ASKI

Analysis of

Sensitivity and

Kernel

Inversion

User Manual

ASKI – version 0.3

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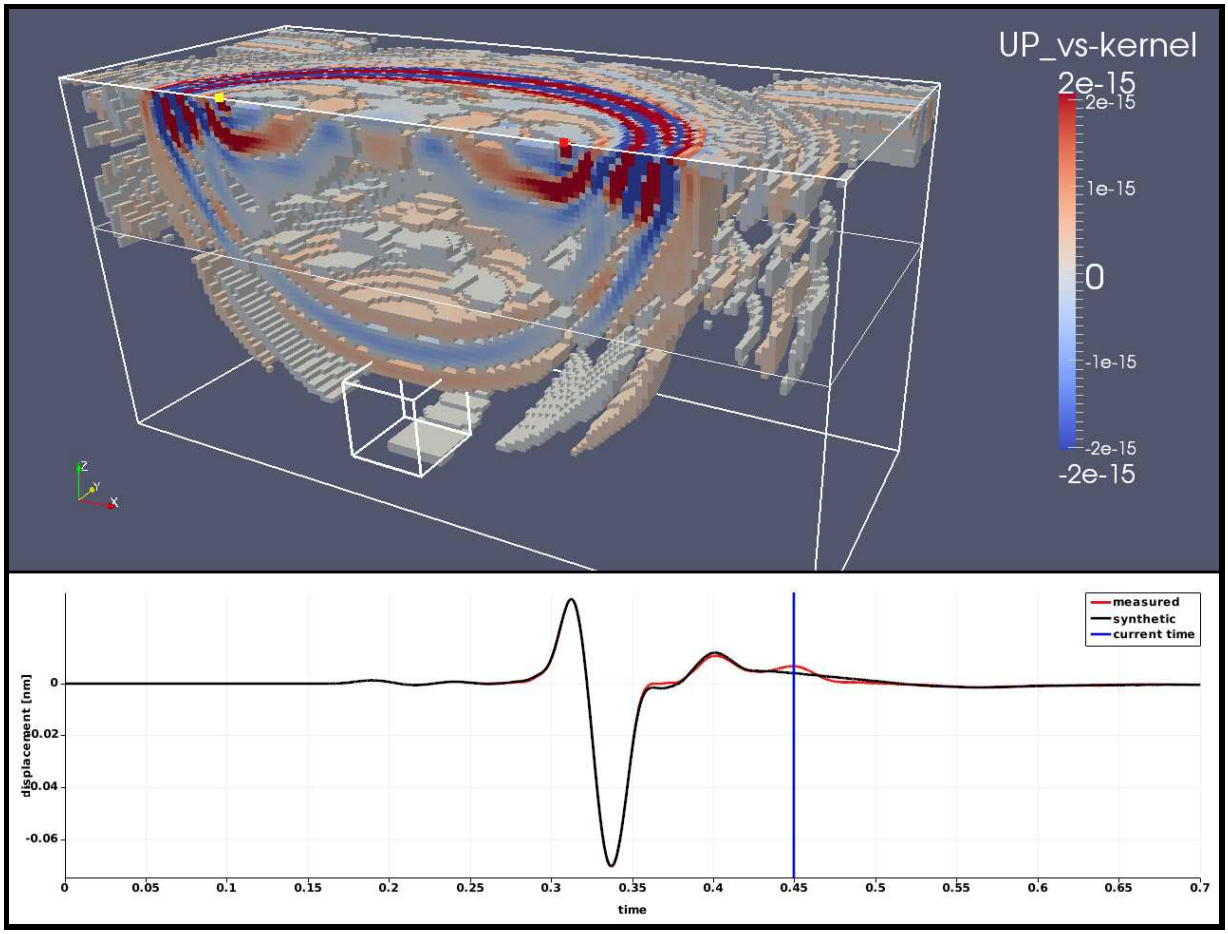

This documentation was written in the hope that it will be useful to the user, but it *cannot be assured* that it is accurate in every respect or complete in any sense.
Please do not hesitate to improve this documentation by incorporating your experiences with `ASKI` and your personal experience of getting used to it. When you have developed new `ASKI` components or have modified existing once, please extend / modify this document accoringly.

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

The LaTeXsource files and all related components of this document are available via `http://www.rub.de/ASKI`

Florian Schumacher, 2013

How to use this manual

Only chapter Guide (page 7) is intended to be read through which, for this reason, is held as compact as possible. This chapter may itself be regarded as "the manual", with the appending chapters only containing more specific detail on processes or objects which chapter Guide refers to.

