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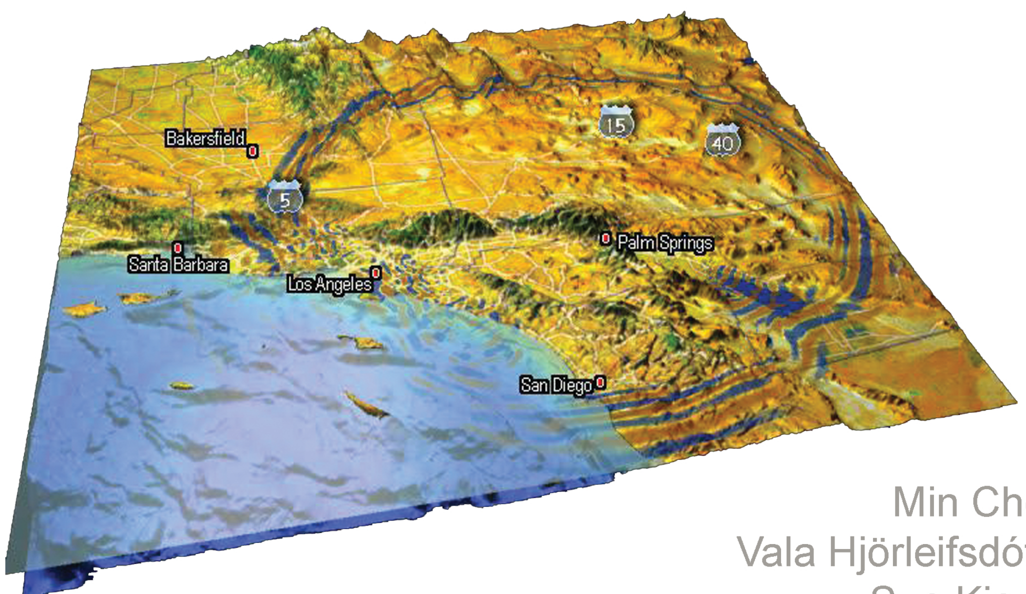
SPECFEM 3D

User Manual

Version 2.0.0



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Version 2.0.0

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Chapter 1

Introduction

The software package SPECFEM3D simulates seismic wave propagation at the local or regional scale based upon the spectral-element method (SEM). The SEM is a continuous Galerkin technique, which can easily be made discontinous [Bernardi et al., 1994, Kopriva et al., 2002, Chaljub et al., 2003, Kopriva, 2006]; it is then a particular case of the discontinuous Galerkin technique [Reed and Hill, 1973, Falk and Richter, 1999, Hu et al., 1999, Cockburn et al., 2000, Giraldo et al., 2002, Rivière and Wheeler, 2003, Monk and Richter, 2005, Grote et al., 2006, Bernacki et al., 2006, Dumbser and Käser, 2006, De Basabe et al., 2008, Wilcox et al., 2010, De Basabe and Sen, 2010], with optimized efficiency because of its tensorized basis functions. Effects due to lateral variations in compressional-wave speed, shear-wave speed, density, a 3D crustal model, topography and bathymetry are included. For a detailed introduction to the SEM as applied to regional seismic wave propagation, please consult Komatitsch and Vilotte [1998], Komatitsch and Tromp [1999], Chaljub et al. [2007], Tromp et al. [2008] and in particular Komatitsch et al. [2004]. If you use the 3D southern California model, please cite Süss and Shaw [2003] (LA), Lovely et al. [2006] (Salton Trough), and Hauksson [2000] (southern California). The Moho map was determined by Zhu and Kanamori [2000]. The 1D SoCal model was developed by Dreger and Helmberger [1990]. The package can accommodate full 21-parameter anisotropy (see Chen and Tromp [2007]) as well as lateral variations in attenuation. Adjoint capabilities and finite-frequency kernel simulations are included [Liu and Tromp, 2006, Tromp et al., 2008].

All SPECFEM3D_GLOBE software is written in Fortran90 with full portability in mind, and conforms strictly to the Fortran95 standard. It uses no obsolete or obsolescent features of Fortran77. The package uses parallel programming based upon the Message Passing Interface (MPI) [Gropp et al., 1994, Pacheco, 1997].

SPECFEM3D won the Gordon Bell award for best performance at the SuperComputing 2003 conference in Phoenix, Arizona (USA) by running at 5 teraflops (sustained) on 1944 processors of the Japanese Earth Simulator using 14.6 billion degrees of freedom stored in 2.5 terabytes of memory; see Komatitsch et al. [2003] and the Gordon Bell Awards News Release (`www.sc-conference.org/sc2003/nr_finalaward.html`) for details. It was a finalist again in 2008 for a run at 0.16 petaflops (sustained) on 149,784 processors of the 'Jaguar' Cray XT5 system at Oak Ridge National Laboratories (USA) [Carrington et al., 2008].

The next release of the code will include support for GPU graphics card acceleration [Komatitsch et al., 2009, 2010a, Michéa and Komatitsch, 2010] as well as Convolutional or Auxiliary Differential Equation Perfectly Matched absorbing Layers (C-PML or ADE-PML) [Komatitsch and Martin, 2007, Martin et al., 2008a,b, Martin and Komatitsch, 2009, Martin et al., 2010]. The next release will use the PT-Scotch and ParMetis parallel libraries for mesh partitioning.

1.1 Citation

If you use SPECFEM3D for your own research, please cite at least one of the following articles: Tromp et al. [2008], Vai et al. [1999], Lee et al. [2008, 2009a,b], Komatitsch et al. [2009, 2010a,b], van Wijk et al. [2004], Komatitsch et al. [2004], Chaljub et al. [2007], Madec et al. [2009], Komatitsch et al. [2010c], Carrington et al. [2008], Tromp et al. [2010], Komatitsch et al. [2002], Komatitsch and Tromp [2002a,b, 1999] or Komatitsch and Vilotte [1998]. If you work on geophysical applications, you may be interested in citing some of these application articles as well, among others: van Wijk et al. [2004], Ji et al. [2005], Krishnan et al. [2006a,b], Lee et al. [2008, 2009a,b], Chevrot et al. [2004], Favier et al. [2004], Ritsema et al. [2002], Godinho et al. [2009], Tromp and Komatitsch [2000], Savage et al. [2010]. The corresponding BibTEX entries may be found in file `USER_MANUAL/bibliography.bib` or in comments at the beginning of file `specfem3D.f90`.

1.2 Support

This material is based upon work supported by the USA National Science Foundation under Grants No. EAR-0406751 and EAR-0711177, by the French CNRS, French INRIA Sud-Ouest MAGIQUE-3D, French ANR NUMASIS under Grant No. ANR-05-CIGC-002, and European FP6 Marie Curie International Reintegration Grant No. MIRG-CT-2005-017461. Older versions of the code were initially developed by Dimitri Komatitsch at Institut de Physique du Globe (France) and then by Dimitri Komatitsch and Jeroen Tromp at Harvard University (USA). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the USA National Science Foundation, CNRS, INRIA, ANR or the European Marie Curie program.

Chapter 2

Getting Started

The SPECFEM3D software package comes in a gzipped tar ball. In the directory in which you want to install the package, type

```
tar -zxvf SPECFEM3D_V2.0.0.tar.gz
```

The directory `SPECFEM3D_V2.0.0` will then contain the source code. To configure the software for your system, run the `configure` shell script. This script will attempt to guess the appropriate configuration values for your system. However, at a minimum, it is recommended that you explicitly specify the appropriate command names for your Fortran90 compiler and MPI package:

```
./configure FC=ifort MPIFC=mpif90
```

The SPECFEM3D software package relies on the Scotch library to partition the meshes created with CUBIT. Because it is not standard, the path of this library needs to be set with the option `--with-scotch-lib`. Just as an example:

```
./configure FC=ifort MPIFC=mpif90 --with-scotch-lib=/opt/scotch/gcc64/lib
```

To compile a serial version of the code for small meshes that fit on one compute node and can therefore be run serially, run `configure` with the `--without-mpi` option to suppress all calls to MPI.

A summary of the most important configuration variables follows.

`F90` Path to the Fortran90 compiler.

`MPIF90` Path to MPI Fortran90.

`MPI_FLAGS` Some systems require this flag to link to MPI libraries.

`FLAGS_CHECK` Compiler flag for non-critical subroutines.

`FLAGS_NO_CHECK` Compiler flag for creating fast, production-run code for critical subroutines.

The `Makefile` contains a number of suggested entries for various compilers, e.g., Portland, Intel, Absoft, NAG, and Lahey. The software has run on a wide variety of compute platforms, e.g., various PC clusters and machines from Sun, SGI, IBM, Compaq, and NEC. Select the compiler you wish to use on your system and choose the related optimization flags. Note that the default flags in the `Makefile` are undoubtedly not optimal for your system, so we encourage you to experiment with these flags and to solicit advice from your systems administrator. Selecting the right compiler and optimization flags can make a tremendous difference in terms of performance. We welcome feedback on your experience with various compilers and flags.

Now that you have set the compiler information, you need to select a number of flags in the `constants.h` file depending on your system:

LOCAL_PATH_IS_ALSO_GLOBAL Set to `.false.` on most cluster applications. For reasons of speed, the (parallel) mesher typically writes a (parallel) database for the solver on the local disks of the compute nodes. Some systems have no local disks, e.g., BlueGene or the Earth Simulator, and other systems have a fast parallel file system, in which case this flag should be set to `.true.`. Note that this flag is not used by the mesher or the solver; it is only used for some of the post-processing.

