factor`: one single factor
`absmax_per_param`, `param_factors`: one factor per parameter name of current parametrization (in conventional order)
`none` : values given here are ignored

`-smoothbnd type_smoothing_boundary` `type_smoothing_boundary` defines the way (non-existing) neighbours are treated in smoothing conditions at outer/inner boundaries of the inversion grid. Supported types:
`zero_all_outer_bnd`: apply zero smoothing conditions at *all* outer boundaries.
`zero_burried_outer_bnd`, `cont_free_surface`: apply zero smoothing conditions

at all outer boundaries *except* on free surfaces.
If not set, standard average is used everywhere (equivalent to continuity boundary conditions).
Option `-smoothbnd` is only allowed to be set, if option `-smoothing` was set.

`-damping scaling_values` If set, damping conditions are applied. `scaling_values` is a vector of scaling values consistent with `-regscal`:
`absmax_per_param,overall_factor`: one single factor
`absmax_per_param,param_factors`: one factor per parameter name of current parametrization (in conventional order)
`none` : values given here are ignored

`-odir` If set, `outfile_base` will be assumed relatively to iteration step output files directory.

`-startsol file_name_starting_solution` The `.kim` file `file_name_starting_solution` defines the starting solution of linear system.

`-normalize type_data_normalization` *For now, this feature is only supported if your dataset contains only a single station component (e.g. only vertical "UP" components for all event-station paths)!*
If set, each equation of the linear system is scaled by a specific factor and thus normalized in a certain sense. `type_data_normalization` defines the type of normalization. *This functionality has not yet been applied in field studies, but don't hesitated to experiment.*
Supported types and their descriptions:
`maxamp_mdata_by_paths`: Separately for each event-station path, find the datum of maximum amplitude, say datum `i_max`. All measured data of this path are then divided through by this amplitude, hence, normalized w.r.t. this amplitude. All synthetic data and all kernel value of this path are divided through by the amplitude of the synthetic datum `i_max`, i.e. the synthetic data and kernel values are scaled w.r.t. the synthetics amplitude at `i_max`, which does not necessarily represents the synthetics maximum amplitude of the path!
`maxamp_mdata_by_paths_and_frequency`: Separately for each event-station path and each frequency, the measured data is divided through by its amplitude and the synthetic data and the kernels are divided through by the amplitude of the synthetic data.
`scale_maxamp_mdata_by_paths`: Separately for each event-station path, the measured data, the synthetic data and the kernels are divided through by the maximum amplitude of the measured data. Hence, for this type of normalization, all scaling factors (for measured data, synthetic data and kernels) are the same, normalizing w.r.t. the maximum amplitude of the measured data.

The parameter file `CG_parfile` (third positional argument)

In the following, the required keywords of the parameter file given as third positional argument is described (documenting commentary is also contained in the template parfile `template/solveCglsKernelSystem_parfile_template`).

`MAX_NUM_CG_ITERATIONS`
This integer gives the upper limit of number of iterations (CG algorithm will stop then, even if convergence criterion is not yet met). This mechanism cannot be switched off! So, set to

a ridiculously high value if you don't want to use it. The maximum possible value that can be used is approx. 2 147 483 647 (4 byte signed integer) If you require more iterations, you should modify the source code. Alternatively, you need to continue the algorithm by passing the solution to option `-startsol`, as described above.

`NITER_WINDOW_STA,NITER_WINDOW_LTA`
These two integers define window sizes of short-term average (`sta`) and long-term average (`lta`) of the residual norm of the linear system, which are used to evaluate a termination criterion of the conjugate-gradient algorithm. The algorithm assumes a monotonically decreasing residual norm, i.e. `sta < lta`. It terminates when `sta`/`lta` equals 1 (in terms of single precision), i.e. when `sta` becomes close enough to `lta`, or when `lta` is not monotonically decreasing anymore, i.e. starts to increase. The numbers `NITER_WINDOW_STA, NITER_WINDOW_LTA` define the number of iterations over which the averrages are computed. Which values are sensible actually depends on the linear system. The termination checks based on `sta`, `lta` cannot be taken into account before iteration `NITER_WINDOW_LTA + 1`. It is required to define
`NITER_WINDOW_STA < NITER_WINDOW_LTA`. A ratio of
`NITER_WINDOW_LTA/NITER_WINDOW_STA = 10` was experienced to be feasible. E.g. define `NITER_WINDOW_STA = 20` and `NITER_WINDOW_LTA = 200`.