In other words: just start reading the respective section of chapter Guide, 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 repuirements for your operation.

All chapters appending chapter Guide are not intended to be read through section by section but may well serve the user as a reference.

Contents

Chapter 0

Guide

This chapter is intended to guide you, dependent on what you want to do, through all necessary steps to achieve your goals.

If you don't know about ASKI yet, we recommend you to quickly read through the next section, 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 15).
Make sure to read through a complete item before hastily doing anything!

Good Luck!

What is ASKI ?

ASKI is a modularized software package which offers analysis tools of seismic data and a full waveform inversion concept based on waveform sensitivity kernels derived from Born scattering theory.

Instead of using time-dependent values of ground motion (i.e. samples of a time-series of seismic data), ASKI uses freqency-dependent complex values of ground motion at a certain receiver excited by a certain seismic source. This, mainly, has reasons of computational feasibility and does not mean any draw-back (e.g. in the sense that no time-windowing is possible etc.), since ASKI aims at taking into account *all* available information contained in a waveform.

Using sensitivity kernels K, change in a data sample Δd_i is connected to model uptdates Δm by an integral relation $\Delta d_i = \int_\Omega \Delta\vec{m}\,\vec{K}_i$. 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 $\int_{\Omega_j} K_i$.

The sensitivity kernels K are computed from forward wavefields produced on a set of points in space, which is dependent on the particular forward method. This set of points is refered to as *wavefield points*. The wavefields are written to file, by the respective forward method, which may require very large discspace. Providing methods for constructing integration rules for arbitrary point sets contained in arbitrary volumes, ASKI computes integration weights for integration of functions on the wavefield points over the volumetric cells of the inversion grid. Thereby, 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, some combinations of

wavefield points (i.e. forward methods), integration weight types and inversion grid types are not possible.

The preintegrated kernel values are also written to files, which may be flexibly read in for arbitrary subsets of data by the binary programs conducting any sensitivity analysis or an interation step 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 a data residuum Δd_i to a model update Δm. After updating the model, wavefields may be computed with respect to the new model, which again may be improved in the same way, possibly using higher frequencies and smaller scatteres.

Any details on `ASKI` and the theory behind, may be found in the near future in respective journal publications.

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 12). For this purpose, apply the steps "Transforming to Time-Domain Sensitivity Kernels" (below) after you computed the standard 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.

In addition to ASKI → 1.1 (page 15), you will need software to solve the forward problem → 1.10 (page 23).

Preliminary 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) → 1.2 (page 15). 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 → 1.4 (page 15)

- Even if you do not have any measured data, it might still be beneficial for you to make yourself (roughly) familiar with the from of data used in ASKI → 1.5 (page 16).
  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 PATH_EVENT_FILTER and PATH_STATION_FILTER in your main parameter file. The transformation of the standard frequency-domain sensitivity kernels to the time domain, *always* requires event filters (i.e. source-time functions) and station filters (i.e. receiver responses). Even if you do not want to apply those values, you need to artificially create the required files in pahts PATH_EVENT_FILTER and PATH_STATION_

FILTER and may set the spectral filter values to the real value $1 \in \mathbb{R}$, i.e. $(1\ 0) \in \mathbb{C}$ for all frequencies.

- 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
- Define the inversion grid → 1.7 (page 17), 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.
- Set all parameters in the specific iteration step parameter file to correct values → 1.3 (page 15), 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 23). For defining a starting model, see → 1.8 (page 23).

Computing Standard Frequency-Domain Sensitivity Kernels

- Compute forward wavefields and Green tensors 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 1.5 (page 16) and 2.5 (page 34)). Refer to the documentation of your method on how to do it.
- Set filename FILE_INTEGRATION_WEIGHTS in your main parameter file (can be any name, will be created), as well as TYPE_INTEGRATION_WEIGHTS → 1.11 (page 24)
- Initiate basic requirements for all programs and scripts → 1.13 (page 25)
- If you have many paths, you may define a data and model space concentrating on defining paths → 1.12 (page 24) If you have only one path or just a few, it 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) and your set of model parameters → 1.14 (page 25)
  If desired, you may have a look at the standard frequency-domain kernels → 1.16 (page 26)

Transforming to Time-Domain Sensitivity Kernels

- Transform the standard frequency-domain waveform kernels to time domain → 1.15 (page 26). Note that the transformation *always* requires event filters (i.e. source-time functions) and station filters (i.e. receiver responses), which in case they are not required may artificially all have real value $1 \in \mathbb{R}$, i.e. $(1\ 0) \in \mathbb{C}$ for all frequencies.