The package can run either in single or in double precision. The default is single precision mode because this requires exactly half as much memory. Select your preference by selecting the appropriate setting in the `constants.h` file:

CUSTOM_REAL Set to `SIZE_REAL` for single precision and `SIZE_DOUBLE` for double precision.

In the `precision.h` file:

CUSTOM_MPI_TYPE Set to `MPI_REAL` for single precision and `MPI_DOUBLE_PRECISION` for double precision.

On a new system, it is definitely worth experimenting with single versus double precision simulations to determine which is faster. Note that on many current processors (e.g., Intel, AMD, IBM Power), single precision calculations are often significantly faster; the difference can typically be 10% to 25%. It is therefore often worth using single precision if you can. We recommend running the same calculation once in single precision and in double precision on your system and comparing the seismograms. If they are identical, you should probably select single precision for your future runs.

When running on an SGI add "`setenv TRAP_FPE OFF`" to your .cshrc file *before* compiling in order to turn underflow trapping off.

Finally, before compiling make sure that the subdirectories `obj` and `OUTPUT_FILES` exist within the directory with the source code (`SPECFEM3D_V2.0.0`). The `go_mesher` script discussed in Chapter 3.2 automatically takes care of creating the `OUTPUT_FILES` directory.

Note that if you run very large meshes on a relatively small number of processors, the memory size needed on each processor might become greater than 2 gigabytes, which is the upper limit for 32-bit addressing; in this case, on some compilers you may need to add "`-mcmodel=medium`" to the compiler options otherwise the compiler will display an error message.

Chapter 3

Mesh Generation

3.1 Meshing with CUBIT

3.1.1 Exporting the Mesh

3.1.2 Partitioning the Mesh with xdecompose_mesh_SCOTCH

The SPECFEM3D software package performs large scale simulations in a parallel 'Single Process Multiple Data' way. The spectral element mesh created with CUBIT needs to be distributed on the processors. This partitioning is executed once and for all prior to the execution of the solver so it is referred to as a static mapping.

An efficient partitioning is important because it leverages the overall running time of the application. It amounts to balance the number of elements in each slice while minimizing the communication coasts resulting from the placement of adjacent elements to different processors. decompose_mesh_SCOTCH depends on the Scotch library which provides efficent static mapping, graph and mesh partitioning routines. Scotch is a free software package downloadable from the web page https://gforge.inria.fr/projects/scotch/.

Prior to compiling decompose_mesh_SCOTCH, make sure you have correctly specified the path of the Scotch library with the option --with-scotch-lib of the configure script. Then you are ready to compile, in the directory decompose_mesh_SCOTCH type 'make decompose_mesh_SCOTCH'. If all paths and flags have been set correctly, the executable xdecompose_mesh_SCOTCH should be produced.

The partitioning is done in serial, the synopsis is :

```
./decompose_mesh_SCOTCH nparts input_directory output_directory
```

All the files generated by the Python scripts must be placed in the input_directory folder before running the program.

3.2 Meshing with xmeshfem3D

You are now ready to compile the internal mesher. This is an alternative to CUBIT for the mesh generation of relatively simple geological models. The mesher is no longer dedicated to Southern California and more flexiblity is provided in this version of the package.

In the directory meshfem3D type 'make meshfem3D'. If all paths and flags have been set correctly, the mesher should now compile and produce the executable xmeshfem3D.

Input for the mesh generation program is provided through the parameter file Par_file, which resides in the subdirectory meshfem3D/DATA. Before running the mesher, a number of parameters need to be set in the Par_file. This requires a basic understanding of how the SEM is implemented, and we encourage you to read Komatitsch and Vilotte [1998], Komatitsch and Tromp [1999] and Komatitsch et al. [2004].

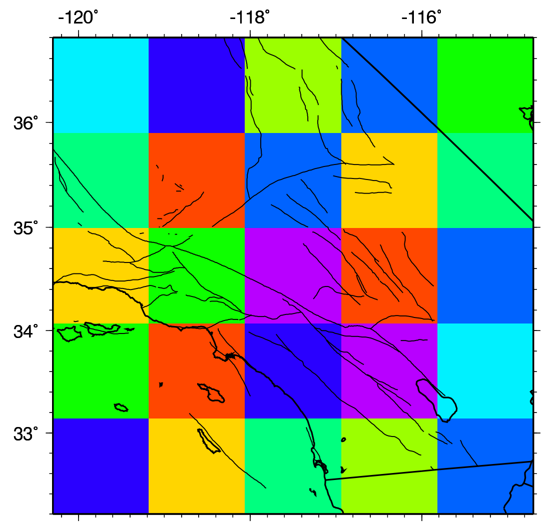

Figure 3.1: For parallel computing purposes, the model block is subdivided in NPROC_XI $\times$ NPROC_ETA slices of elements. In this example we use $5^2 = 25$ processors.

The mesher and the solver use UTM coordinates internally, therefore you need to define the zone number for the UTM projection (e.g., zone 11 for Los Angeles). Use decimal values for latitude and longitude (no minutes/seconds). These values are approximate; the mesher will round them off to define a square mesh in UTM coordinates. When running benchmarks on rectangular models, turn the UTM projection off by using the flag SUPPRESS_UTM_PROJECTION, in which case all 'longitude' parameters simply refer to the x axis, and all 'latitude' parameters simply refer to the y axis. To run the mesher for a global simulation, the following parameters need to be set in the Par_file:

LATITUDE_MIN Minimum latitude in the block (negative for South).

LATITUDE_MAX Maximum latitude in the block.

LONGITUDE_MIN Minimum longitude in the block (negative for West).

LONGITUDE_MAX Maximum longitude in the block.

DEPTH_BLOCK_KM Depth of bottom of mesh in kilometers.

UTM_PROJECTION_ZONE UTM projection zone in which your model resides, only valid when SUPPRESS_UTM_PROJECTION is .false..

SUPPRESS_UTM_PROJECTION set to be .false. when your model range is specified in the geographical coordinates, and needs to be .true. when your model is specified in a cartesian coordinates. UTM PROJECTION ZONE IN WHICH YOUR SIMULATION REGION RESIDES.

INTERFACES_FILE File in which contains the description of the topography and of the interfaces between the different layers of the model, if any. The number of spectral elements in the vertical direction within each layer is also defined in this file.

NEX_XI The number of spectral elements along one side of the block. This number *must* be 8 $\times$ a multiple of NPROC_XI defined below. Based upon benchmarks against semi-analytical discrete wavenumber synthetic seismograms [Komatitsch et al., 2004], determined that a NEX_XI $= 288$ run is accurate to a shortest period of roughly 2 s. Therefore, since accuracy is determined by the number of grid points per shortest wavelength, for any particular value of NEX_XI the simulation will be accurate to a shortest period determined by

$$\text{shortest period (s)} = (288/\texttt{NEX\_XI}) \times 2. \tag{3.1}$$

The number of grid points in each orthogonal direction of the reference element, i.e., the number of Gauss-Lobatto-Legendre points, is determined by NGLLX in the constants.h file. We generally use NGLLX $= 5$, for a total of $5^3 = 125$ points per elements. We suggest not to change this value.

NEX_ETA The number of spectral elements along the other side of the block. This number *must* be $8 \times$ a multiple of NPROC_ETA defined below.

NPROC_XI The number of processors or slices along one side of the block (see Figure 3.1); we must have NEX_XI $= 8 \times c \times$ NPROC_XI, where $c \geq 1$ is a positive integer.

NPROC_ETA The number of processors or slices along the other side of the block; we must have NEX_ETA $= 8 \times c \times$ NPROC_ETA, where $c \geq 1$ is a positive integer.

USE_REGULAR_MESH set to be .true. if you want a perfectly regular mesh or .false. if you want to add doubling horizontal layers to coarsen the mesh. In this case, you also need to provide additional information by setting up the next three parameters.

NDOUBLINGS The number of horizontal doubling layers. Must be set to 1 or 2 if USE_REGULAR_MESH is set to .true..

NZ_DOUBLING_1 The position of the first doubling layer (only interpreted if USE_REGULAR_MESH is set to .true.).

NZ_DOUBLING_2 The position of the second doubling layer (only interpreted if USE_REGULAR_MESH is set to .true. and if NDOUBLINGS is set to 2).

CREATE_ABAQUS_FILES Set this flag to .true. to save Abaqus FEA (www.simulia.com) mesh files for subsequent viewing. Turning the flag on generates files in the LOCAL_PATH directory. See Section 7.1 for a discussion of mesh viewing features.

CREATE_DX_FILES Set this flag to .true. to save OpenDX (www.opendx.org) mesh files for subsequent viewing.

LOCAL_PATH Directory in which the databases generated by the mesher will be written. Generally one uses a directory on the local disk of the compute nodes, although on some machines these databases are written on a parallel (global) file system (see also the earlier discussion of the LOCAL_PATH_IS_ALSO_GLOBAL flag in Chapter 2). The mesher generates the necessary databases in parallel, one set for each of the NPROC_XI $\times$ NPROC_ETA slices that constitutes the mesh (see Figure 3.1). After the mesher finishes, you can log in to one of the compute nodes and view the contents of the LOCAL_PATH directory to see the (many) files generated by the mesher.