`USE_BLAS_LEVEL_1,USE_BLAS_LEVEL_2`
Logicals indicating whether to use BLAS Level 1 and Level 2 routines for vector and matrix-vector operations in the course of the CG algorithm. If `.false.`, intrinsic Fortran functionality will be used for those kinds of operations (e.g. `matmul` and explicit summation etc.), which for small problems might be more efficient than using BLAS. For large problems, at least BLAS Level 2 routines are recommended, i.e. `USE_BLAS_LEVEL_2 = .true.`. You might aswell test the performance of your particular application by profiling runs with and without these flages switched on.

`NITER_RECOMPUTE_RESIDUAL`
This feature seems not to work, hence it is disabled in the code so that the value of `NITER_RECOMPUTE_RESIDUAL` *does not have any effect at al!* If you want to use it anyway, you need to enable it in the source code. It should be easy to find for you. If you cannot find it easily, it is probably best for you not to use it (no offense). Description of the parameter (if enabled):
`NITER_RECOMPUTE_RESIDUAL` gives the number of iterations after which (circularly repeating) a true residual vector should be computed from the current solution of the system, instead of only updating it (i.e. approximating it) as defined by the original algorithm by [BES98]. If *no* recomputation should be done (i.e. original algorithm), set `NITER_RECOMPUTE_RESIDUAL` to some value ≤ 0.

3.1.24 `solveKernelSystem`

Do inversion step by solving the kernel linear system defined by data model space info and regularization constraints. This program is executed in a serial way using the LAPACK library.

Positional arguments

`dmspace_file` Data-model-space-info file which defines data and model space.

outfile Basename of output model files (will be used for all files, with suitable extensions) – output model will additionally be written as vtk.

main_parfile Main parameter file of inversion.

Optional options

-regscal type_regul_scaling `type_regul_scaling` is the type of scaling of regularization constraints, at the moment only `absmax_per_param`, `overall_factor`, `absmax_per_param`, `param_factors` and `none` are supported Option `-regscal` can only be requested when adding damping or smoothing conditions by options `-smooth` or `-damp`.

-smoothing scaling_values If set, smoothing conditions are applied. `scaling_values` is a vector of scaling values consistent with `-regscal`:
`absmax_per_param`, `overall_factor`: one single factor
`absmax_per_param`, `param_factors`: one factor per parameter name of current parametrization (in conventional order)
`none` : values given here are ignored

-smoothbnd type_smoothing_boundary `type_smoothing_boundary` defines the way (non-existing) neighbours are treated in smoothing conditions at outer/inner boundaries of the inversion grid. Supported types:
`zero_all_outer_bnd`: apply zero smoothing conditions at *all* outer boundaries.
`zero_burried_outer_bnd`, `cont_free_surface`: apply zero smoothing conditions at all outer boundaries *except* on free surfaces.
If not set, standard average is used everywhere (equivalent to continuity boundary conditions). Option `-smoothbnd` is only allowed to be set, if option `-smoothing` was set.

-damping scaling_values If set, damping conditions are applied. `scaling_values` is a vector of scaling values consistent with `-regscal`:
`absmax_per_param`, `overall_factor`: one single factor
`absmax_per_param`, `param_factors`: one factor per parameter name of current parametrization (in conventional order)
`none` : values given here are ignored

-odir If set, `outfile_base` will be assumed relatively to iteration step output files directory.

-normalize type_data_normalization *For now, this feature is only supported if your dataset contains only a single station component (e.g. only vertical "UP" components for all event-station paths)!*
If set, each equation of the linear system is scaled by a specific factor and thus normalized in a certain sense. `type_data_normalization` defines the type of normalization. *This functionality has not yet been applied in field studies, but don't hesitated to experiment.*
Supported types are (see for descriptions above in section about executable

solveCglsKernelSystem):
maxamp_mdata_by_paths
maxamp_mdata_by_paths_and_frequency
scale_maxamp_mdata_by_paths

3.1.25 solveParKernelSystem

Solves linear system of sensitivity kernel equations in parallel by ScaLAPACK libraries.

