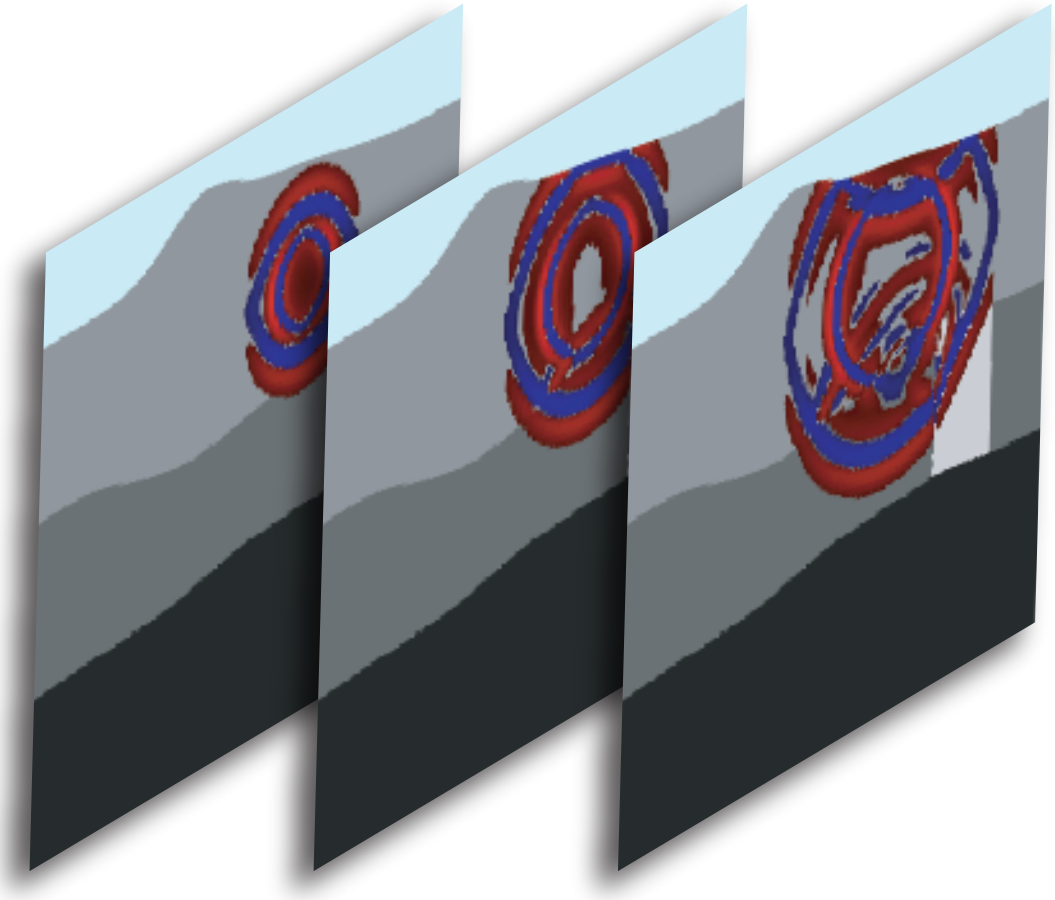
COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)
CNRS (FRANCE)
PRINCETON UNIVERSITY (USA)

SPECFEM 2D



SPECFEM2D
User Manual

Version 8.1

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Authors

The SPECFEM2D package was first developed by Dimitri Komatitsch and Jean-Pierre Vilotte at Institut de Physique du Globe (IPGP) in Paris, France from 1995 to 1997 and then by Dimitri Komatitsch at Harvard University (USA), Caltech (USA) and then CNRS and University of Pau (France) from 1998 to 2005. The story started on April 4, 1995, when Prof. Yvon Maday from CNRS and University of Paris, France, gave a lecture to Dimitri Komatitsch and Jean-Pierre Vilotte at IPG about the nice properties of the Legendre spectral-element method with diagonal mass matrix that he had used for other equations. We are deeply indebted and thankful to him for that. That followed a visit by Dimitri Komatitsch to OGS (Istituto Nazionale di Oceanografia e di Geofisica Sperimentale) in Trieste, Italy, in February 1995 to meet with Géza Seriani and Enrico Priolo, who introduced him to their 2D Chebyshev version of the spectral-element method with a non-diagonal mass matrix. We are deeply indebted and thankful to them for that.

Since then it has been developed and maintained by a development team: in alphabetical order, Étienne Bachmann, Alexis Bottero, Quentin Brissaud, Bryant Chow, Paul Cristini, Rene Gassmoeller, Hom Nath Gharti, Michael Gineste, Felix Halpaap, Dimitri Komatitsch, Jesús Labarta, Matthieu Lefebvre, Nicolas Le Goff, Pieyre Le Loher, Qiancheng Liu, Qinya Liu, Youshan Liu, Zhaolun Liu, David Luet, Roland Martin, René Matzen, Ryan Modrak, Christina Morency, Masaru Nagaso, Daniel Peter, Eric Rosenkrantz, Herurisa Rusmanugroho, Elliott Sales de Andrade, Carl Tape, Jeroen Tromp, Eduardo Valero Cano, Jean-Pierre Vilotte, Zhinan Xie, Zhendong Zhang.

Current and past main participants or main sponsors of the SPECFEM project (in no particular order)

Contents

Chapter 1

Introduction

SPECFEM2D allows users to perform 2D and 2.5D (i.e., axisymmetric) simulations of acoustic, elastic, viscoelastic, and poroelastic seismic wave propagation as well as full waveform imaging (FWI) or adjoint tomography.

In fluids, SPECFEM2D uses the classical linearized Euler equation; thus if you have sharp local variations of density in the fluid (highly heterogeneous fluids in terms of density) or if density becomes extremely small in some regions of your model (e.g. for upper-atmosphere studies), before using the code please make sure the linearized Euler equation is a valid approximation in the case you want to study. For more details on that see e.g. Jensen et al. [2011].