NMATERIALS The number of different materials in your model. In the following lines, each material needs to be defined as :

```
material_ID rho vp vs Q_flag anisotropy_flag domain_ID
```

where

- Q_flag : 0=no attenuation / standard Q attenutation value
- anisotropy_flag : 0=no anisotropy / 1,2,.. check with implementation in aniso_model.f90
- domain_id : 1=acoustic / 2=elastic / 3=poroelastic

NMATERIALS The number of regions in the mesh. In the following lines, because the mesh is regular or 'almost regular', each region is defined as :

```
XI_begin XI_end ETA_begin ETA_end material_ID
```

The topography of the model is defined as a set of elevation values on a regular 2D grid. It is also posible to define interfaces between the layers of the model in the same way.

The file defined in `INTERFACES_FILE` contains the settings of the topography grid and of the interfaces grids. The number of interfaces, including the topography, needs to be set at the first line. Then, from the bottom to the top of the model, you need to define the grids with several parameters : number of points along x and y, minimal x and y coordinates, spacing between points and the file in which the elevation values are stored. At the end of this file, you simply need to set the number of spectral elements in the vertical direction for each layer.

Finally, depending on your system, you might need to provide a file that tells MPI what compute nodes to use for the simulations. The file must have a number of entries (one entry per line) at least equal to the number of processors needed for the run. A sample file is provided in the file `mymachines`. This file is not used by the mesher or solver, but is required by the `go_mesher` and `go_solver` default job submission scripts. See Chapter 8 for information about running the code on a system with a scheduler, e.g., LSF.

Now that you have set the appropriate parameters in the `Par_file` and have compiled the mesher, you are ready to launch it! This is most easily accomplished based upon the `go_mesher` script. When you run on a PC cluster, the script assumes that the nodes are named n001, n002, etc. If this is not the case, change the `tr -d 'n'` line in the script. You may also need to edit the last command at the end of the script that invokes the `mpirun` command. See Chapter 8 for information about running the code on a system with a scheduler, e.g., LSF.

Mesher output is provided in the `OUTPUT_FILES` directory in `output_mesher.txt`; this file provides lots of details about the mesh that was generated. Alternatively, output can be directed to the screen instead by uncommenting a line in `constants.h`:

```
! uncomment this to write messages to the screen
! integer, parameter :: IMAIN = ISTANDARD_OUTPUT
```

The quality of the mesh may be inspected more precisely based upon the serial code `check_mesh_quality_CUBIT_Abaqus.f` In the directory `check_mesh_quality_CUBIT_Abaqus`, type

```
make check_mesh_quality_CUBIT_Abaqus
```

and then use

```
xcheck_mesh_quality_CUBIT_Abaqus
```

to generate an AVS output file (`AVS_meshquality.inp` in AVS UCD format) or OpenDX output file (`DX_meshquality.dx`) that can be used to investigate mesh quality, e.g, skewness of elements and a Gnuplot histogram (`mesh_quality_histogram.txt`) that can be plotted with gnuplot (type '`gnuplot plot_mesh_quality_histogram.gnu`'). The histogram is also printed to the screen. If you want to start designing your own meshes, this tool is useful for viewing your creations. You are striving for meshes with elements with 'cube-like' dimensions, e.g., the mesh should contain no very elongated or skewed elements.

Running this code is optional because no information needed by the solver is generated.

Chapter 4

Creating the Distributed Databases

Either you previously used `xmeshfem3D` or `xdecompose_mesh_SCOTCH`, the next step in the workflow is to compile `xgenerate_databases`. This program is going to create all the missing information needed by the SEM solver. In the main directory type '`make generate_databases`'. Input for the program is provided through the main parameter file `Par_file`, which resides in the subdirectory `DATA`. Before running `xgenerate_databases`, a number of parameters need to be set in the `Par_file`:

SIMULATION_TYPE is set to 1 for forward simulations, 2 for adjoint simulations (see Section 6.2) and 3 for kernel simulations (see Section 7.3).

SAVE_FORWARD is only set to `.true.` for a forward simulation with the last frame of the simulation saved, as part of the finite-frequency kernel calculations (see Section 7.3). For a regular forward simulation, leave `SIMULATION_TYPE` and `SAVE_FORWARD` at their default values.

UTM_PROJECTION_ZONE UTM projection zone in which your model resides, only valid when `SUPPRESS_UTM_PROJECTION` is `.false.`.

SUPPRESS_UTM_PROJECTION set to be `.false.` when your model range is specified in the geographical coordinates, and needs to be `.true.` when your model is specified in a cartesian coordinates. UTM PROJECTION ZONE IN WHICH YOUR SIMULATION REGION RESIDES.

NPROC The number of MPI processors, each one is assigned one slice of the whole mesh.

NSTEP The number of time steps of the simulation. This controls the length of the numerical simulation, i.e., twice the number of time steps requires twice as much CPU time. This feature is not used at the time of meshing but is required for the solver, i.e., you may change this parameter after running `xgenerate_databases`.

DT The length of each time step in seconds. If you used xmeshfem3D to generate your mesh, you should set the value suggested in `meshfem3D/OUTPUT_FILES/output_mesher.txt`.

OCEANS Set to `.true.` if the effect of the oceans on seismic wave propagation should be incorporated based upon the approximate treatment discussed in Komatitsch and Tromp [2002b]. This feature is inexpensive from a numerical perspective, both in terms of memory requirements and CPU time. This approximation is accurate at periods of roughly 20 s and longer. At shorter periods the effect of water phases/reverberations is not taken into account, even when the flag is on.

TOPOGRAPHY Set to `.true.` if topography and bathymetry should be incorporated based upon model ETOPO5 [NOAA, 1988]. This feature adds no cost to the simulation.

ATTENUATION Set to `.true.` if attenuation should be incorporated. Turning this feature on increases the memory requirements significantly (roughly by a factor of 1.5), and is numerically fairly expensive. See Komatitsch and Tromp [1999, 2002a] for a discussion on the implementation of attenuation based upon standard linear solids.

USE_OLSEN_ATTENUATION Set to `.true.` if you want to use the attenuation model that scaled from the velocity model using Olsen's empirical relation (reference).

ABSORBING_CONDITIONS Set to .true. to turn on Clayton-Enquist absorbing boundary conditions (see Komatitsch and Tromp [1999]).

RECORD_LENGTH_IN_MINUTES Choose the desired record length of the synthetic seismograms (in minutes). This controls the length of the numerical simulation, i.e., twice the record length requires twice as much CPU time. This feature is not used at the time of meshing but is required for the solver, i.e., you may change this parameter after running xgenerate_databases.

MOVIE_SURFACE Set to .false., unless you want to create a movie of seismic wave propagation on the Earth's surface. Turning this option on generates large output files. See Section 7.2 for a discussion on the generation of movies. This feature is only relevant for the solver.

MOVIE_VOLUME Set to .false., unless you want to create a movie of seismic wave propagation in the Earth's interior. Turning this option on generates huge output files. See Section 7.2 for a discussion on the generation of movies. This feature is only relevant for the solver.

NTSTEP_BETWEEN_FRAMES Determines the number of timesteps between movie frames. Typically you want to save a snapshot every 100 timesteps. The smaller you make this number the more output will be generated! See Section 7.2 for a discussion on the generation of movies. This feature is only relevant for the solver.

CREATE_SHAKEMAP Set this flag to .true. to create a ShakeMap®, i.e., a peak ground velocity map of the maximum absolute value of the two horizontal components of the velocity vector.

SAVE_DISPLACEMENT Set this flag to .true. if you want to save the displacement instead of velocity for the movie frames.

USE_HIGHRES_FOR_MOVIES Set this flag to .true. if you want to save the values at all the NGLL grid points for the movie frames.

SAVE_MESH_FILES Set this flag to .true. to save AVS (www.avs.com), OpenDX (www.opendx.org), or ParaView (www.paraview.org) mesh files for subsequent viewing. Turning the flag on generates large (distributed) files in the LOCAL_PATH directory. See Section 7.1 for a discussion of mesh viewing features.

LOCAL_PATH Directory in which the databases and the synthetics will be written. Generally one uses a directory on the local disk of the compute nodes, although on some machines these databases are written on a parallel (global) file system (see also the earlier discussion of the LOCAL_PATH_IS_ALSO_GLOBAL flag in Chapter 2). xgenerate_databases generates the necessary databases in parallel, one set for each of the NPROC_XI × NPROC_ETA slices that constitutes the mesh (see Figure 3.1). After the mesher finishes, you can log in to one of the compute nodes and view the contents of the LOCAL_PATH directory to see the (many) files generated by xgenerate_databases.

NTSTEP_BETWEEN_OUTPUT_INFO This parameter specifies the interval at which basic information about a run is written to the file system (timestamp* files in the OUTPUT_FILES directory). If you have access to a fast machine, set NTSTEP_BETWEEN_OUTPUT_INFO to a relatively high value (e.g., at least 100, or even 1000 or more) to avoid writing output text files too often. This feature is not used at the time of meshing. One can set this parameter to a larger value than the number of time steps to avoid writing output during the run.