This executable is parallelized using BLACS libraries which usually are based on MPI. Hence, it should probably be called like
mpirun -np 8 solveParKernelSystem (followed by respective arguments)
The executable uses the maximum number of parallel slots being available in the MPI environment, in the above example this would be 8. solveParKernelSystem minimally requires NPROC_ROWS*NPROC_COLUMNS parallel slots, as defined by the mpi_parfile. *If there are less slots availble than required, the program will raise an error.*

Positional arguments

dmsi_file Data-model-space-info file

outfile_base Base name of output files (will be used for all files, with suitable extensions)

mpi_parfile Parameter file defining everything related to the ScaLAPACK parallelization of the linear system. A description of its content can be found at the end of this subsection and a template is provided:
template/solveParKernelSystem_parfile_template

main_parfile Main parameter file of inversion.

Optional options

-regscal type_regul_scaling type_regul_scaling is the type of scaling of regularization constraints, at the moment only absmax_per_param,overall_factor, absmax_per_param,param_factors and none are supported Option -regscal can only be requested when adding damping or smoothing conditions by options -smooth or -damp.

-smoothing scaling_values If set, smoothing conditions are applied. scaling_values is a vector of scaling values consistent with -regscal:
absmax_per_param,overall_factor: one single factor
absmax_per_param,param_factors: one factor per parameter name of current parametrization (in conventional order)
none : values given here are ignored

-smoothbnd type_smoothing_boundary type_smoothing_boundary defines the way (non-existing) neighbours are treated in smoothing conditions at outer/inner boundaries of the inversion grid. Supported types:
zero_all_outer_bnd: apply zero smoothing conditions at *all* outer boundaries.
zero_burried_outer_bnd,cont_free_surface: apply zero smoothing conditions at all outer boundaries *except* on free surfaces.
If not set, standard average is used everywhere (equivalent to continuity boundary conditions).
Option -smoothbnd is only allowed to be set, if option -smoothing was set.

-damping scaling_values If set, damping conditions are applied. scaling_values is a vector of scaling values consistent with -regscal:
absmax_per_param,overall_factor: one single factor
absmax_per_param,param_factors: one factor per parameter name of current parametrization (in conventional order)
none : values given here are ignored

-odir If set, outfile_base will be assumed relatively to iteration step output files directory.

-normalize type_data_normalization *For now, this feature is only supported if your dataset contains only a single station component (e.g. only vertical "UP" components for all event-station paths)!*
If set, each equation of the linear system is scaled by a specific factor and thus normalized in a certain sense. type_data_normalization defines the type of normalization. *This functionality has not yet been applied in field studies, but don't hesitated to experiment.*
Supported types are (see for descriptions above in section about executable solveCglsKernelSystem):
maxamp_mdata_by_paths
maxamp_mdata_by_paths_and_frequency
scale_maxamp_mdata_by_paths

The parameter file mpi_parfile (third first positional argument)

In the following, the required keywords of the parameter file given as third positional argument is described (documenting commentary is also contained in the template parfile template/solveParKernelSystem_parfile_template). **NPROC_ROWS, NPROC_COLUMNS**
Number of processes in the rows/columns of the 2D process grid as used by the BLACS libraries. The total number of required MPI processes is NPROC_ROWS * NPROC_COLUMNS (if the MPI environment provides more ranks, those are ignored).

NROW_PER_BLOCK,NCOL_PER_BLOCK
Integer values giving the number of rows and columns per submatrix block- ScaLAPACK subdivides the linear system matrix into a block matrix, each block being a submatrix of size NROW_PER_BLOCK-times-NCOL_PER_BLOCK. The total numbers of rows (columns) of the global system matrix, however, does not need to be a multiple of NROW_PER_BLOCK (NCOOL_PER_BLOCK), there will be fractional blocks at the bottom (or right end) of the matrix. There is not yet an automated ScaLAPACK functionality telling you the optimal block

sizes, which are dependent on the linear system and your parallel environment. Anything from 200 to 500 should be sensible (?!). For more information, browse the web, e.g. `http://www.netlib.org/utk/papers/scalapack/node19.html`

NROW_TO_PROCESS_AT_ONCE
Integer value giving the number of rows of the kernel matrix which are handled by the master process at a time. The larger this number is, the more memory is required for the master process to keep those rows in the memory, e.g.

- The master process will read this number of rows of the kernel matrix from the kernel files before distributing it onto the process grid. For this operation it is efficient if `NROW_TO_PROCESS_AT_ONCE` is a multiple of the number of data samples per data path (in case all data paths have the same number of data samples, i.e. the same number of frequencies and components). Otherwise kernel files might be opened and closed several times, which could cost extra performance.
- The regularization equations will also be requested by the master process and then distributed onto the process grid. This will be done in sections of rows, each containing `NROW_TO_PROCESS_AT_ONCE` rows.