The 2D spectral-element solver accommodates regular and unstructured meshes, generated for example by Cubit, Gmsh or GiD. Even mesh creation packages that generate triangles, for instance Delaunay-Voronoi triangulation codes, can be used because each triangle can then easily be decomposed into three quadrangles by linking the barycenter to the center of each edge; while this approach does not generate quadrangles of optimal quality, it can ease mesh creation in some situations and it has been shown that the spectral-element method can very accurately handle distorted mesh elements.

Furthermore, the 2D spectral-element solver accommodates Convolution PML absorbing layers as well as higher-order time schemes (4th order Runge-Kutta and LDDRK4-6). Convolution or Auxiliary Differential Equation Perfectly Matched absorbing Layers (C-PML or ADE-PML) are described in Martin et al. [2008b,c], Martin and Komatitsch [2009], Martin et al. [2010], Komatitsch and Martin [2007].

The solver has adjoint capabilities and can calculate finite-frequency sensitivity kernels [Tromp et al., 2008, Peter et al., 2011] for acoustic, (an)elastic, and poroelastic media. The package also considers 2D SH and P-SV wave propagation. Finally, the solver can run both in serial and in parallel. See the github repository SPECFEM2D for the source code.

The SEM is a continuous Galerkin technique [Tromp et al., 2008, Peter et al., 2011], which can easily be made discontinuous [Bernardi et al., 1994, Chaljub, 2000, Kopriva et al., 2002, Chaljub et al., 2003, Legay et al., 2005, Kopriva, 2006, Wilcox et al., 2010, Acosta Minolia and Kopriva, 2011]; it is then close to a particular case of the discontinuous Galerkin technique [Reed and Hill, 1973, Lesaint and Raviart, 1974, Arnold, 1982, Johnson and Pitkäranta, 1986, Bourdel et al., 1991, 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, Ainsworth et al., 2006, Bernacki et al., 2006, Dumbser and Käser, 2006, De Basabe et al., 2008, de la Puente et al., 2009, Wilcox et al., 2010, De Basabe and Sen, 2010, Étienne et al., 2010], with optimized efficiency because of its tensorized basis functions [Wilcox et al., 2010, Acosta Minolia and Kopriva, 2011]. In particular, it can accurately handle very distorted mesh elements [Oliveira and Seriani, 2011].

It has very good accuracy and convergence properties [Maday and Patera, 1989, Seriani and Priolo, 1994, Deville et al., 2002, Cohen, 2002, De Basabe and Sen, 2007, Seriani and Oliveira, 2008, Ainsworth and Wajid, 2009, 2010, Melvin et al., 2012]. The spectral element approach admits spectral rates of convergence and allows exploiting hp-convergence schemes. It is also very well suited to parallel implementation on very large supercomputers [Komatitsch

et al., 2003, Tsuboi et al., 2003, Komatitsch et al., 2008, Carrington et al., 2008, Komatitsch et al., 2010b] as well as on clusters of GPU accelerating graphics cards [Komatitsch, 2011, Michéa and Komatitsch, 2010, Komatitsch et al., 2009, 2010a]. Tensor products inside each element can be optimized to reach very high efficiency [Deville et al., 2002], and mesh point and element numbering can be optimized to reduce processor cache misses and improve cache reuse [Komatitsch et al., 2008]. The SEM can also handle triangular (in 2D) or tetrahedral (in 3D) elements [Wingate and Boyd, 1996, Taylor and Wingate, 2000, Komatitsch et al., 2001, Cohen, 2002, Mercerat et al., 2006] as well as mixed meshes, although with increased cost and reduced accuracy in these elements, as in the discontinuous Galerkin method.

Note that in many geological models in the context of seismic wave propagation studies (except for instance for fault dynamic rupture studies, in which very high frequencies or supershear rupture need to be modeled near the fault, see e.g. Benjemaa et al. [2007, 2009], de la Puente et al. [2009], Tago et al. [2010]) a continuous formulation is sufficient because material property contrasts are not drastic and thus conforming mesh doubling bricks can efficiently handle mesh size variations [Komatitsch and Tromp, 2002, Komatitsch et al., 2004, Lee et al., 2008, 2009a,b].

For a detailed introduction to the SEM as applied to regional seismic wave propagation, please consult Peter et al. [2011], Tromp et al. [2008], Komatitsch and Vilotte [1998], Komatitsch and Tromp [1999], Chaljub et al. [2007] and in particular Lee et al. [2009b,a, 2008], Godinho et al. [2009], van Wijk et al. [2004], Komatitsch et al. [2004]. A detailed theoretical analysis of the dispersion and stability properties of the SEM is available in Cohen [2002], De Basabe and Sen [2007], Seriani and Oliveira [2007], Seriani and Oliveira [2008] and Melvin et al. [2012].

The SEM was originally developed in computational fluid dynamics [Patera, 1984, Maday and Patera, 1989] and has been successfully adapted to address problems in seismic wave propagation. Early seismic wave propagation applications of the SEM, utilizing Legendre basis functions and a perfectly diagonal mass matrix, include Cohen et al. [1993], Komatitsch [1997], Faccioli et al. [1997], Casadei and Gabellini [1997], Komatitsch and Vilotte [1998] and Komatitsch and Tromp [1999], whereas applications involving Chebyshev basis functions and a non-diagonal mass matrix include Seriani and Priolo [1994], Priolo et al. [1994] and Seriani et al. [1995]. In the Legendre version that we use in SPECFEM the mass matrix is purposely slightly inexact but diagonal (but can be made exact if needed, see Teukolsky [2015]), while in the Chebyshev version it is exact but non diagonal.