NTSTEP_BETWEEN_OUTPUT_SEISMOS This parameter specifies the interval at which synthetic seismograms are written in the LOCAL_PATH directory. If a run crashes, you may still find usable (but shorter than requested) seismograms in this directory. On a fast machine set NTSTEP_BETWEEN_OUTPUT_SEISMOS to a relatively high value to avoid writing to the seismograms too often. This feature is only relevant for the solver.

PRINT_SOURCE_TIME_FUNCTION Turn this flag on to print information about the source time function in the file OUTPUT_FILES/plot_source_time_function.txt. This feature is only relevant for the solver.

Chapter 5

Running the Solver xspecfem3D

Now that you have successfully generated the databases, you are ready to compile the solver. For reasons of speed, the solver uses static memory allocation. Therefore it needs to be recompiled (type 'make clean' and 'make specfem3D') every time one reruns xgenerate_databases. To compile the solver one needs a file created by xgenerate_databases in the directory OUTPUT_FILES called values_from_mesher.h, which contains parameters describing the static size of the arrays as well as the setting of certain flags.

The solver needs three input files in the DATA directory to run: the Par_file which was discussed in detail in Chapters 3.1 and 3.2, the earthquake source parameter file CMTSOLUTION, and the stations file STATIONS. Most parameters in the Par_file should be set prior to running the mesher. Only the following parameters may be changed after running xgenerate_databases:

- the simulation type control parameters: SIMULATION_TYPE and SAVE_FORWARD
- the time step parameters NSTEP and DT
- the movie control parameters MOVIE_SURFACE, MOVIE_VOLUME, and NTSTEPS_BETWEEN_FRAMES
- the ShakeMap®option CREATE_SHAKEMAP
- the output information parameters NTSTEP_BETWEEN_OUTPUT_INFO and NTSTEP_BETWEEN_OUTPUT_SEISMOS
- the PRINT_SOURCE_TIME_FUNCTION flags

Any other change to the Par_file implies rerunning both the mesher and the solver.

For any particular earthquake, the CMTSOLUTION file that represents the point source may be obtained directly from the Harvard Centroid-Moment Tensor (CMT) web page (www.seismology.harvard.edu). It looks like this:

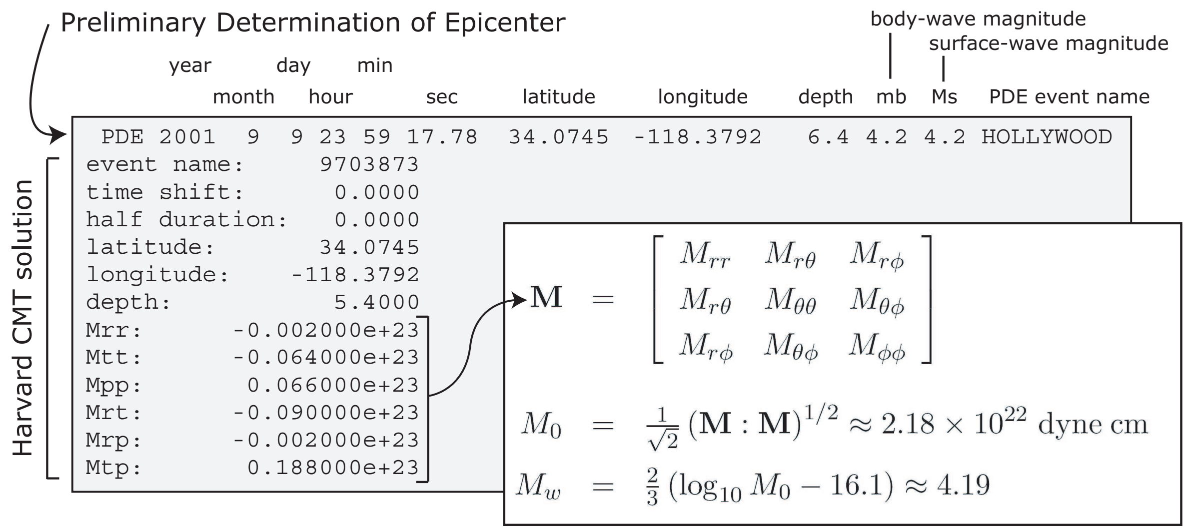

Figure 5.1: `CMTSOLUTION` file based on the format from the Harvard CMT catalog. $\mathbf{M}$ is the moment tensor, M_0 is the seismic moment, and M_w is the moment magnitude.

The `CMTSOLUTION` should be edited in the following way:

- Set the `time shift` parameter equal to 0.0 (the solver will not run otherwise.) The time shift parameter would simply apply an overall time shift to the synthetics, something that can be done in the post-processing (see Section 9.3).

- For point-source simulations (see finite sources, page 15) we recommend setting the source half-duration parameter `half duration` equal to zero, which corresponds to simulating a step source-time function, i.e., a moment-rate function that is a delta function. If `half duration` is not set to zero, the code will use a Gaussian (i.e., a signal with a shape similar to a 'smoothed triangle', as explained in Komatitsch and Tromp [2002a] and shown in Fig 5.2) source-time function with half-width `half duration`. We prefer to run the solver with `half duration` set to zero and convolve the resulting synthetic seismograms in post-processing after the run, because this way it is easy to use a variety of source-time functions (see Section 9.3). Komatitsch and Tromp [2002a] determined that the noise generated in the simulation by using a step source time function may be safely filtered out afterward based upon a convolution with the desired source time function and/or low-pass filtering. Use the serial code `convolve_source_timefunction.f90` and the script `convolve_source_timefunction.csh` for this purpose, or alternatively use signal-processing software packages such as SAC (`www.llnl.gov/sac`). Type

  ```
  make convolve_source_timefunction
  ```

  to compile the code and then set the parameter `hdur` in `convolve_source_timefunction.csh` to the desired half-duration.

- The zero time of the simulation corresponds to the center of the triangle/Gaussian, or the centroid time of the earthquake. The start time of the simulation is $t = -1.5 *$ `half duration` (the 1.5 is to make sure the moment rate function is very close to zero when starting the simulation). To convert to absolute time t_{abs}, set

  $$t_{\text{abs}} = t_{\text{pde}} + \texttt{time shift} + t_{\text{synthetic}}$$

  where t_{pde} is the time given in the first line of the `CMTSOLUTION`, `time shift` is the corresponding value from the original `CMTSOLUTION` file and $t_{\text{synthetic}}$ is the time in the first column of the output seismogram.

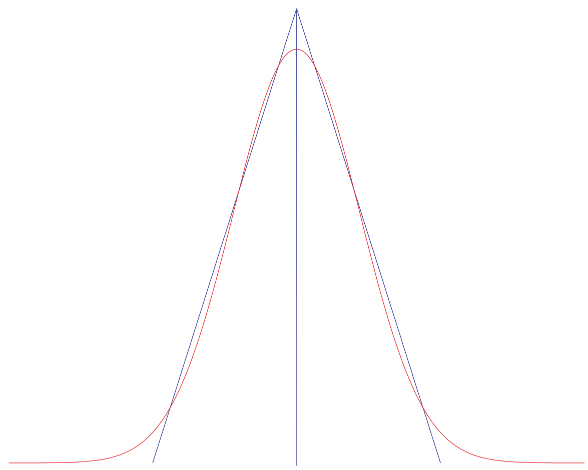

Figure 5.2: Comparison of the shape of a triangle and the Gaussian function actually used.

Centroid latitude and longitude should be provided in geographical coordinates. The code converts these coordinates to geocentric coordinates [Dahlen and Tromp, 1998]. Of course you may provide your own source representations by designing your own `CMTSOLUTION` file. Just make sure that the resulting file adheres to the Harvard CMT conventions (see Appendix A). Note that the first line in the `CMTSOLUTION` file is the Preliminary Determination of Earthquakes (PDE) solution performed by the USGS NEIC, which is used as a seed for the Harvard CMT inversion. The PDE solution is based upon P waves and often gives the hypocenter of the earthquake, i.e., the rupture initiation point, whereas the CMT solution gives the 'centroid location', which is the location with dominant moment release. The PDE solution is not used by our software package but must be present anyway in the first line of the file.

To simulate a kinematic rupture, i.e., a finite-source event, represented in terms of $N_{\rm sources}$ point sources, provide a `CMTSOLUTION` file that has $N_{\rm sources}$ entries, one for each subevent (i.e., concatenate $N_{\rm sources}$ `CMTSOLUTION` files to a single `CMTSOLUTION` file). At least one entry (not necessarily the first) must have a zero `time shift`, and all the other entries must have non-negative `time shift`. Each subevent can have its own half duration, latitude, longitude, depth, and moment tensor (effectively, the local moment-density tensor).

Note that the zero in the synthetics does NOT represent the hypocentral time or centroid time in general, but the timing of the *center* of the source triangle with zero `time shift` (Fig 5.3).

Although it is convenient to think of each source as a triangle, in the simulation they are actually Gaussians (as they have better frequency characteristics). The relationship between the triangle and the gaussian used is shown in Fig 5.2. For finite fault simulations it is usually not advisable to use a zero half duration and convolve afterwards, since the half duration is generally fixed by the finite fault model.