- Plot the time kernels → 1.17 (page 26)

Full Waveform Inversion - Classical Waveform Sensitivity Kernels

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

In addition to ASKI → 1.1 (page 15), you will need software to solve the forward problem → 1.10 (page 23).

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) → 1.2 (page 15). 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 the expected number of iteration steps of your inversion → 1.4 (page 15)

- Make yourself familiar with the from of data used in ASKI → 1.5 (page 16).
  Set 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 → 1.6 (page 17)

- 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 17)

- Set all parameters in the specific iteration step parameter file to correct values → 1.3 (page 15), 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 23). Before the first iteration, however, you need to define some starting model → 1.8 (page 23).

Conducting An Iteration Step

- Compute forward wavefields and Green tensors 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 1.5 (page 16) and 2.5 (page 34)). Refer to the documentation of your method on how to do it.

- Set filename `FILE_INTEGRATION_WEIGHTS` in your main parameter file (can be any name, will be created), as well as `TYPE_INTEGRATION_WEIGHTS` → 1.11 (page 24)

- Initiate basic requirements for all programs and scripts → 1.13 (page 25)

- Define data and model space, whereby the paths are mainly important for now → 1.12 (page 24)

- Compute sensitivity kernels for your specific set of paths and your set of model parameters → 1.14 (page 25)
  If desired, you may have a look at your kernels → 1.16 (page 26)

- 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

- Finally compute the inverted model by solving the kernel system → 1.18 (page 27)

Chapter 1

Basic Steps

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 Installing `ASKI`

- Download here: `http://www.rub.de/ASKI`
- Unpack tar ball somewhere
- Follow the directions in file `ASKI_0.3/README`

1.2 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 29) and 2.1.1 (page 29).

1.3 Iteration Step Parameter Files

Having created a directory environment for your operation, as described in section 1.4 (page 15), 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 29) and 2.1.2 (page 31).

1.4 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 1.2 (page 15)) 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.

1.5 Data in ASKI

One certain data sample in ASKI is characterized by a seismic *source*, a *component* of a seismic *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 Receivers

The events file (2.2 (page 33)) and stations file (2.3 (page 33)) 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).

Receiver Components

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

Cartesian receivers

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 receivers

`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 i, the corresponding frequency f_i [Hz] computes as $f_i = i \cdot \Delta f$. E.g. $\Delta f = 10$ Hz and frequency indices $i = 2,\ 3,\ 5,\ 7,\ 10$ define the set of discrete frequencies $f_i = 20.0,\ 30.0,\ 50.0,\ 70.0,\ 100.0$ [Hz].

1.6 Prepare Measured Data

In the future, we plan to have a binary program `createMeasuredData`, which converts time-domain data to the special frequency-domain form required by `ASKI`. It is planned to supporte measured data given in some basic data formats like Seismic Unix and time-series given as textfiles per trace.

For now, you must prepare measured data files on your own as required by `ASKI`, see sections 1.5 (page 16) and 2.4 (page 34).

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 scartInversionGrid

A Simple CARTesian 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 23)) 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).

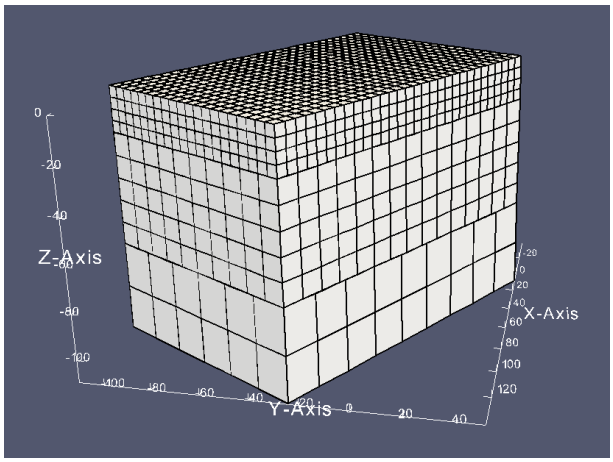

Figure 1.1: Example of a simple Cartesian inversion grid

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 1.1 (page 18).