Beware that, in a spectral-element method, some spurious modes (that have some similarities with classical so-called "Hourglass modes" in finite-element techniques, although in the SEM they are not zero-energy modes) can appear in some (but not all) cases in the spectral element in which the source is located. Fortunately, they do not propagate away from the source element. However, this means that if you put a receiver in the same spectral element as a source, the recorded signals may in some cases be wrong, typically exhibiting some spurious oscillations, which are often even non causal. If that is the case, an easy option is to slightly change the mesh in the source region in order to get rid of these Hourglass-like spurious modes, as explained in Duczek et al. [2014], in which this phenomenon is described in details, and in which practical solutions to avoid it are suggested.

All SPECFEM2D software is written in Fortran2003 with full portability in mind, and conforms strictly to the Fortran2003 standard. It uses no obsolete or obsolescent features of Fortran. The package uses parallel programming based upon the Message Passing Interface (MPI) [Gropp et al., 1994, Pacheco, 1997].

This new release of the code includes support for GPU graphics card acceleration [Komatitsch, 2011, Michéa and Komatitsch, 2010, Komatitsch et al., 2009, 2010a].

The code uses the plane strain convention when the standard P-SV equation case is used, i.e., the off-plane strain ϵ_{zz} is zero by definition of the plane strain convention but the off-plane stress σ_{zz} is not equal to zero, one has $\sigma_{zz} = \lambda(\epsilon_{xx}+\epsilon_{yy})$. This implies, as in any plain strain software package, that the P-SV source is a line source along the direction perpendicular to the plane (see file discussion_of_2D_sources_and_approximations_from_Pilant_1979.pdf for more details).

1.1 Citation

You can find all the references below in BibTeXformat in file `doc/USER_MANUAL/bibliography.bib`.

If you use this code for your own research, please cite at least one article written by the developers of the package, for instance:

- Tromp et al. [2008],
- Peter et al. [2011],
- Vai et al. [1999],
- Lee et al. [2009a],
- Lee et al. [2008],
- Lee et al. [2009b],
- Komatitsch et al. [2010a],
- Komatitsch et al. [2009],
- Liu et al. [2004],
- Chaljub et al. [2007],
- Komatitsch and Vilotte [1998],
- Komatitsch and Tromp [1999],
- Komatitsch et al. [2004],
- Morency and Tromp [2008],
- Blanc et al. [2016],
- and/or other articles from `https://specfem.github.io/komatitsch.free.fr/publications.html`.

If you use the C-PML absorbing layer capabilities of the code, please cite at least one article written by the developers of the package, for instance:

- Xie et al. [2014],
- Xie et al. [2016].

If you use the UNDO_ATTENUATION option of the code in order to produce full anelastic/viscoelastic sensitivity kernels, please cite at least one article written by the developers of the package, for instance (and in particular):

- Komatitsch et al. [2016].

More generally, if you use the attenuation (anelastic/viscoelastic) capabilities of the code, please cite at least one article written by the developers of the package, for instance:

- Komatitsch et al. [2016],
- Blanc et al. [2016].

If you use the kernel capabilities of the code, please cite at least one article written by the developers of the package, for instance:

- Tromp et al. [2008],

- Peter et al. [2011],
- Liu and Tromp [2006],
- Morency et al. [2009].

If you use the SCOTCH / CUBIT non-structured capabilities, please cite:

- Martin et al. [2008a].

If you use axisymmetric geometries please also cite:

- Bottero et al. [2016]

The corresponding BibTeX entries may be found in file `doc/USER_MANUAL/bibliography.bib`.

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. 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

To download the SPECFEM2D software package, type this:

```
git clone --recursive --branch devel https://github.com/SPECFEM/specfem2d.git
```

Then, 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 Fortran compiler (another option is to define FC, CC and MPIF90 in your .bash_profile or your .cshrc file):

```
./configure FC=gfortran CC=gcc
```

If you want to run in parallel, i.e., using more than one processor core, then you would type

```
./configure FC=gfortran CC=gcc MPIFC=mpif90 --with-mpi
```

You can replace the GNU compilers above (gfortran and gcc) with other compilers if you want to; for instance for Intel ifort and icc use FC=ifort CC=icc instead.

Before running the `configure` script, you should probably edit file `flags.guess` to make sure that it contains the best compiler options for your system. Known issues or things to check are:

`Intel ifort compiler` See if you need to add `-assume byterecl` for your machine. In the case of that compiler, we have noticed that initial release versions sometimes have bugs or issues that can lead to wrong results when running the code, thus we *strongly* recommend using a version for which at least one service pack or update has been installed. In particular, for version 17 of that compiler, users have reported problems (making the code crash at run time) with the `-assume buffered_io` option; if you notice problems, remove that option from file `flags.guess` or change it to `-assume nobuffered_io` and try again.

`IBM compiler` See if you need to add `-qsave` or `-qnosave` for your machine.

`Mac OS` You will probably need to install `Xcode`.

The SPECFEM2D software package relies on the SCOTCH library to partition meshes. The SCOTCH library [Pellegrini and Roman, 1996] provides efficient static mapping, graph and mesh partitioning routines. SCOTCH is a free software package developed by François Pellegrini et al. from LaBRI and Inria in Bordeaux, France, downloadable from the web page `https://gitlab.inria.fr/scotch/scotch`. In case no SCOTCH libraries can be found on the system, the configuration will bundle the version provided with the source code for compilation. The path to an existing SCOTCH installation can to be set explicitly with the option `--with-scotch-dir`. Just as an example:

```
./configure FC=ifort MPIFC=mpif90 --with-mpi --with-scotch-dir=/opt/scotch
```

If you use the Intel ifort compiler to compile the code, we recommend that you use the Intel icc C compiler to compile Scotch, i.e., use:

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

For further details about the installation of SCOTCH, go to subdirectory `scotch_5.1.11/` and read `INSTALL.txt`. You may want to download more recent versions of SCOTCH in the future from SCOTCH gitlab repository. Support for the METIS graph partitioner has been discontinued because SCOTCH is more recent and performs better.