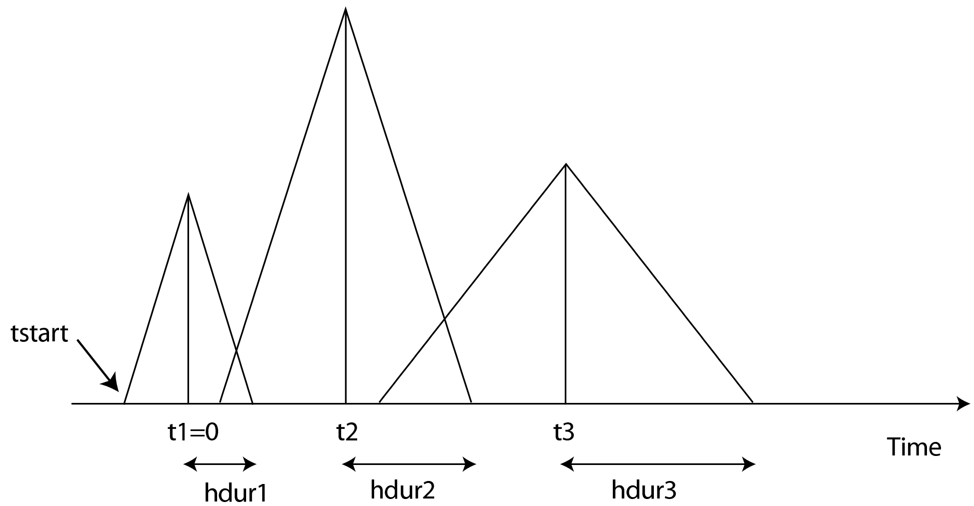

Figure 5.3: Example of timing for three sources. The center of the first source triangle is defined to be time zero. Note that this is NOT in general the hypocentral time, or the start time of the source (marked as tstart). The parameter `time shift` in the `CMTSOLUTION` file would be t1(=0), t2, t3 in this case, and the parameter `half duration` would be hdur1, hdur2, hdur3 for the sources 1, 2, 3 respectively.

The solver can calculate seismograms at any number of stations for basically the same numerical cost, so the user is encouraged to include as many stations as conceivably useful in the `STATIONS` file, which looks like this:

Station	Network	Latitude (deg)	Longitude (deg)	Elevation (m)	Burial (m)
ASBS	AZ	33.6208	-116.4664	0.0	0.0
BZN	AZ	33.4915	-116.6670	0.0	0.0
CRY	AZ	33.5654	-116.7373	0.0	0.0
ELKS	AZ	33.5813	-116.4496	0.0	0.0
AGA	CI	33.6384	-116.4011	0.0	0.0
AGO	CI	34.1465	-118.7670	0.0	0.0
ALP	CI	34.6870	-118.2995	0.0	0.0
BAK	CI	35.3444	-119.1044	0.0	0.0
BAR	CI	32.6801	-116.6722	0.0	0.0
BBA	CI	34.1955	-118.3534	0.0	0.0
BBB	CI	33.3526	-115.7332	0.0	0.0
BBR	CI	34.2623	-116.9207	0.0	0.0
BBS	CI	33.9214	-116.9805	0.0	0.0
⋮	⋮	⋮	⋮	⋮	⋮

Figure 5.4: Sample `STATIONS` file. Station latitude and longitude should be provided in geographical coordinates. The width of the station label should be no more than 32 characters (see `MAX_LENGTH_STATION_NAME` in the `constants.h` file), and the network label should be no more than 8 characters (see `MAX_LENGTH_NETWORK_NAME` in the `constants.h` file).

Each line represents one station in the following format:

```
Station Network Latitude (degrees) Longitude (degrees) Elevation (m) burial (m)
```

The mesher filters the list of stations in file `DATA/STATIONS` to exclude stations that are not located within the region given in the `Par_file` (between `LATITUDE_MIN` and `LATITUDE_MAX` and between `LONGITUDE_MIN` and `LONGITUDE_MAX`). The filtered file is called `DATA/STATIONS_FILTERED`.

Solver output is provided in the `OUTPUT_FILES` directory in the `output_solver.txt` file. Output can be directed to the screen instead by uncommenting a line in `constants.h`:

```
! uncomment this to write messages to the screen
! integer, parameter :: IMAIN = ISTANDARD_OUTPUT
```

On PC clusters the seismogram files are generally written to the local disks (the path `LOCAL_PATH` in the `Par_file`) and need to be gathered at the end of the simulation.

While the solver is running, its progress may be tracked by monitoring the '`timestamp*`' files in the `OUTPUT_FILES` directory. These tiny files look something like this:

```
Time step #          10000
Time:     108.4890      seconds
Elapsed time in seconds =    1153.28696703911
Elapsed time in hh:mm:ss =     0 h 19 m 13 s
Mean elapsed time per time step in seconds =     0.115328696703911
Max norm displacement vector U in all slices (m) =    1.0789589E-02
```

The `timestamp*` files provide the `Mean elapsed time per time step in seconds`, which may be used to assess performance on various machines (assuming you are the only user on a node), as well as the `Max norm displacement vector U in all slices (m)`. If something is wrong with the model, the mesh, or the source, you will see the code become unstable through exponentially growing values of the displacement and fluid potential with time, and ultimately the run will be terminated by the program. You can control the rate at which the timestamp files are written based upon the parameter `NTSTEP_BETWEEN_OUTPUT_INFO` in the `Par_file`.

Having set the `Par_file` parameters, and having provided the `CMTSOLUTION` and `STATIONS` files, you are now ready to launch the solver! This is most easily accomplished based upon the `go_solver` script (See Chapter 8 for information about running through a scheduler, e.g., LSF). You may need to edit the last command at the end of the script that invokes the `mpirun` command. The `runall` script compiles and runs both mesher and solver in sequence. This is a safe approach that ensures using the correct combination of mesher output and solver input.

It is important to realize that the CPU and memory requirements of the solver are closely tied to choices about attenuation (`ATTENUATION`) and the nature of the model (i.e., isotropic models are cheaper than anisotropic models). We encourage you to run a variety of simulations with various flags turned on or off to develop a sense for what is involved.

For the same model, one can rerun the solver for different events by simply changing the `CMTSOLUTION` file, or for different stations by changing the `STATIONS` file. There is no need to rerun the mesher. Of course it is best to include as many stations as possible, since this does not add to the cost of the simulation.

Chapter 6

Adjoint Simulations

Adjoint simulations are generally performed for two distinct applications. First, they can be used for earthquake source inversions, especially earthquakes with large ruptures such as the Lander's earthquake [Wald and Heaton, 1994]. Second, they can be used to generate finite-frequency sensitivity kernels that are a critical part of tomographic inversions based upon 3D reference models [Tromp et al., 2005, Liu and Tromp, 2006, Tromp et al., 2008, Liu and Tromp, 2008]. In either case, source parameter or velocity structure updates are sought to minimize a specific misfit function (e.g., waveform or traveltime differences), and the adjoint simulation provides a means of computing the gradient of the misfit function and further reducing it in successive iterations. Applications and procedures pertaining to source studies and finite-frequency kernels are discussed in Sections 6.1 and 6.2, respectively. The two related parameters in the `Par_file` are `SIMULATION_TYPE` (1 or 2) and the `SAVE_FORWARD` (boolean).

6.1 Adjoint Simulations for Sources

In the case where a specific misfit function is minimized to invert for the earthquake source parameters, the gradient of the misfit function with respect to these source parameters can be computed by placing time-reversed seismograms at the receivers and using them as sources in an adjoint simulation, and then the value of the gradient is obtained from the adjoint seismograms recorded at the original earthquake location.

1. **Prepare the adjoint sources**

   (a) First, run a regular forward simlation (`SIMULATION_TYPE = 1` and `SAVE_FORWARD = .false.`). You can automatically set these two variables using the `UTILS/change_simulation_type.pl` script:

   ```
   UTILS/change_simulation_type.pl -f
   ```

   and then collect the recorded seismograms at all the stations given in `DATA/STATIONS`.

   (b) Then select the stations for which you want to compute the time-reversed adjoint sources and run the adjoint simulation, and compile them into the `DATA/STATIONS_ADJOINT` file, which has the same format as the regular `DATA/STATIONS` file.

   - Depending on what type of misfit function is used for the source inversion, adjoint sources need to be computed from the original recorded seismograms for the selected stations and saved in the `SEM/` directory with the format `STA.NT.BH?.adj`, where `STA`, `NT` are the station name and network code given in the `DATA/STATIONS_ADJOINT` file, and `BH?` represents the component name of a particular adjoint seismogram.
   - The adjoint seismograms are in the same format as the original seismogram (`STA.NT.BH?.sem?`), with the same start time, time interval and record length.

   (c) Notice that even if you choose to time reverse only one component from one specific station, you still need to supply all three components because the code is expecting them (you can set the other two components to be zero).

(d) Also note that since time-reversal is done in the code itself, no explicit time-reversing is needed for the preparation of the adjoint sources, i.e., the adjoint sources are in the same forward time sense as the original recorded seismograms.

2. **Set the related parameters and run the adjoint simulation**
   In the `DATA/Par_file`, set the two related parameters to be `SIMULATION_TYPE = 2` and `SAVE_FORWARD = .false.`. More conveniently, use the scripts `UTILS/change_simulation_type.pl` to modify the `Par_file` automatically (`change_simulation_type.pl -a`). Then run the solver to launch the adjoint simulation.