3.1.26 spec2timeKernels

Compute `time_kernel` files from existing `spectral_kernel` files (by inverse Fourier transform) for the time windows as specified by options t0,dt,nt1,nt2: The total set of time samples consists of `n` time windows. nt1,nt2 are strings containing `n` integers defining the start (`nt1`) and end (`nt2`) each time window by a time sample index. Times compute as `t = t0 + jt*dt` where $\texttt{nt1} \leq \texttt{jt} \leq \texttt{nt2}$. There are two possibele ways to define a set of kernels that are transformed:

(way 1): compute kernel for only one path, defined by eventID and station name using options `-evid`, `-staname`, `-comp` and `-param`

(way 2): use flag `-dmsapce` in connection with optional range definition of the path index (flags `-ipath1` `-ipath2`)
in order to define a subset of the paths contained in the given data-model-space description. If the upper (lower) limit of the path range is not defined (i.e. `-ipath1` (`-ipath2`) not set), the maximum (minimum) possible value is used. Then, all kernels for the defined range of paths in the given data-model-space description are computed.

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

-evid event_id Defines the event id of the one path (must belong to an event in main event list). (way 1)

-staname station_name Defines the station name of the one path (must belong to a station in main station list). (way 1)

-comp "comp_1 ... comp_n" Vector of station components for which time kernel should be transformed. For valid components see 1.4 (page 26). (way 1)

-param "param_1 ... param_n" Vector of parameter names for which time kernel should be transformed. Only valid parameter names of the chosen model parametrization are accepted. (way 1)

-dmspace Data model space input file to define a set of paths. (way 2)

-dt time_step Global time step of time discretization of time kernels.

-nt1 "idx_1 .. idx_n" Vector of `n` time indices defining the start indices of the `n` time windows within which time kernels will be computed.

-nt2 "idx_1 .. idx_n" Vector of `n` time indices defining the start indices of the `n` time windows within which time kernels will be computed.

Optional options

-ipath1 path1 `path1` is the first index of the path loop. By default, `path1 = 1` (way 2)

-ipath2 path2 `path2` is the last index of the path loop. By default, `path2 = max_number_of_paths` as to data-model-space description. (way 2)

-t0 tzero Optional global time shift which is added to all times defined by `dt`, `nt1`, `nt2` (default `t0=0`)

-wp If set, then 'ON-WP' spectral kernel files are produced, containing plain kernel values on wavefield points. If not set, normal kernel files (pre-integrated) are transformed.

3.1.27 timeKernel2vtk

Produces vtk files from *one existing* binary time sensitivity kernel file for a selection of time steps defined by vectors of starting and end indices `-nt1` , `-nt2`.

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

-evid event_id Defines the event id of the one path. (must belong to an event in main event list)

-staname station_name Defines the station name of the one path. (must belong to a station in main station list)

-comp "comp_1 ... comp_n" Vector of station components for which vtk files should be generated. For valid components see 1.4 (page 26).

-param "param_1 ... param_n" Vector of parameter names for which vtk files should be generated. Only valid parameter names of the chosen model parametrization are accepted.

-nt1 "idx_1 .. idx_n" Vector of `n` time indices defining the start indices of the `n` time windows within which vtk files should be generated (the resulting set of time indices must be contained in the binary time kernel files generated by `spec2timeKernels`.

-nt2 "idx_1 .. idx_n" Vector of `n` time indices defining the start indices of the `n` time windows within which vtk files should be generated (the resulting set of time indices must be contained in the binary time kernel files generated by `spec2timeKernels`.

Optional options

-wp If set, time waveform kernel files 'ON-WP' (plain kernel values on wavefield points) will be read (assuming these files exist!) and writte as vtk files. If not set, normal time kernel files (pre-integrated) are read in and written as vtk files.

3.1.28 `transformMeasuredData`

Fourier transform of time-domain data to `ASKI`-conform frequency-domain measured data; frequency discretization of measured data as defined in main parfile.

Positional arguments

main_parfile Main parameter file of inversion.

Mandatory options

-txt parfile_txt Input data files are plain text files, containing one time series per file. `parfile_txt` is the filename of a parameter file with details on location, naming and content of the files, as provided by `template/transformMeasuredData_parfile_txt_template` . The content of this parameter file is described below. Exactly one of options `-txt`, `-su` must be set.