When compiling the SCOTCH source code, if you get a message such as: "ld: cannot find -lz", the Zlib compression development library is probably missing on your machine and you will need to install it or ask your system administrator to do so. On Linux machines the package is often called "zlib1g-dev" or similar (thus "sudo apt-get install zlib1g-dev" would install it).

You can add `--enable-vectorization` to the configuration options to speed up the code in the fluid (acoustic) and elastic parts. This works fine if (and only if) your computer always allocates a contiguous memory block for each allocatable array; this is the case for most machines and most compilers, but not all. To check if that option works fine on your machine, run the code with and without it for an acoustic/elastic model and make sure the seismograms are identical.

You may edit the `Makefile` for more specific modifications. Especially, there are several options available:

- `-DUSE_MPI` compiles with use of an MPI library.
- `-DUSE_SCOTCH` enables use of graph partitioner SCOTCH.

After these steps, go back to the main directory of SPECFEM2D/ and type

```
make
```

to create all executables which will be placed into the folder `./bin/`.

By default, the solver runs in single precision. This is fine for most application, but if for some reason you want to run the solver in double precision, run the `configure` script with option "`--enable-double-precision`". Keep in mind that this will of course double total memory size and will also make the solver around 20 to 30% slower on many processors.

If your compiler has problems with the `use mpi` statements that are used in the code, use the script called `replace_use_mpi_with_include_mpif_dot_h.pl` in the root directory to replace all of them with `include 'mpif.h'` automatically.

If you have problems configuring the code on a Cray machine, i.e. for instance if you get an error message from the `configure` script, try exporting these two variables: `MPI_INC=$CRAY_MPICH2_DIR/include` and `FCLIBS=" "`, and for more details if needed you can refer to the `utils/infos/Cray_compiler_information` directory. You can also have a look at the configure script called `utils/infos/Cray_compiler_information/configure_SPECFEM_for_Piz_Daint.bash`.

For people who would like to run the package on Windows rather than on Unix machines, you can install Docker or VirtualBox (installing a Linux in VirtualBox in that latter case) and run it easily from inside that.

We recommend that you add `ulimit -S -s unlimited` to your `.bash_profile` file and/or `limit stacksize unlimited` to your `.cshrc` file to suppress any potential limit to the size of the Unix stack.

2.1 Using the GPU version of the code

SPECFEM2D supports GPU acceleration by CUDA. When compiling for GPU cards, you can enable the CUDA version with:

```
./configure --with-cuda ..
```

or

```
./configure --with-cuda=cuda9 ..
```

where for example `cuda4,cuda5,cuda6,cuda7,..` specifies the target GPU architecture of your card, (e.g., with CUDA 9 this refers to Volta V100 cards), rather than the installed version of the CUDA toolkit. Before CUDA version 5, one version supported basically one new architecture and needed a different kind of compilation. Since version 5, the compilation has stayed the same, but newer versions supported newer architectures. However at the moment, we still have one version linked to one specific architecture:

```
- CUDA 4 for Tesla,   cards like K10, Geforce GTX 650, ..
- CUDA 5 for Kepler,  like K20
- CUDA 6 for Kepler,  like K80
- CUDA 7 for Maxwell, like Quadro K2200
- CUDA 8 for Pascal,  like P100
- CUDA 9 for Volta,   like V100
- CUDA 10 for Turing, like GeForce RTX 2080
- CUDA 11 for Ampere, like A100
- CUDA 12 for Hopper, like H100
```

So even if you have the new CUDA toolkit version 11, but you want to run on say a K20 GPU, then you would still configure with:

```
./configure --with-cuda=cuda5
```

The compilation with the cuda5 setting chooses then the right architecture (`-gencode=arch=compute_35,code=sm_35` for K20 cards).

2.2 Adding OpenMP support in addition to MPI

OpenMP support can be enabled in addition to MPI. However, in many cases performance will not improve because our pure MPI implementation is already heavily optimized and thus the resulting code will in fact be slightly slower. A possible exception could be IBM BlueGene-type architectures.

To enable OpenMP, add the flag `--enable-openmp` to the configuration:

```
./configure --enable-openmp ..
```

This will add the corresponding OpenMP flag for the chosen Fortran compiler. Please note that only the elastic domain solver has OpenMP support for now.

2.3 Visualizing the subroutine calling tree of the source code

Packages such as `doxywizard` can be used to visualize the subroutine calling tree of the source code. `Doxywizard` is a GUI front-end for configuring and running `doxygen`.
To visualize the call tree (calling tree) of the source code, you can see the Doxygen tool available in directory `doc/call_trees_of_the_source_code`.

2.4 Becoming a developer of the code, or making small modifications in the source code

If you want to develop new features in the code, and/or if you want to make small changes, improvements, or bug fixes, you are very welcome to contribute! To do so, i.e. to access the development branch of the source code with read/write access (in a safe way, no need to worry too much about breaking the package, there are CI tests based on

BuildBot, Travis-CI and Jenkins in place that are checking and validating all new contributions and changes), please visit this Web page:
https://github.com/SPECFEM/specfem2d/wiki

Chapter 3

Mesh Generation

3.1 How to use SPECFEM2D

The first step in running a spectral-element simulation consists of constructing a high-quality mesh for the region under consideration. We provide two possibilities to do so: (1) relying on an external, hexahedral mesher, like Gmsh and CUBIT, or (2) using the provided, internal capabilities. To run the mesher, please edit the main input file `DATA/Par_file`, describing the setup of your simulation. Then type:

```
./bin/xmeshfem2D
```

to create the mesh, which will be stored in directory `OUTPUT_FILES/`. `xmeshfem2D` will output several files called `Database??????.bin`, one for each process. These files are required for running the solver in a subsequent step.