3. **Collect the seismograms at the original source location**

   After the adjoint simulation has completed successfully, collect the seismograms from `LOCAL_PATH`.

   - These adjoint seismograms are recorded at the locations of the original earthquake sources given by the `DATA/CMTSOLUTION` file, and have names of the form `S?????.NT.S??.sem` for the six-component strain tensor (`SNN,SEE,SZZ,SNE,SNZ,SEZ`) at these locations, and `S?????.NT.BH?.sem` for the three-component displacements (`BHN,BHE,BHZ`) recorded at these locations.
   - `S?????` denotes the source number; for example, if the original `CMTSOLUTION` provides only a point source, then the seismograms collected will start with `S00001`.
   - These adjoint seismograms provide critical information for the computation of the gradient of the misfit function.

6.2 Adjoint Simulations for Finite-Frequency Kernels (Kernel Simulation)

Finite-frequency sensitivity kernels are computed in two successive simulations (please refer to Liu and Tromp [2006] and Tromp et al. [2008] for details).

1. **Run a forward simulation with the state variables saved at the end of the simulation**

   Prepare the `CMTSOLUTION` and `STATIONS` files, set the parameters `SIMULATION_TYPE = 1` and `SAVE_FORWARD = .true.` in the `Par_file` (`change_simulation_type -F`), and run the solver.

   - Notice that attenuation is not implemented yet for the computation of finite-frequency kernels; therefore set `ATTENUATION = .false.` in the `Par_file`.
   - We also suggest you modify the half duration of the `CMTSOLUTION` to be similar to the accuracy of the simulation (see Equation 3.1) to avoid too much high-frequency noise in the forward wavefield, although theoretically the high-frequency noise should be eliminated when convolved with an adjoint wavefield with the proper frequency content.
   - This forward simulation differs from the regular simulations (`SIMULATION_TYPE = 1` and `SAVE_FORWARD = .false.`) described in the previous chapters in that the state variables for the last time step of the simulation, including wavefields of the displacement, velocity, acceleration, etc., are saved to the `LOCAL_PATH` to be used for the subsequent simulation.
   - For regional simulations, the files recording the absorbing boundary contribution are also written to the `LOCAL_PATH` when `SAVE_FORWARD = .true.`.

2. **Prepare the adjoint sources**

   The adjoint sources need to be prepared the same way as described in the Section 1.

   - In the case of travel-time finite-frequency kernel for one source-receiver pair, i.e., point source from the `CMTSOLUTION`, and one station in the `STATIONS_ADJOINT` list, we supply a sample program in `UTILS/xcut_velocity` to cut a certain portion of the original displacement seismograms and convert it into the proper adjoint source to compute the finite-frequency kernel.

     ```
     xcut_velocity t1 t2 ifile[0-5] E/N/Z-ascii-files [baz]
     ```

where `t1` and `t2` are the start and end time of the portion you are interested in, `ifile` denotes the component of the seismograms to be used (0 for all three components, 1 for East, 2 for North, and 3 for vertical, 4 for transverse, and 5 for radial component), `E/N/Z-ascii-files` indicate the three-component displacement seismograms in the right order, and `baz` is the back-azimuth of the station. Note that `baz` is only supplied when `ifile` = 4 or 5.

3. **Run the kernel simulation**

   With the successful forward simulation and the adjoint source ready in `SEM/`, set `SIMULATION_TYPE = 3` and `SAVE_FORWARD = .false.` in the `Par_file(change_simulation_type.pl -b), and` rerun the solver.

   - The adjoint simulation is launched together with the back reconstruction of the original forward wavefield from the state variables saved from the previous forward simulation, and the finite-frequency kernels are computed by the interaction of the reconstructed forward wavefield and the adjoint wavefield.
   - The back-reconstructed seismograms at the original station locations are saved to the `LOCAL_PATH` at the end of the kernel simulations, and can be collected to the local disk.
   - These back-constructed seismograms can be compared with the time-reversed original seismograms to assess the accuracy of the backward reconstruction, and they should match very well.
   - The arrays for density, P-wave speed and S-wave speed kernels are also saved in the `LOCAL_PATH` with the names `proc??????_rho(alpha,beta)_kernel.bin`, where `proc??????` represents the processor number, `rho(alpha,beta)` are the different types of kernels.

In general, the three steps need to be run sequentially to assure proper access to the necessary files. If the simulations are run through some cluster scheduling system (e.g., LSF), and the forward simulation and the subsequent kernel simulations cannot be assigned to the same set of computer nodes, the kernel simulation will not be able to access the database files saved by the forward simulation. Solutions for this dilemma are provided in Chapter 8. Visualization of the finite-frequency kernels is discussed in Section 7.3.

Chapter 7

Graphics

7.1 Meshes

Use the serial code combine_AVS_DX.f90 (type 'make combine_AVS_DX' and then 'xcombine_AVS_DX') to generate AVS (www.avs.com) output files (in AVS UCD format) or OpenDX (www.opendx.org) output files showing the mesh, the MPI partition (slices), the NCHUNKS chunks, the source and receiver location, etc. Use the AVS UCD files AVS_continent_boundaries.inp and AVS_plate_boundaries.inp or the OpenDX files DX_continent_boundaries.dx and DX_plate_boundaries.dx for reference.

7.2 Movies

To make a surface or volume movie of the simulation, set parameters MOVIE_SURFACE, MOVIE_VOLUME, and NTSTEP_BETWEEN_FRAMES in the Par_file. Turning on the movie flags, in particular MOVIE_VOLUME, produces large output files. MOVIE_VOLUME files are saved in the LOCAL_PATH directory, whereas MOVIE_SURFACE output files are saved in the OUTPUT_FILES directory. We save the velocity field. The look of a movie is determined by the half-duration of the source. The half-duration should be large enough so that the movie does not contain frequencies that are not resolved by the mesh, i.e., it should not contain numerical noise. This can be accomplished by selecting a CMT HALF_DURATION > 1.1 $\times$ smallest period (see figure 5.1). When MOVIE_SURFACE = .true., the half duration of each source in the CMTSOLUTION file is replaced by

$$\sqrt{(\mathtt{HALF\_DURATION}^2 + \mathtt{HDUR\_MOVIE}^2)}$$

> **NOTE:** If HDUR_MOVIE is set to 0.0, the code will select the appropriate value of 1.1 $\times$ smallest period. As usual, for a point source one can set HALF_DURATION in the Par_file to be 0.0 and HDUR_MOVIE = 0.0 to get the highest frequencies resolved by the simulation, but for a finite source one would keep all the HALF_DURATIONs as prescribed by the finite source model and set HDUR_MOVIE = 0.0.

7.2.1 Movie Surface

When running xspecfem3D with the MOVIE_SURFACE flag turned on, the code outputs moviedata?????? files in the OUTPUT_FILES directory. The files are in a fairly complicated binary format, but there are two programs provided to convert the output into more user friendly formats. The first one, create_movie_AVS_DX.f90, outputs data in ASCII, OpenDX, AVS, or ParaView format. Run the code from the source directory (type 'make create_movie_AVS_DX' first) to create an input file in your format of choice. The code will prompt the user for input parameters. The second program create_movie_GMT.f90 outputs ascii xyz files, convenient for use with GMT. This code uses significantly less memory than create_movie_AVS_DX.f90 and is therefore useful for high resolution runs.

The SPECFEM3D code is running in near real-time to produce animations of southern California earthquakes via the web; see Southern California ShakeMovie®(www.shakemovie.caltech.edu).

7.3 Finite-Frequency Kernels

The finite-frequency kernels computed as explained in Section 6.2 are saved in the `LOCAL_PATH` at the end of the simulation. Therefore, we first need to collect these files on the front end, combine them into one mesh file, and visualize them with some auxilliary programs.

1. **Create slice files**

   We will only discuss the case of one source-receiver pair, i.e., the so-called banana-doughnut kernels. Although it is possible to collect the kernel files from all slices on the front end, it usually takes up too much storage space (at least tens of gigabytes). Since the sensitivity kernels are the strongest along the source-receiver great circle path, it is sufficient to collect only the slices that are along or close to the great circle path.

   A Perl script `UTILS/slice_number.pl` that calls MATLAB can help to figure out the slice numbers that lie along the great circle path (both the minor and major arcs), as well as the slice numbers required to produce a full picture of the inner core if your kernel also illuminates the inner core.

   (a) On machines where you have MATLAB access, copy the `CMTSOLUTION` file, `STATIONS_ADJOINT`, and `Par_file`, and run:

   ```
   UTILS/slice_number.pl Par_file output_solver.txt slice_file
   ```

   which will generate a `slices_file`.

   (b) For cases with multiple sources and multiple receivers, you need to provide a slice file before proceeding to the next step.

2. **Collect the kernel files**

   After obtaining the slice files, you can collect the corresponding kernel files from the given slices.

   (a) You can use or modify the script `UTILS/copy_databases.pl` to accomplish this:

   ```
   UTILS/copy_database.pl slice_file lsf_machine_file filename [jobid]
   ```

   where `lsf_machine_file` is the machine file generated by the LSF scheduler, `filename` is the kernel name (e.g., `rho_kernel`, `alpha_kernel` and `beta_kernel`), and the optional `jobid` is the name of the subdirectory under `LOCAL_PATH` where all the kernel files are stored.