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.`

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
```

1.7.2 ecartInversionGrid

WARNING, EXPERIMENTAL FEATURE: *so far, this type of inversion grid works for tetrahedral cells only, since support for hexahedreal cells is not completed throughout. However, even for tetrahedra the automatic detection of neighbours did not work properly in some test cases! So if you intend to use this inversion grid, please have a look at the grid and all neighbours (neighbours only required for model smoothing in case of solving the Kernel system of equations). You can do that by using binary program* `invgrid2vtk` *along with option* `-nb`. *Call* `invgrid2vtk -h` *for further details on how to use it.*

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 2.8 (page 36) 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 23)) 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).

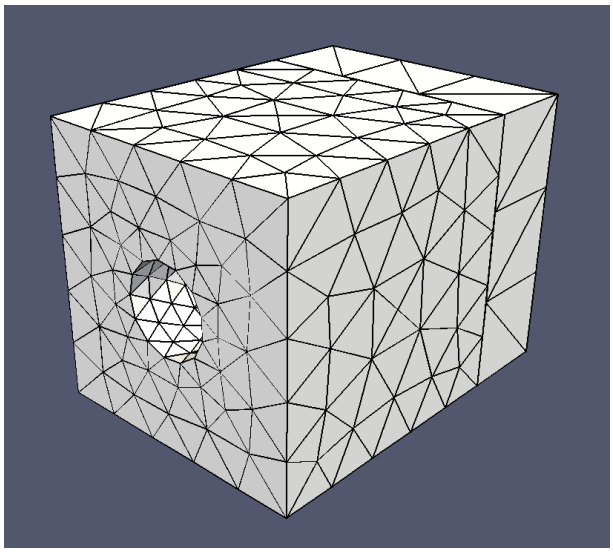

Figure 1.2: Example of an external Cartesian inversion grid created by Cubit

The nodes and cell files, e.g. produced by `Cubit`, are referred to in a parameter file, a template 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 1.2 (page 21).

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 25)), this file is recreated.

ECART_INVGRID_FILE_NEIGHBOURS_IS_BINARY

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

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

1.7.3 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).

Please refer to the documentation of your SPECFEM3D forward method (1.10 (page 23)) on how to define an inversion grid of type specfem3dInversionGrid.

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 binary 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. createStartmodelKim -h will print a help message how to use the program. Afterwards you may export the produced model file to your forward method as explained in section 1.9 (page 23).

1.9 Export Inverted Model

The binary program 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. exportKim -h will print a help message how to use it. Template files of starting model descriptions may be found in template/.

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 is not yet fully supported in this release version. For some test cases, waveform kernels were successfully computed using Gemini II in Cartesian as well as spherical setting. We hope to provide the Gemini II interface for ASKI soon.

SPECFEM3D_Cartesian

The Cartesian spectral element code SPECFEM3D_Cartesian is supported by ASKI , cf. [Sch13]

SPECFEM3D_GLOBE

The global spectral element code SPECFEM3D_GLOBE is not yet fully supported in this release version. For some test cases, waveform kernels were successfully computed using SPECFEM3D_GLOBE. We hope to provide the SPECFEM3D_GLOBE interface for ASKI soon.

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 1.7.3 (page 22))

A detailed description of some of the integration weights, especially the weights after [Lev99] can be found in section 3.1 (page 39).

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 parameters 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 parameters, the model lives in $\mathbb{R}^n$). You only need to define which data sample (model parameter) refers to which dimension (i.e. entry in vector) of the data space (model space).
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, we describe how data samples and model parameters are defined in this software package and how you can choose specific subsets to be used.

1.12.1 Definition of Data Samples

As the sensitivities are calculated in frequency domain, the data live in frequency domain, too. A data sample is uniquely characterized by a seismic *source*, a *component* of a seismic *receiver*, and a *frequency*, as well as if it is *real* or *imaginary* part of the complex spectral values. Refer to 1.5 (page 16) for details on data in `ASKI` .

1.12.2 Definition of Model Parameters

A model parameter is uniquely characterized by a parameter name (mus be a valid parameter name of the model parametrization as defined by `MODEL_PARAMETRIZATION` 2.1.1 (page 30)) and an inversion grid cell index in valid range.

1.12.3 Choosing a Set of Data Samples and Model Parameters

Create a text file as described in section 2.7 (page 35).

1.13 Initiate Basic Requirements

Run binary `initBasics`, `initBasics -h` will print a help message how to use it.

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, whereby 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!

1.14 Compute Standard Sensitivity Kernels

The kernels are computed by combining green tensor and forward wavefield for a given path, and by integration over all inverison grid cells. I.e. there is one sensitivity kernel file for a specific path. This file contains sensitivity values of the three Cartesian receiver components `CX`, `CY`, `CZ` for all model parameters of your model parametrization, with the values living on the inverison grid cells.

Use binary `computeKernels`. `computeKernels -h` will print a help message how to use it. It makes sense, to only compute kernel files for those paths that you are going to use (defined by your data model space file).

You can define the set of paths for which sensitivities should be computed in two ways:

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

way 2 input a data and model space file (as defined by 1.12 (page 24)) by option `-dmspace`, defining all paths for which kernels should be computed; optionally define range of path index by `-ipath1`, `-ipath2`

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. The transforation is done for specific data components (e.g. `N`, `DOWN`, `CY`, ..), where first the spectra for the standard component `CX`, `CY`, `CZ` are rotated and afterwards the respective event filter and station component filter are applied before the actual Fourier transform takes place.

Use binary `spec2timeKernels`. `spec2timeKernels -h` will print a help message how to use it. It makes sense, to only compute kernel files for those paths that you are going to use (defined by your data model space file).

You can define the set of paths for which the time-domain kernels should be computed in two ways:

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

way 2 input a data and model space file (as defined by 1.12 (page 24)) by option `-dmspace`, defining all paths for which kernels should be transformed; optionally define range of path index by `-ipath1`, `-ipath2`

1.16 Plot Standard Sensitivity Kernels

One way to plot a specific sensitivity Kernel in frequency domain, i.e. the sensitivity spectra for a specific path, is to procuce vtk files with binary `kernel2vtk`. `kernel2vtk -h` will print a help message how to use it.
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.

1.17 Plot Time Sensitivity Kernels

One way to plot a specific sensitivity Kernel in time domain, is to procuce vtk files with binary `timeKernel2vtk`. `timeKernel2vtk -h` will print a help message how to use it.
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.

1.18 Solve Kernel System

Call binary `solveKernelSystem` to set up the kerne matrix, read in synthetic and real data, add smoothing (if required). `solveKernelSystem -h` will print a help message how to use it.

Chapter 2

Files

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 , SPECFEM3D_GLOBE

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

MODEL_PARAMETRIZATION

isoLame → isotropic Lame parameters ρ, λ, μ

isoVelocity → isotropic seismic velocities ρ, v_p, v_s

Nothing else supported yet

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 = /scratch/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: 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, PATH_EVENT_FILTER, PATH_STATION_FILTER

Paths where ASKI finds files related to the measured data files. These paths can be everywhere, e.g. close to where you have stored/processed your (time domain) data, or in directory MAIN_PATH_INVERSION, etc. ... The naming convention of files in these directories is: FILE_MEASURED_DATA: data_EVENTID_STATIONNAME_COMP, FILE_EVENT_FILTER: filter_EVENTID, FILE_STATION_FILTER: filter_STATIONNAME_COMP, where 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 supported by module componentTransformation
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

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.

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 <= 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 write their output (relatively small output like models, coefficients etc., NO wavefields/kernels etc.!), relative to MAIN_PATH_INVERSION/ITERATION_STEP_PATH. Be 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. Be 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. Be 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. Be 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. Be 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)
typ	source type: 0 = force, 1 = moment tensor, -1: not specified
mag	factor on source mechanism
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 in the directory `PATH_MEASURED_DATA` as defined in the main parameter file.

One measured data file contains all data values for one specific receiver 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.

Line `i` contains measured data values 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 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 path (i.e. a specific source-receiver combination). Its filename is by convention `synthetics_EVENTID_STATIONNAME`

The files are text files containing `ITERATION_STEP_NUMBER_OF_FREQ` lines and 3 columns of complex numbers, which can be understood by `FORTRAN read` command:

Line `i` contains synthetic data values for the i^{th} frequency, as defined by vector of indices `ITERATION_STEP_INDEX_OF_FREQ` and frequency step `MEASURED_DATA_FREQUENCY_STEP`. The 3 complex numbers on a line refer to the 3 Cartesian components `CX`, `CY`, `CX`.

2.6 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, we use the

vtk file format.
General information on this file format may be found under www.vtk.org/VTK/img/file-formats.pdf

PUT HERE:
General info about the two types of vtk files (invgridVtk, wavefield points Vtk files)
Some basic content description about some special vtk files.

2.7 Data and Model Space File

Files in which a data and model space is defined have the following form. Also have a look at example template files template/data_model_space_info_template_*