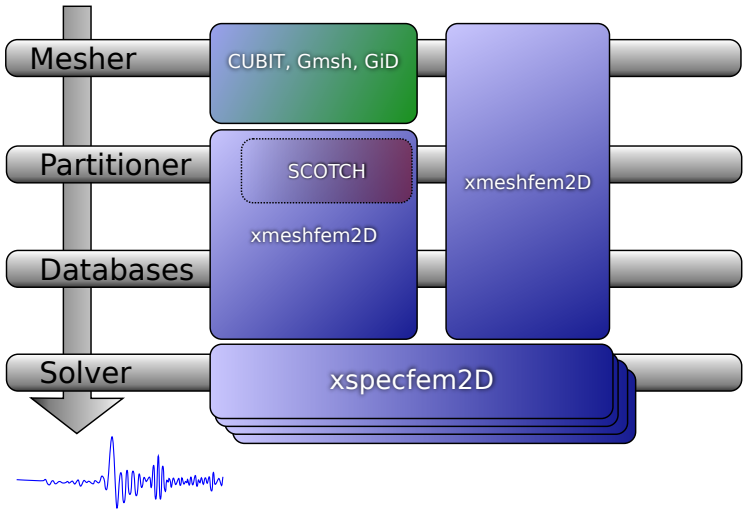


Figure 3.1: Schematic workflow for a SPECFEM2D simulation. The executable `xmeshfem2D` creates the GLL mesh points and assigns specific model parameters. The executable `xspecfem2D` solves the seismic wave propagation.

Notes about `DATA/Par_file` parameters

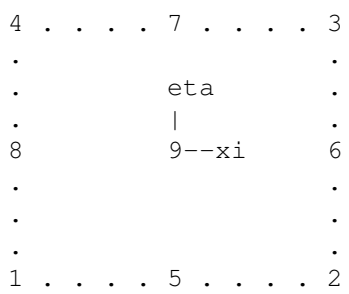
The default `DATA/Par_file` provided in the root directory of the code contains detailed comments and should be almost self-explanatory (note that some of the older `DATA/Par_file` files provided in the `EXAMPLES` directory work fine but some of the comments they contain may be obsolete or even wrong; thus refer to the default

DATA/Par_file instead for reliable explanations).

If you need more details we do not have a detailed description of all the parameters for the 2D version in this manual but you can find useful information in the manuals of the 3D versions, since many parameters and the general philosophy is similar. They are available at SPECFEM3D Cartesian user manual.

NPROC If you have the code compiled with MPI support, you can specify the number of processes (> 1) for the simulation to run on. Otherwise, this has to be set to 1 for a serial run. The mesher will use the partitioner specified by parameter PARTITIONING_TYPE to load-balance the mesh for multiple processes.

NGNOD Regarding mesh point numbering in the files created by the mesher, we use the classical convention of 4-node and 9-node finite elements (NGNOD = 4 or NGNOD = 9, respectively):



the local coordinate system being ξ and η (xi and eta). Note that this convention is used to describe the geometry only. In the solver the wave field is then described based on high-order Lagrange interpolants at Gauss-Lobatto-Legendre points, as is classical in spectral-element methods.

MODEL With MODEL = default chosen, a variety of simple velocity and density models can be defined using the nbmodels section in the Par_file.

The material types can be specified by one of the following line formats:

```
I:  model_number 1 rho Vp Vs 0 0 QKappa Qmu 0 0 0 0 0 0
II:  model_number 2 rho c11 c13 c15 c33 c35 c55 c12 c23 c25 0 QKappa Qmu
III: model_number 3 rhos rhof phi c kxx kxz kzz Ks Kf Kfr etaf mufr Qmu
IV: model_number -1 0 0 A 0 0 0 0 0 0 0 0 0 0
```

I: To make a given region acoustic, use (I) and make Vs be zero. To make a given region isotropic elastic, use (I) and make Vs be nonzero. See Section 4.1 for more details.

Thus, to create acoustic (fluid) regions, just set the S wave speed to zero and the code will see that these elements are fluid and switch to the right equations there automatically, and automatically match them with the solid regions.

II: To make a given region anisotropic, use (II). See Section 4.3 for more details.

III: To make a given region poroelastic, use (III). See Section 4.4 for more details.

IV: To impose a tomographic model on a given region, use (IV). For now, we only allow for a single tomography file and region. Note that the model_number must be strictly positive, but the following domain number must be negative (-1) for tomographic models. The values for density (rho) and Vp are ignored, however the value for Vs, i.e., A, must be either zero (0.0) to be recognized as an acoustic region or a positive non-zero value (e.g., 1.0) for an elastic region. The tomographic model values are overimposed on this region, and defined in the file specified by the parameter TOMOGRAPHY_FILE.

When viscoelasticity is turned on, the Vp and Vs values that are read here are the UNRELAXED ones i.e. the values at infinite frequency unless the READ_VELOCITIES_AT_f0 parameter is set to true, in which case they are the values at frequency f_0. Please also note that Qmu is always equal to Qs, but Qkappa is

in general not equal to Qp. To convert one to the other see doc/note_on_Qkappa_versus_Qp.pdf and utils/attenuation/conversion_from_Qkappa_Qmu_to_Qp_Qs_from_Dahlen_Tromp_959_960.f90.

With MODEL = default chosen, a variety of simple layered model configurations can be specified using the nbregions section in the Par_file. Please see the comment in the Par_file how to specify different material regions in the mesh for internal meshes. Meshes defined by an external mesher will have to specify these informations in separate files, please find more explanations below for the parameter read_external_mesh.