   (b) After executing this script, all the necessary mesh topology files as well as the kernel array files are collected to the local directory of the front end.

3. **Combine kernel files into one mesh file**

   We use an auxilliary program `combine_paraview_data.f90` to combine the kernel files from all slices into one mesh file.

   (a) Compile it in the global code directory:

   ```
   make combine_paraview_data
   xcombine_paraview_data slice_list filename input_dir output_dir high/low-resolution
   ```

   where `input_dir` is the directory where all the individual kernel files are stored, and `output_dir` is where the mesh file will be written.

   (b) Use 1 for a high-resolution mesh, outputting all the GLL points to the mesh file, or use 0 for low resolution, outputting only the corner points of the elements to the mesh file.

   (c) The output mesh file will have the name `filename_rho(alpha,beta).mesh`

4. **Convert mesh files into .vtu files**

   (a) We next convert the `.mesh` file into the VTU (Unstructured grid file) format which can be viewed in ParaView, for example:

   ```
   UTILS/mesh2vtu.pl -i file.mesh -o file.vtu
   ```

(b) Notice that this Perl script uses a program `mesh2vtu` in the `UTILS/mesh2vtu` directory, which further uses the VTK (`http://www.vtk.org/`) run-time library for its execution. Therefore, make sure you have them properly set in the script according to your system.

5. **Copy over the source and receiver .vtk file**

   In the case of a single source and a single receiver, the simulation also generates the `OUTPUT_FILES/sr.vtk` file to describe the source and receiver locations, which can also be viewed in Paraview in the next step.

6. **View the mesh in ParaView**

   Finally, we can view the mesh in ParaView (`www.paraview.org`).

   (a) Open ParaView.

   (b) From the top menu, File →Open data, select `file.vtu`, and click the Accept button.

   - If the mesh file is of moderate size, it shows up on the screen; otherwise, only the bounding box is shown.

   (c) Click Display Tab → Display Style → Representation and select wireframe of surface to display it.

   (d) To create a cross-section of the volumetric mesh, choose Filter → cut, and under Parameters Tab, choose Cut Function → plane.

   (e) Fill in center and normal information given by the `global_slice_number.pl` script (either from the standard output or from `normal_plane.txt` file).

   (f) To change the color scale, go to Display Tab → Color → Edit Color Map and reselect lower and upper limits, or change the color scheme.

   (g) Now load in the source and receiver location file by File → Open data, select `sr.vtk`, and click the Accept button. Choose Filter → Glyph, and represent the points by 'spheres'.

   (h) For more information about ParaView, see the ParaView Users Guide (`www.paraview.org/files/v1.6/ParaViewUsersGuide.PDF`).

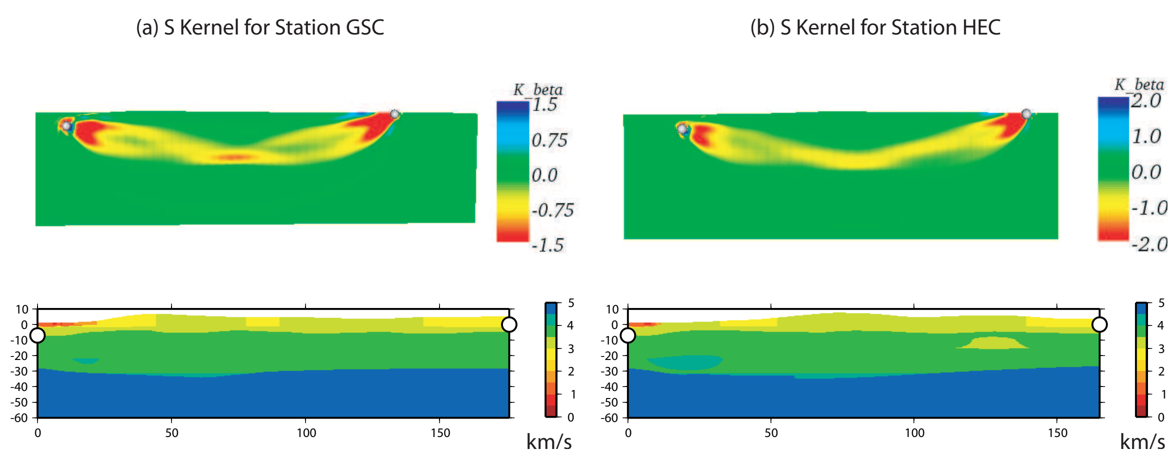

Figure 7.1: (a) Top Panel: Vertical source-receiver cross-section of the S-wave finite-frequency sensitivity kernel K_β for station GSC at an epicentral distance of 176 km from the September 3, 2002, Yorba Linda earthquake. Lower Panel: Vertical source-receiver cross-section of the 3D S-wave velocity model used for the spectral-element simulations [Komatitsch et al., 2004]. (b) The same as (a) but for station HEC at an epicentral distance of 165 km [Liu and Tromp, 2006].

Chapter 8

Running through a Scheduler

The code is usually run on large parallel machines, often PC clusters, most of which use schedulers, i.e., queuing or batch management systems to manage the running of jobs from a large number of users. The following considerations need to be taken into account when running on a system that uses a scheduler:

- The processors/nodes to be used for each run are assigned dynamically by the scheduler, based on availability. Therefore, in order for the mesher and the solver (or between successive runs of the solver) to have access to the same database files (if they are stored on hard drives local to the nodes on which the code is run), they must be launched in sequence as a single job.

- On some systems, the nodes to which running jobs are assigned are not configured for compilation. It may therefore be necessary to pre-compile both the mesher and the solver. A small program provided in the distribution called `create_header_file.f90` can be used to directly create `OUTPUT_FILES/values_from_mesher.h` using the information in the `DATA/Par_file` without having to run the mesher (type '`make create_header_file`' to compile it and '`xcreate_header_file`' to run it; refer to the sample scripts below). The solver can now be compiled as explained above.

- One feature of schedulers/queuing systems is that they allow submission of multiple jobs in a "launch and forget" mode. In order to take advantage of this property, care needs to be taken that output and intermediate files from separate jobs do not overwrite each other, or otherwise interfere with other running jobs.

We describe here in some detail a job submission procedure for the Caltech 1024-node cluster, CITerra, under the LSF scheduling system. We consider the submission of a regular forward simulation. The two main scripts are `run_lsf.bash`, which compiles the Fortran code and submits the job to the scheduler, and `go_mesher_solver_lsf.bash`, which contains the instructions that make up the job itself. These scripts can be found in `UTILS/` directory and can straightforwardly be modified and adapted to meet more specific running needs.

8.1 run_lsf.bash

This script first sets the job queue to be 'normal'. It then compiles the mesher and solver together, figures out the number of processors required for this simulation from the `DATA/Par_file`, and submits the LSF job.

```
#!/bin/bash
# use the normal queue unless otherwise directed queue="-q normal"
if [ $# -eq 1 ]; then
        echo "Setting the queue to $1"
        queue="-q $1"
fi

# compile the mesher and the solver
d=`date' echo "Starting compilation $d"
```

```
make clean
make meshfem3D
make create_header_file
xcreate_header_file
make specfem3D
d=`date'
echo "Finished compilation $d"

# compute total number of nodes needed
NPROC_XI=`grep NPROC_XI DATA/Par_file | cut -c 34- '
NPROC_ETA=`grep NPROC_ETA DATA/Par_file | cut -c 34- '

# total number of nodes is the product of the values read
numnodes=$(( $NPROC_XI * $NPROC_ETA ))

echo "Submitting job"
bsub $queue -n $numnodes -W 60 -K <go_mesher_solver_lsf.bash
```

8.2 go_mesher_solver_lsf.bash

This script describes the job itself, including setup steps that can only be done once the scheduler has assigned a job-ID and a set of compute nodes to the job, the run_lsf.bash commands used to run the mesher and the solver, and calls to scripts that collect the output seismograms from the compute nodes and perform clean-up operations.

1. First the script directs the scheduler to save its own output and output from stdout into OUTPUT_FILES/%J.o, where %J is short-hand for the job-ID; it also tells the scheduler what version of mpich to use (mpich_gm) and how to name this job (go_mesher_solver_lsf).

2. The script then creates a list of the nodes allocated to this job by echoing the value of a dynamically set environment variable LSB_MCPU_HOSTS and parsing the output into a one-column list using the Perl script UTILS/remap_lsf_machines.pl. It then creates a set of scratch directories on these nodes (/scratch/ $USER/DATABASES_MPI) to be used as the LOCAL_PATH for temporary storage of the database files. The scratch directories are created using shmux, a shell multiplexor that can execute the same commands on many hosts in parallel. shmux is available from Shmux (web.taranis.org/shmux/). Make sure that the LOCAL_PATH parameter in DATA/Par_file is also set properly.