The blocks described in the subsections below should be put into a file, one after another. The header block must come first, then the data space block and model parameter block. The order of the latter two is arbitrary, both orders are allowed, however if the model parameters block is defined first, an additional check for empty kernel file names will be done in the processing of the data samples block.

2.7.1 Header Block

line 1: currently ignored (file format version specification possible, header comment)

line 2: must either contain ASCII or BINARY
currently ignored (possible form definition like ASCII / mixed ASCII/BINARY (similar to in vtk(?)))
At the moment, this file must be a formatted text file.

2.7.2 Model Parameters Block

line: MODEL PARAMETERS
this defines that the definition of the model parameters 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 pmtrization_1 param_1 ... pmtrization_n param_n
defines the parametrization used for all inversion grid cells.

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 pmtrization_1 param_1 ... pmtrization_n param_n
defining the parameters to be used for this specific inversion grid cell.

2.7.3 Data Samples Block

line “DATA SAMPLES” 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.

2.8 `ecartInversionGrid` Files

2.8.1 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.

2.8.2 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.

2.8.3 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.

Chapter 3

Programs, Scripts and Modules

This chapter collects some scripts, binary programs or modular program components contained in the `ASKI` package, for which some more detail on arguments and basic functionality is required by expert users.
It is not refered to any code, here.

3.1 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`):

3.1.0 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).

3.1.1 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 $\mathbf{x}_i^S = T(\mathbf{x}_i)$ 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

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

whereby $\mathcal{J}_{T^{-1}}$ 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 $J = \begin{pmatrix} d+m \\ m \end{pmatrix}$ is the dimension of space Π_m. $A_i^{(k)}$ are then defined as the components $a_i = A_i^{(k)}$ of vector $\bar{a} = D^{-1}E\left(E^t D^{-1} E\right)^{-1}\bar{c}$, where

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

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

$$\Omega^S = [-1,1]^3 = \left\{ \left(\begin{array}{c} x \\ y \\ z \end{array} \right) \middle| -1 \leq x,y,z \leq 1 \right\}$$

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 $E^t D^{-1} E$ 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 $w_i^S = A_i,\ 1 \leq i \leq n_c$

Application to Tetrahedral Inversion Grid Cells

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

$$\left(\begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right), \left(\begin{array}{c} 1 \\ 0 \\ 0 \end{array} \right), \left(\begin{array}{c} 0 \\ 1 \\ 0 \end{array} \right), \left(\begin{array}{c} 0 \\ 0 \\ 1 \end{array} \right)$$

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

$$\left(\begin{array}{c} 0.25 \\ 0.25 \\ 0.25 \end{array} \right)$$

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

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

Scattered Data Integration, Order 1

`intw_type = 1`

In the context of this subsection 3.1.1, $m = 1$ 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 $J = \left(\begin{array}{c} 3+m \\ m \end{array} \right) = \left(\begin{array}{c} 4 \\ 1 \end{array} \right) = 4$. 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 3.1.1, $m = 2$ 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 $J = \begin{pmatrix} 3+m \\ m \end{pmatrix} = \begin{pmatrix} 5 \\ 2 \end{pmatrix} = 10$. As a basis of Π_2 we choose $\left\{1, x, y, z, x^2, xy, xz, y^2, yz, z^2\right\}$.

Scattered Data Integration, Order 3

`intw_type = 3`
In the context of this subsection 3.1.1, $m = 3$ 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 $J = \begin{pmatrix} 3+m \\ m \end{pmatrix} = \begin{pmatrix} 6 \\ 3 \end{pmatrix} = 20$. As a basis of Π_3 we choose $\left\{1, x, y, z, x^2, xy, xz, y^2, yz, z^2, x^3, x^2y, x^2z, xy^2, xyz, xz^2, y^3, y^2z, yz^2, z^3\right\}$.

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 $E_{i,j} = p_j\left(x_i\right)$ 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.

3.1.2 Linear (first order) Integration

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

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

in each inversion grid cell Ω_c, where $\mathrm{vol}\left(\Omega_c\right)$ 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 $\sum_{i=1}^{n_c} w_i K\left(\mathbf{x}_i^G\right) = \mathrm{vol}\left(\Omega_c\right) \frac{1}{n_c} \sum_{i=1}^{n_c} K\left(\mathbf{x}_i^G\right)$ yields the average kernel value in Ω_c 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 $\mathrm{vol}\left(\mathcal{T}\right) \frac{1}{4} \sum_{i=1}^{4} f(\mathbf{t}_i)$.

3.1.3 External Integration Weights

In case of `intw_type = 6`, function `createIntegrationWeights` does not actually compute any integration weights. Instead, it calls function `transformToStandardCellInversionGri`

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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