The parameter MODEL can also have other values specified than default. Possible selections are:

- ascii: for reading in a single ASCII model file (DATA/proc***_rho_vp_vs.dat)
- binary or gll: for reading in binary model files (DATA/proc***_rho.bin, DATA/proc***_vp.bin, DATA/proc***_vs.bin)
  In case attenuation is turned on for the simulation, it will also read in attenuation files (DATA/proc***_Qmu.bin, DATA/proc***_Qkappa.bin)
- binary_voigt: for reading in an anisotropic model specified by binary files (DATA/proc***_rho.bin, DATA/proc***_c11.bin, DATA/proc***_c13.bin, DATA/proc***_c15.bin DATA/proc***_c33.bin, DATA/proc***_c35.bin, DATA/proc***_c55.bin)
- external: for reading in a velocity model specified in the source code routine define_external_model() in file src/specfem2d/define_external_model.f90. The user can implement his own routine here as explained in the source file. By default, the routine implements the spherically symmetric isotropic AK135 model.
- legacy: for reading in a single ASCII model file with a legacy format of very old SPECFEM2D versions (DATA/proc***_model_velocity.dat_input)

read_external_mesh If you are using an external mesher (like Gmsh, CUBIT/Trelis or GiD), you should set this parameter to .true., with the following files defined for the mesher:

mesh_file is the file describing the mesh : first line is the number of elements, then a list of 4 nodes (quadrilaterals only) forming each elements on each line.

nodes_coords_file is the file containing the coordinates (x and z) of each node: number of nodes on the first line, then coordinates x and z on each line.

materials_file is the number of the material for every element : an integer ranging from 1 to nbmodels on each line.

nummaterial_velocity_file specifies the material properties for each material of the nbmodels defined in the materials file. The material specification follows a format slightly different than the nbmodels section in the Par_file, but identical to the SPECFEM3D Cartesian version where you can find more informations about it. Also, examples of such nummaterial_velocity_file files can be found in the EXAMPLES/meshing/ folder and the format is described in more detail therein in the header of the files.

free_surface_file is the file describing the edges forming the acoustic free surface: number of edges on the first line, then on each line: number of the element, number of nodes forming the free surface (1 for a point, 2 for an edge), the nodes forming the free surface for this element. If you do not want any free surface, just put 0 on the first line; you then get a rigid surface instead.

axial_elements_file is the file describing the axial elements in the case of an axisymmetric simulation. See Section 4.2.

absorbing_surface_file is the file describing the edges forming the absorbing boundaries: number of edges on the first line, then on each line: number of the element, number of nodes forming the absorbing edge (must always be equal to 2), the two nodes forming the absorbing edge for this element, and then the type of absorbing edge: 1 for BOTTOM, 2 for RIGHT, 3 for TOP and 4 for LEFT. Only two nodes per element can be listed, i.e., the second parameter of each line must always be equal to 2. If one of your elements has more than one edge along a given absorbing contour (e.g., if that contour has a corner) then

list it twice, putting the first edge on the first line and the second edge on the second line. Do not list the same element with the same absorbing edge twice or more, otherwise absorption will not be correct because the edge integral will be improperly subtracted several times. If one of your elements has a single point along the absorbing contour rather than a full edge, do NOT list it (it would have no weight in the contour integral anyway because it would consist of a single point). If you use 9-node elements, list only the first and last points of the edge and not the intermediate point located around the middle of the edge; the right 9-node curvature will be restored automatically by the code.

tangential_detection_curve_file contains points describing the envelope, that are used for the source_normal_to_surface and rec_normal_to_surface. Should be fine grained, and ordered clockwise. Number of points on the first line, then (x,z) coordinates on each line.

READ_VELOCITIES_AT_f0 shift (i.e. change) velocities read from the input file to take average physical dispersion into account, i.e. if needed change the reference frequency at which these velocities are defined internally in the code: by default, the velocity values that are read at the end of this Par_file of the code are supposed to be the unrelaxed values, i.e. the velocities at infinite frequency. If you set this flag to .true., the values read are then those for a given frequency called ATTENUATION_f0_REFERENCE.

Note this only has an effect, if attenuation is turned on for the simulation, i.e., either ATTENUATION_VISCOELASTIC or ATTENUATION_VISCOACOUSTIC is set to .true.. Otherwise, the simulation is for a purely elastic or acoustic medium and the concept of a reference frequency is not needed.

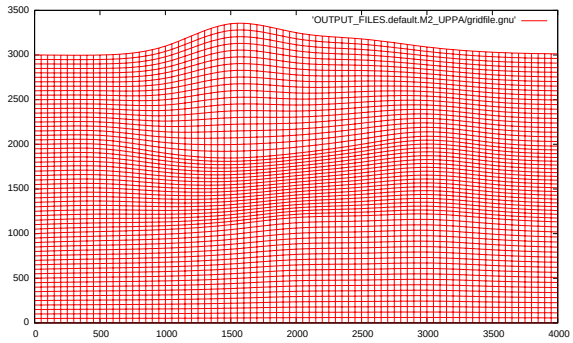


Figure 3.2: Example of a grid file generated by xmeshfem2D when parameter output_grid_Gnuplot is set to .true., and visualized with gnuplot (within gnuplot, type 'plot "OUTPUT_FILES/gridfile.gnu" w l').

3.2 How to use Gmsh to generate an external mesh

Gmsh[1] is a 3D finite element grid generator which can be used for the generation of quadrangle and hexahedral meshes. It is therefore a good candidate for generating meshes which can be processed by SPECFEM2D. Only two modules of Gmsh are of interest for the SPECFEM2D users : the geometry and the mesh modules. An example is given in directory EXAMPLES/applications/meshing/Gmsh_example* which illustrates the generation of an external mesh using these two modules. The model that is considered consists of a homogeneous square containing two circles filled with a different material.