-su su_files_path Input data files are seismic unix. su_files_path is the path where seismic unix files can be found which have filenames of form eventID_COMP.su. Every such seismic unix file is assumed to contain the same number of data traces, one trace for each station as defined in the ASKI stations file (in that order). The time discretization of the time series will be taken from each file separately, but it is assumed that all traces contained in a seismic unix file have the very same time discretization (time step and number of samples are always taken from the first trace of a file). Exactly one of options -txt, -su must be set.

Optional options

-htaper taper_portion If set, a cosign-hanning taper is applied to time-domain traces before Fourier Transform. The argument taper_portion gives the portion of the end of the time-series (between 0.0 and 1.0) to which the taper is applied. If not set, a taper *is* applied with default portion of 0.05 (i.e. 5 percent).

The parameter file for option -txt

In the following, the required keywords of the parameter file for option -txt are described (documenting commentary is also contained in the template parfile template/transformMeasuredData_parfile_txt_template).

PATH_TXT_TRACES
Path where all .txt trace files can be found (must end on /). The trace files in that path are expected to have filenames of form EVID_STANAME_COMP.txt .

FILE_DATA_MODEL_SPACE_INFO
Data model space info file defining the set of data samples for which the conversion will be done: For all receiver components (present in the file) of all data paths (present in the file), the complete spectrum will be generated as defined by global frequency discretization from main parfile. I.e. any specific frequency definition in the data model space info file will be ignored.

DT, NSTEP
Global time discretization (timestep and number of samples) for *all* .txt trace files. If some of your data have other time discretizations than others, you would need to re-run this executable for each time discretization, properly re-defining the data subset through the data model space info file file.

COLUMN_OF_TRACE
Integer value defining the column of the .txt trace files in which the actual time-series is found. E.g. if the files contain the time as first column and amplitude values as second column, set COLUMN_OF_TRACE = 2; if only one column with amplitude values is contained in the files, set COLUMN_OF_TRACE = 1.

3.2 Python Scripts and Applications

3.2.1 create_ASKI_dir.py

For description see → 1.3 (page 25)

3.2.2 create_shore_lines.py

This application creates a `.vtk` file containing shore lines trimmed to the domain of the currently used inversion grid and transformed to the currently used `VTK_PROJECTION`. It is based on the Fortran-to-python interface generator `f2py` and thus needs special attention for compiling an additionally required module (see → 1.20.2 (page 48) if you have not yet compiled it).

Positional arguments

`filename_GSHHS_bin` Name of GSHHS file in native binary format, containing the shore line data. Such files can be downloaded via `https://www.ngdc.noaa.gov/mgg/shorelines/data/gshhg/latest/`. you should download the dataset in form of native binary files (probably package named like `gshhg-bin-?.?.?.zip`) and choose here a file of specific resolution e.g. `gshhs_c.b`, `gshhs_l.b`, `gshhs_i.b`, `gshhs_h.b`, `gshhs_f.b`. If you are interested in the file format of GSHHS native binary files, as expected by `ASKI`, see 2.10 (page 60).

`outfile_base` Absolute output file base (will be concatenated by "`.vtk`" for vtk output). Existing output files will *not* be overwritten, but an alternative non-existend extension of the filename will be used.

`main_parfile` Main parameter file of inversion.

3.2.3 plot_ASKI_data_spectrum.py

This application plots text files containing complex spectral values (in Fortran format) as ocurring in `ASKI` for e.g. measured and synthetic data or filters. Executing `plot_ASKI_data_spectrum.py` without arguments will plot a usage message.

Positional arguments

`spectrum_file` Filename of file to be plotted

`column_to_plot` Optional positional argument (integer value), defining which column of complex numbers contained in the file should be plotted. If not given, the first column is plotted.