3. The next portion of the script launches the mesher and then the solver using run_lsf.bash.

4. The final portion of the script collects the seismograms and performs clean up on the nodes, using the Perl scripts collect_seismo_lsf_multi.pl and cleanmulti.pl.

```
#!/bin/bash -v
#BSUB -o OUTPUT_FILES/%J.o
#BSUB -a mpich_gm
#BSUB -J go_mesher_solver_lsf

# set up local scratch directories
BASEMPIDIR=/scratch/$USER/DATABASES_MPI
mkdir -p OUTPUT_FILE
echo "$LSB_MCPU_HOSTS" > OUTPUT_FILES/lsf_machines
echo "$LSB_JOBID" > OUTPUT_FILES/jobid
remap_lsf_machines.pl OUTPUT_FILES/lsf_machines >OUTPUT_FILES/machines
shmux -M50 -Sall -c "rm -r -f /scratch/$USER; \
      mkdir -p /scratch/$USER; mkdir -p $BASEMPIDIR" \
      - < OUTPUT_FILES/machines >/dev/null
```

```
# run the specfem program
current_pwd=$PWD
run_lsf.bash --gm-no-shmem --gm-copy-env $current_pwd/xmeshfem3D
run_lsf.bash --gm-no-shmem --gm-copy-env $current_pwd/xspecfem3D

# collect seismograms and clean up
mkdir -p SEM
cd SEM
collect_seismo.pl ../OUTPUT_FILES/lsf_machines
cleanbase.pl ../OUTPUT_FILES/machines
```

Chapter 9

Post-Processing Scripts

Several post-processing scripts/programs are provided in the `UTILS/` directory, and most of them need to be adjusted when used on different systems, for example, the path of the executable programs. Here we only list the available scripts and provide a brief description, and you can either refer to the related sections for detailed usage or, in a lot of cases, type the script/program name without arguments for its usage.

9.1 Collect Synthetic Seismograms

The forward and adjoint simulations generate synthetic seismograms in the `LOCAL_PATH`. For the forward simulation, the files are named `STA.NT.BH?.semd` for two-column time series, or `STA.NT.BH?.semd.sac` for ASCII SAC format, where STA and NT are the station name and network code, and `BH?` stands for the component name. The adjont simulations generate synthetic seismograms with the name `S?????.NT.S??.sem` (refer to Section 6.1 for details). The kernel simulations output the back-reconstructed synthetic seismogram in the name `STA.NT.BH?.semd`, mainly for the purpose of checking the accuracy of the reconstruction. Refer to Section 6.2 for further details.

To collect the synthetics onto the frontend, you can use the `UTILS/collect_seismo.pl` machines script:

```
collect_seismo.pl machines
```

9.2 Clean Local Database

After all the simulations are done, the seismograms are collected, and the useful database files are copied to the frontend, you may need to clean the local scratch disk for the next simulation. This is especially important in the case of 1- or 2-chunk kernel simulation, where very large files are generated for the absorbing boundaries to help with the reconstruction of the regular forward wavefield. A sample script is provided in `UTILS/`:

```
cleanbase.pl machines
```

9.3 Process Data and Synthetics

In many cases, the SEM synthetics are calculated and compared to data seismograms recorded at seismic stations. Since the SEM synthetics are accurate for a certain frequency range, both the original data and the synthetics need to be processed before a comparison can be made. We generally use the following scripts:

9.3.1 `process_trinet_data.pl`

This script cuts a given portion of the original data, filters it, transfers the data into a displacement record, and picks the first P and S arrivals. For more functionality, type '`process_trinet_data.pl`' without any argument. An example of the usage of the script:

```
process_trinet_data.pl -m CMTSOLUTION -l 0/180 -t 2/40 -i dir -p -x bp  9703873*.BH?.SAC
```

which has cut all the sac files between 0 and 180 seconds, filtered them between 2 and 40 seconds, transfered them into displacement records using the polezero files in `dir` directory, picked the first P and S arrivals, and added suffix '`bp`' to the file names.

Note that all of the scripts in this section actually use the SAC and/or IASP91 to do the core operations; therefore make sure that the SAC and IASP91 packages are installed properly on your system, and that all the environment variables are set properly before running these scripts.

9.3.2 `process_trinet_syn.pl`

This script converts the synthetic output from the SEM code from ASCII to SAC format, and performs similar operations as '`process_trinet_data.pl`'. An example of the usage of the script:

```
process_trinet_syn.pl -m CMTSOLUTION -a STATIONS -l 0/180 -t 2/40 -p -x bp syn/*.BH?.semd
```

which will convert the synthetics into SAC format, add event and station information into the SAC headers, cut the SAC files between 0 and 180 seconds, filter them between 2 and 40 seconds, pick the first P and S arrivals, and add the suffix '`bp`' to the file names.

More options are available for this script, such as adding time shift to the origin time of the synthetics, convolving the synthetics with a triangular source time function with a given half duration, etc. Type `process_trinet_syn.pl` without any argument for a detailed usage.

9.3.3 `rotate.pl`

The original data and synthetics have three components: vertical (BHZ), north (BHN) and east (BHE). However, for most seismology applications, transverse and radial components are also desirable. Therefore, we need to rotate the horizontal components of both the data and the synthetics to the transverse and radial direction, and `rotate.pl` can be used to accomplish this:

```
rotate.pl -l 0 -L 180 -d DATA/*.BHE.SAC.bp
rotate.pl -l 0 -L 180 SEM/*.BHE.semd.sac.bp
```

where the first command performs rotation on the SAC data obtained through Seismogram Transfer Program (STP) (`http://www.data.scec.org/STP/stp.html`), while the second command rotates the processed SEM synthetics.

9.4 Plot Movie Snapshots and Synthetic Shakemaps

9.4.1 `movie2gif.pl`

With the movie data saved in `OUTPUT_FILES/` at the end of a movie simulation (`MOVIE_SURFACE=.true.`), you can run the '`create_movie_GMT`' code to convert these binary movie data into GMT xyz files for futher processing. A sample script `movie2gif.pl` is provided to do this conversion, and then plot the movie snapshots in GMT, for example:

```
movie2gif.pl -m CMTSOLUTION -g -f 1/40 -n -2 -p
```

which for the first through the 40th movie frame, converts the `moviedata` files into GMT xyz files, interpolates them using the 'nearneighbor' command in GMT, and plots them on a 2D topography map. Note that '`-2`' and '`-p`' are both optional.

9.4.2 plot_shakemap.pl

With the shakemap data saved in OUTPUT_FILES/ at the end of a shakemap simulation (CREATE_SHAKEMAP=.true.), you can also run 'create_movie_GMT' code to convert the binary shakemap data into GMT xyz files. A sample script plot_shakemap.pl is provided to do this conversion, and then plot the shakemaps in GMT, for example:

```
plot_shakemap.pl data_dir type(1,2,3) CMTSOLUTION
```

where type=1 for a displacement shakemap, 2 for velocity, and 3 for acceleration.

9.5 Map Local Database

A sample program remap_database is provided to map the local database from a set of machines to another set of machines. This is especially useful when you want to run mesher and solver, or different types of solvers separately through a scheduler (refer to Chapter 8).

```
run_lsf.bash --gm-no-shmem --gm-copy-env remap_database old_machines 150
```

where old_machines is the LSF machine file used in the previous simulation, and 150 is the number of processors in total.

Bug Reports and Suggestions for Improvements

To report bugs or suggest improvements to the code, please send an e-mail to the CIG Computational Seismology Mailing List (`cig-seismo@geodynamics.org`) or Jeroen Tromp (`jtromp-AT-princeton.edu`), and/or use our online bug tracking system Roundup (`www.geodynamics.org/roundup`).

Notes & Acknowledgments

In order to keep the software package thread-safe in case a multithreaded implementation of MPI is used, developers should not add modules or common blocks to the source code but rather use regular subroutine arguments (which can be grouped in "derived types" if needed for clarity).

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OpenDX (`http://www.opendx.org`) is open-source based on IBM Data Explorer, AVS (`http://www.avs.com`) is a trademark of Advanced Visualization Systems, and ParaView (`http://www.paraview.com`) is an open-source visualization platform.

The main developers of the `SPECFEM3D` source code are Dimitri Komatitsch, Jeroen Tromp, and Qinya Liu. The following individuals (listed in alphabetical order) have also contributed to the development or improvement of the source code: Min Chen, Vala Hjörleifsdóttir, Jesús Labarta, and Leif Strand. The following individuals (listed in alphabetical order) contributed to this manual: Min Chen, Vala Hjörleifsdóttir, Sue Kientz, Dimitri Komatitsch, Qinya Liu, Alessia Maggi, Carl Tape, and Jeroen Tromp. The manual's cover graphic was created by Santiago Lombeyda from Caltech's Center for Advanced Computing Research (CACR) (`http://www.cacr.caltech.edu`). Older versions of the code were initially developed by Dimitri Komatitsch at Institut de Physique du Globe (France) and then by Dimitri Komatitsch and Jeroen Tromp at Harvard University (USA).

Please e-mail your feedback, questions, comments, and suggestions to Jeroen Tromp (`jtromp-AT-princeton.edu`) or to the CIG Computational Seismology Mailing List (`cig-seismo@geodynamics.org`).

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Appendix A

Reference Frame Convention

The code uses the following convention for the Cartesian reference frame:

- the x axis points East
- the y axis points North
- the z axis points up

Note that this convention is different from both the Aki and Richards [1980] convention and the Harvard Centroid-Moment Tensor (CMT) convention. The Aki & Richards convention is

- the x axis points North
- the y axis points East
- the z axis points down

and the Harvard CMT convention is

- the x axis points South
- the y axis points East
- the z axis points up

Appendix B

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