The geometry is generated by loading file SqrCirc.geo into Gmsh. The end of the .geo file contains several lines which are required in order to define the sides of the box and the media. This is done using the following conventions :

```
Physical Line("Top") = {1};    line corresponding to the top of the box
Physical Line("Left") = {2};   line corresponding to the left side of the box
Physical Line("Bottom") = {3}; line corresponding to the bottom of the box
```

[1] freely available at the following address : http://gmsh.info/

```
Physical Line("Right") = {4};  line corresponding to the right side of the box
Physical Surface("M1") = {10};  surrounding medium
Physical Surface("M2") = {11,12};  interior of the two circles
```

For instance, if you want to fill the two circles with two different materials, you will have to write :

```
Physical Surface("M1") = {10};  surrounding medium
Physical Surface("M2") = {11};  interior of the big circle
Physical Surface("M3") = {12};  interior of the small circle
```

and, consequently, you will have to define a new medium numbered `3` in the `Par_file`.

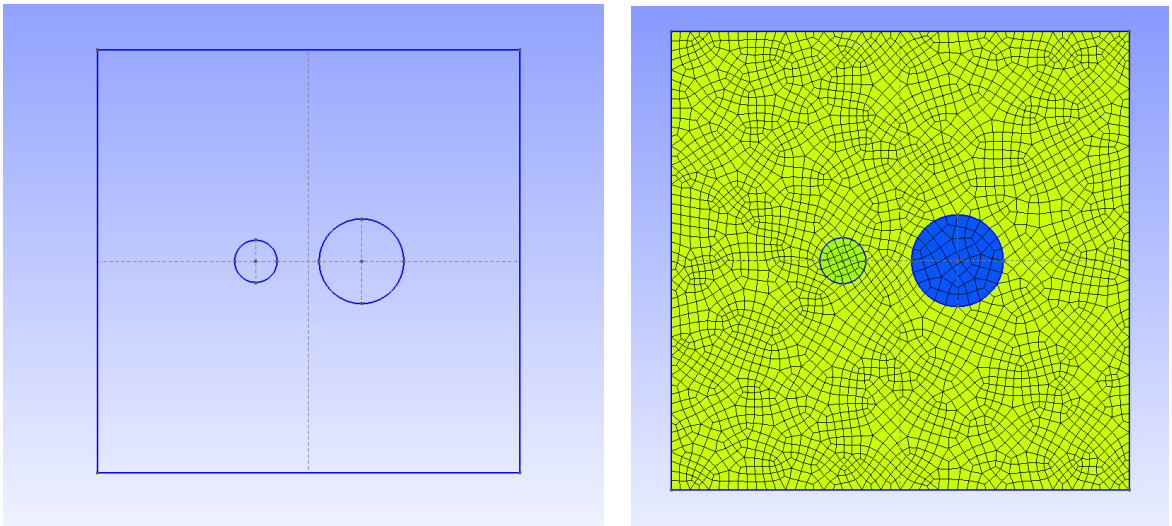


Figure 3.3: Geometry and mesh of the two circle model generated with Gmsh

Then, a 2D mesh can be created and saved after selecting the appropriate options in Gmsh : `All quads` in `Subdivision algorithm` and `1` or `2` in `Element order` whether you want a 4 or 9 node mesh. This operation will generate a `SqrCirc.msh` file which must be processed to get all the files required by SPECFEM2D when using an external mesh (see previous section). This is done by running a python script called `LibGmsh2Specfem.py`, located in directory `utils/Gmsh`:

```
python LibGmsh2Specfem.py SqrCirc -t A -b A -r A -l A
```

Where the options `-t`, `-b`, `-r` and `-l` represent the different sides of the model (top, bottom, right and left) and can take the values `A` or `F` if the corresponding side is respectively absorbing or free. All boundaries are absorbing by default. The connections of the generated filenames to the filenames indicated in the previous section are :

- `Mesh_SqrCirc` is the **`mesh_file`**
- `Material_SqrCirc` is the **`material_file`**
- `Nodes_SqrCirc` is the **`nodes_coords_file`**
- `Surf_abs_SqrCirc` is the **`absorbing_surface_file`**
- `Surf_free_SqrCirc` is the **`free_surface_file`**

In addition, four files like `free_surface_file` corresponding to the sides of the model are generated.

3.3 How to use Cubit/Trelis to generate an external mesh

Cubit (or Trelis)[2] is a 2D/3D finite element grid generator distributed which can be used for the generation of quadrangle and hexahedral meshes. Cubit has a convenient interface with Python (module cubit) which allows to create meshes from Python scripts. To get started with Cubit/Trelis we recommend you the step-by-step tutorials available at: https://coreform.com/coreform-cubit-tutorials/ Many powerful graphical tools are available, and very useful, but we will focus here on the command line functionalities and especially the Python interface which is the real force of Cubit/Trelis.

To get started we recommend to the inpatients to open Cubit/Trelis and to click on the following symbol:  . Then select the files of type Python Files (*.py) and play the following script:

```
utils/cubit2specfem2d/simplest2DexampleWithPmls.py
```

In the case you want to perform an axisymmetric simulation, we recommend you rather to play:

```
utils/cubit2specfem2d/simpleAxisym2dMesh.py
```

It will create a simple mesh with PMLs. Then re-click on  and play:

```
utils/cubit2specfem2d/cubit2specfem2d.py
```

This script will create (in current directory) all the mesh files necessary for a SPECFEM2D simulation. Other commented examples are available. We particularly recommend you to look at the folder `EXAMPLES/reproducible_study/Bottero2016_axisymmetry_example` beginning by reading the README available there. Read carefully the comments in these scripts, they are helpful. Another way to use Python together with Cubit/Trelis is to use the script tab. This tab is a real Python terminal that can be used to pass command line python instruction to Cubit/Trelis through the cubit module. In the case of the Script tab is not visible in the command line panel (at the bottom of the screen) do:

```
Tools -> Options... -> Layout [-> Cubit Layout] -> Show script tab
```

This tab will allow you to play the scripts one line after another directly in Cubit/Trelis. With this you should be able to understand how to create meshes and export them under SPECFEM2D format.