3.3 Integration Weights

The `ASKI` module `integrationWeights` computes integration weights for the set of wavefield points in order to integrate the kernels over the inversion grid. As we need to calculate the integrals of the kernels over each inversion grid cell separately, the integration weights are computed for each cell in such a way that weighting the summation of the kernel values yields the desired integral value:

For each inversion grid cell $\Omega_c \subset \mathbb{R}^3$ which contains wavefield points $\mathbf{x}_1, \ldots, \mathbf{x}_{n_c}$ the weights $w_1, \ldots, w_{n_c}$ are computed such that

$$\int_{\Omega_c} K(\mathbf{x})\, d\mathbf{x} \simeq \sum_{i=1}^{n_c} w_i K(\mathbf{x}_i) \tag{3.1}$$

There are several types of integration weights supported (indicated by dummy variable `intw_type` of subroutine `createIntegrationWeights`):

3.3.0 Compute Average (no integration)

In case of `intw_type = 0`, function `createIntegrationWeights` sets

$$w_i = \frac{1}{n_c} \quad , i = 1, \ldots, n_c$$

in each inversion grid cell Ω_c.
This way, the summation $\sum_{i=1}^{n_c} w_i K\left(\mathbf{x}_i^G\right) = \frac{1}{n_c} \sum_{i=1}^{n_c} K\left(\mathbf{x}_i^G\right)$ yields the average kernel value in Ω_c.

This type of integration weights (which are actually no integration weights) may be used to perform some sort of interpolation of kernel values onto the inversion grid (e.g. in order to compare kernel values from different methods which use different sets of wavefield points).

3.3.1 Scattered Data Integration

In case of `intw_type = 1...4`, a method by David Levin [Lev99] is apllied to a standardized inversion grid cell Ω^S. For different shapes of inversion grid cells, different types of standard cells are used, which are referred to below.

For each inversion grid cell $\Omega_c \subset \mathbb{R}^3$ containing wavefield points $\mathbf{x}_1, \ldots, \mathbf{x}_{n_c}$, a transformation $T : \Omega_c \to \Omega^S$ is used to transform cell Ω_c into the standard cell Ω^S and to compute the respective transformed wavefield points $\mathbf{x}_i^S = T\left(\mathbf{x}_i\right)$ contained in Ω^S.

Then [Lev99] is applied to points $\mathbf{x}_1^S, \ldots, \mathbf{x}_{n_c}^S$ and volume Ω^S to compute integration weights $w_1^S, \ldots, w_{n_c}^S$ such that

$$\begin{aligned} \int_{\Omega_c} K(\mathbf{x})\, d\mathbf{x} &= \int_{\Omega^S} K\left(T^{-1}\left(\mathbf{x}^S\right)\right) \mathcal{J}_{T^{-1}}\left(\mathbf{x}^S\right)\, d\mathbf{x}^S \\ &\simeq \sum_{i=1}^{n_c} w_i^S\, \mathcal{J}_i\, K(\mathbf{x}_i) \\ &= \sum_{i=1}^{n_c} w_i K(\mathbf{x}_i) \end{aligned} \tag{3.2}$$

where $\mathcal{J}_{T^{-1}}$ denotes the Jacobian of the inverse transformation T^{-1}, $\mathcal{J}_i = \mathcal{J}_{T^{-1}}\left(\mathbf{x}_i^S\right)$ and the desired weights compute as $w_i = w_i^S\, \mathcal{J}_i$. The method of computing such integration weights $w_1^S, \ldots, w_{n_c}^S$, as presented in [Lev99], is explained in the following.

The Method of Scattered Data Integration

[Lev99] follows a composite rule strategy for building the integration weights. For subsets of the volume of interest it constructs integration formulae which are as local and as stable as possible and are exact for polyinomials p of a certain fixed degree m. It is assumed that the integrals of these polynomials $p \in \Pi_m$ over the subsets are easily computable.

In notation of [Lev99], the integration weights A_i for a function f on domain $\Omega \subset \mathbb{R}^d$ which is given on a set $\{x_i\}_{i=1}^N \subset \Omega$ are constructed as

$$A_i = \sum_{k=1}^{K} A_i^{(k)}\,, \quad 1 \le i \le N\,,$$

where Ω is subdivided into K disjoint subsets E_k. For each E_k, the N weights $A_i^{(k)}$ are calculated as follows.

We choose a basis $\{p_i\}_{i=1}^J$ of the space Π_m of all polynomials in $\mathbb{R}^d$ with maximum total degree m, where $J = \binom{d+m}{m}$ is the dimension of space Π_m. $A_i^{(k)}$ are then defined as the components $a_i = A_i^{(k)}$ of vector $\bar{a} = D^{-1}E\left(E^tD^{-1}E\right)^{-1}\bar{c}$, where

$$\begin{aligned} D &= 2\text{Diag}\left\{\eta\left(\|x^* - x_1\|\right), \ldots, \eta\left(\|x^* - x_N\|\right)\right\} \\ E_{i,j} &= p_j\left(x_i\right)\,, \quad 1 \le i \le N,\ 1 \le j \le J \end{aligned}$$

and $\bar{c}$ contains the integrals of the p_i over E_k, i.e. $c_i = \int_{E_k} p_i$. $\eta(r) = \exp\left(r^2/h^2\right)$ is a fast increasing weight function which gives the localizing properties of the weights. h is approximately the diameter of subsets E_k and x^* is some center of E_k.

This composite local approach of calculating global integration weights involves K solutions of a full linear system of order J.

Application to Hexahedral Inversion Grid Cells

For inversion grid cells of general hexahedral shape, the 3-dimensional cube

$$\Omega^S = [-1,1]^3 = \left\{ \begin{pmatrix} x \\ y \\ z \end{pmatrix} \middle| -1 \le x, y, z \le 1 \right\}$$

is used as the standard cell. For every such inversion grid cell Ω_c, module `inversionGrid` is expected to provide its transformed wavefield points $\mathbf{x}_1^S, \ldots, \mathbf{x}_{n_c}^S$ and their corresponding values of Jacobian $\mathcal{J}_i$.

In the context of Scattered Data Integration, the inversion domain $\Omega = \Omega^S = [-1,1]^3$ is subdivided into $K = n_h^3$ subcubes E_k of edge length $h = 2/n_h$. $n_h = \max\left\{\left\lfloor \sqrt[3]{\frac{n_c}{J}} \right\rfloor, 1\right\}$ is chosen in such a way that there should be at least J (or all, otherwise) integration points within E_k, as otherwise the damping by matrix D^{-1} might cause numerical instabilities by making matrix $E^tD^{-1}E$ close to singular.

As x^*, the center of the respective subcube is chosen.

The desired weights $w_1^S, \ldots, w_{n_c}^S$ are then given by $w_i^S = A_i$, $1 \le i \le n_c$

Application to Tetrahedral Inversion Grid Cells

For inversion grid cells of general tetrahedral shape, the 3-dimensional simplex with corners

$$\begin{pmatrix}0\\0\\0\end{pmatrix}, \begin{pmatrix}1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\end{pmatrix}$$

is used as the standard cell Ω^S. For every such inversion grid cell Ω_c, module `inversionGrid` is expected to provide its transformed wavefield points $\mathbf{x}_1^S, \ldots, \mathbf{x}_{n_c}^S$ and their corresponding values of Jacobian $\mathcal{J}_i$.

In the context of Scattered Data Integration, here the inversion domain $\Omega = \Omega^S$ is *not* subdivided into any true subsets E_k. It is always $K = 1$ and $E_1 = \Omega$, mainly because a subdivision of the standard tetrahedron is not trivial (compared with e.g. the cube $[-1, 1]^3$), considering that the integrals of the base polynomials must be computed over all subsets E_k.

As x^*, the barycenter

$$\begin{pmatrix}0.25\\0.25\\0.25\end{pmatrix}$$

of the standard simplex is chosen and $h = 1$.

The desired weights $w_1^S, \ldots, w_{n_c}^S$ are then given by $w_i^S = A_i$, $1 \le i \le n_c$

Scattered Data Integration, Order 1

`intw_type = 1`
In the context of this subsection 3.3.1, $m = 1$ is used as the degree of polynomials which are integrated in an exact way and of course $d = 3$. The space Π_1 of all polynomials in $\mathbb{R}^3$ of maximum total degree $m = 1$ has dimension $J = \binom{3+m}{m} = \binom{4}{1} = 4$. As a basis of Π_1 we choose $\{1, x, y, z\}$.

Scattered Data Integration, Order 2

`intw_type = 2`
In the context of this subsection 3.3.1, $m = 2$ is used as the degree of polynomials which are integrated in an exact way and of course $d = 3$. The space Π_2 of all polynomials in $\mathbb{R}^3$ of maximum total degree $m = 2$ has dimension $J = \binom{3+m}{m} = \binom{5}{2} = 10$. As a basis of Π_2 we choose $\{1, x, y, z, x^2, xy, xz, y^2, yz, z^2\}$.

Scattered Data Integration, Order 3

`intw_type = 3`
In the context of this subsection 3.3.1, $m = 3$ is used as the degree of polynomials which are integrated in an exact way and of course $d = 3$. The space Π_3 of all polynomials in $\mathbb{R}^3$ of maximum total degree $m = 3$ has dimension $J = \binom{3+m}{m} = \binom{6}{3} = 20$. As a basis of Π_3 we choose $\{1, x, y, z, x^2, xy, xz, y^2, yz, z^2, x^3, x^2y, x^2z, xy^2, xyz, xz^2, y^3, y^2z, yz^2, z^3\}$.

Scattered Data Integration, Optimal Order

In case of `intw_type = 4`, function `createIntegrationWeights` tries to seperately find for each inversion grid cell the highest possible order of Scattered Data Integration. Starting with highest order $m = 3$, it continues to recompute Scattered Data Integration weights of order $m = 2$ and $m = 1$ until the computation was successful. If the computation for order $m = 1$ fails, the integration weights of that cell will be marked erroneous, the computation of the weights is not successfull in that case.

As the success of the Scattered Data Integration method is strongly dependent on the specific set of points $\mathbf{x}_1^S, \ldots, \mathbf{x}_{n_c}^S$, since matrix $E_{i,j} = p_j(x_i)$ must have full rank, the strategy of choosing the highest possible degree of integration for each cell tries to take all locally availabe information of inversion grid and wavefield points into account.

3.3.2 Linear (first order) Integration

In case of `intw_type = 5`, function `createIntegrationWeights` sets

$$w_i = \frac{1}{n_c}\mathrm{vol}(\Omega_c) \quad , i = 1, \ldots, n_c$$

in each inversion grid cell Ω_c, where $\mathrm{vol}(\Omega_c)$ denotes the volume of inversion grid cell Ω_c, which is expected to be provided by module `inversionGrid` for every cell.
This way, the summation $\sum_{i=1}^{n_c} w_i K\left(\mathbf{x}_i^G\right) = \mathrm{vol}(\Omega_c)\frac{1}{n_c}\sum_{i=1}^{n_c} K\left(\mathbf{x}_i^G\right)$ yields the average kernel value in Ω_c multiplied with the volume of Ω_c.

This somehow approximates the generalization of the trapezoidal rule to 3 dimensions, in which the integral of a function f over some tetrahedron $\mathcal{T}$, which is defined by 4 incoplanar points $\mathbf{t}_1, \ldots, \mathbf{t}_4$, is computed by $\mathrm{vol}(\mathcal{T})\frac{1}{4}\sum_{i=1}^{4} f(\mathbf{t}_i)$.

3.3.3 External Integration Weights

In case of `intw_type = 6`, function `createIntegrationWeights` does not actually compute any integration weights. Instead, it calls function `transformToStandardCellInversionGrid` of module `inversionGrid` with dummy variable `type_standard_cell` set to value `-1`, which requests the routine to return the total integration weights in variable `jacobian` instead the jacobian values. These returned values are then stored as the integration weights.

This functionality must be supported by the type of inversion grid. At the moment only inversion grids of type `specfem3dInversionGrid` support external type integration weights.

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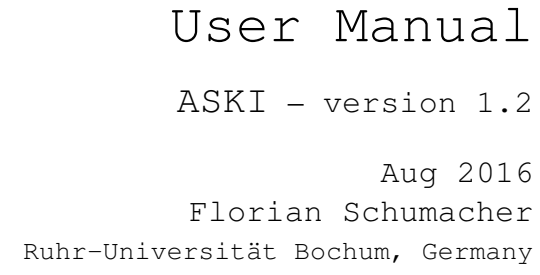

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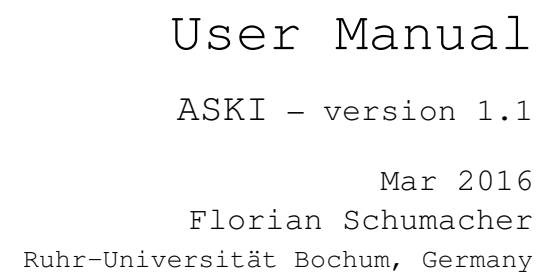

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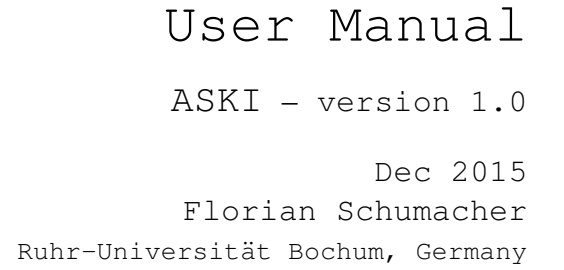

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