3.3.1 Note about Cubit/Trelis built-in Python

Beware, there are some (annoying) differences between cubit built-in Python and the actual Python langage:

- `"aString" + 'anotherString'` can cause problems even after being stored:

  ```
  a = "aString"
  b = a + 'anotherString'
  ```

  Example that is not working:

  ```
  pathToMeshDir = pathToSpecfem + 'EXAMPLES/reproducible_study/Bottero2016_axisymmetry_example/'
  pathToMeshDir = pathToMeshDir + 'MESH'
  cubit.cmd('cd \"'+pathToMeshDir+'\"')
  ```

- No comments after double dots:
  Example that is not working:

  ```
  if True: # Just a dummy comment
      print "Ok!"
  ```

  This example works without the comment.

- `os.makedirs("~/aDirectory/")` does not work. It creates a directory named `~`
  !!!!! To remove that do: `rm -R ./~` AND NEVER `rm -rf ~` !!!!!

- `sys.argv` can not be used

- No comments `""" """` at the beginning of a script

And probably many others! Hopefully, this will be resolved in future.

[2] available at https://coreform.com

3.4 Notes about absorbing PMLs

If you use CPML, an additional file listing the CPML elements is needed. Its first line is the total number of CPML elements, and then a list of all the CPML elements, one per line. The format of these lines is: in the first column the CPML element number, and in the second column a flag as follows:

Table 3.1: Definition of flags for CPML elements

Flag	Meaning
1	element belongs to a X CPML layer only (either in Xmin or in Xmax)
2	element belongs to a Y CPML layer only (either in Ymin or in Ymax)
3	element belongs to both a X and a Y CPML layer (i.e., to a CPML corner)

In order to see how to add PML layers to a mesh / model created with an external mesher such as Gmsh, see the examples in directory `EXAMPLES/applications/meshing/Gmsh_example_CPML_MPI`.

If you use PML, the mesh elements that belong to the PML layers can be acoustic or elastic, but not viscoelastic nor poroelastic. Then, when defining your model, you should define these absorbing elements as either acoustic or elastic. If you forget to do that, the code will fix the problem by automatically converting the viscoelastic or poroelastic PML elements to elastic. This means that strictly speaking the PML layer will not be perfectly matched any more, since the physical model will change from viscoelastic or poroelastic to elastic at the entrance of the PML, but in practice this is sufficient and produces only tiny / negligible spurious reflections.

If you use PML and an external mesh (created using an external meshing tool such as Gmsh, CUBIT/TRELIS or similar), try to have elements inside the PML as regular as possible, i.e. ideally non-deformed rectangles obtained by 'extrusion' of the edge mesh elements meshing the outer edges of the computational domain without PML; by doing so, the PMLs obtained will be far more stable in time (PML being weakly unstable from a mathematical point of view, very deformed mesh elements inside the PMLs can trigger instabilities much more quickly).

If you have an existing CUBIT (or similar) mesh stored in SPECFEM2D format but do not know how to assign CPML flags to it, we have created a small serial Fortran program that will do that automatically for you. That program is `utils/CPML/convert_external_layers_of_a_given_mesh_to_CPML_layers2D.f90`. When you create the PML layers using that script, you do not need to mark (i.e. assign to physical entities with a specific name) those external layers in the mesher. However you still need to specify the boundary of the mesh as you where doing in the case of absorbing conditions. The script will automatically extract the elements on the PML. It will ask you for a thickness for the PML layers. Suppose that you have created a region with a 1-meter size element, when it will prompt for the PML thickness you can enter 3.1 and it will create a PML 3 element thick. Always input a slightly larger (5-10%) size because the element might be slightly skewed, or if you have not created your PML region via extrusion/webcut in CUBIT/TRELIS.

To stabilize PMLs it also helps to add a transition layer of geometrically-regular non-PML elements, in which attenuation is also turned off (i.e. $Q_\kappa = Q_\mu = 9999$ in that layer), as in the red layer of Figure 3.4. Our tools in directory in directory `utils/CPML` will implement that transition layer automatically in future.

To be more precise:

1/ If one wants to use PML layers, they should NOT mark the layers according to that python script - the reason is that the `xmeshfem2d` does not recognize those CPML flags. If whoever developed the script adjusts it to solve this problem - this might be a great relief for users; as of now no physical identifiers are needed for those layers.

2/ HOWEVER, the "Top", "Bottom", "Left"," and "Right" boundaries of the model, need to be re-assigned to outer boundaries of the model - that will be the leftmost boundary of the left -bounding PML , rightmost of the right PML, topmost for the Top PML (if there is one) and the bottom boundary of the bottom layer. Those and only those lines need to have the mentioned identifiers (opposite to the example with the two-holed square with Stacey conditions).

3/ There is no need to create Top PML in case one wants it to be reflective; as the fortran script that assigns the flag will ignore the elements that sit within PML-layer thickness distance to the top.

4/ The Fortran program `utils/CPML/convert_external_layers_of_a_given_mesh_to_CPML_layers2D.f90` that flags the PML elements does not create additional elements; it simply takes the elements within chosen distance from the boundaries, that sit in the interior of model and marks them as absorbing.

If you use PML and an external velocity and density model (e.g., setting flag `MODEL` to `external`), you should be careful because mathematically a PML cannot handle heterogeneities along the normal to the PML edge inside the PML layer. This comes from the fact that the damping profile that is defined assumes a constant velocity and density model along the normal direction. Thus, you need to modify your velocity and density model in order for it to be 1D inside the PML, as shown in Figure 3.5. This applies to the bottom layer as well; there you should make sure that your model is 1D and thus constant along the vertical direction.

To summarize, only use a 2D velocity and density model inside the physical region, and in all the PML layers extend it by continuity from its values along the inner PML edge.

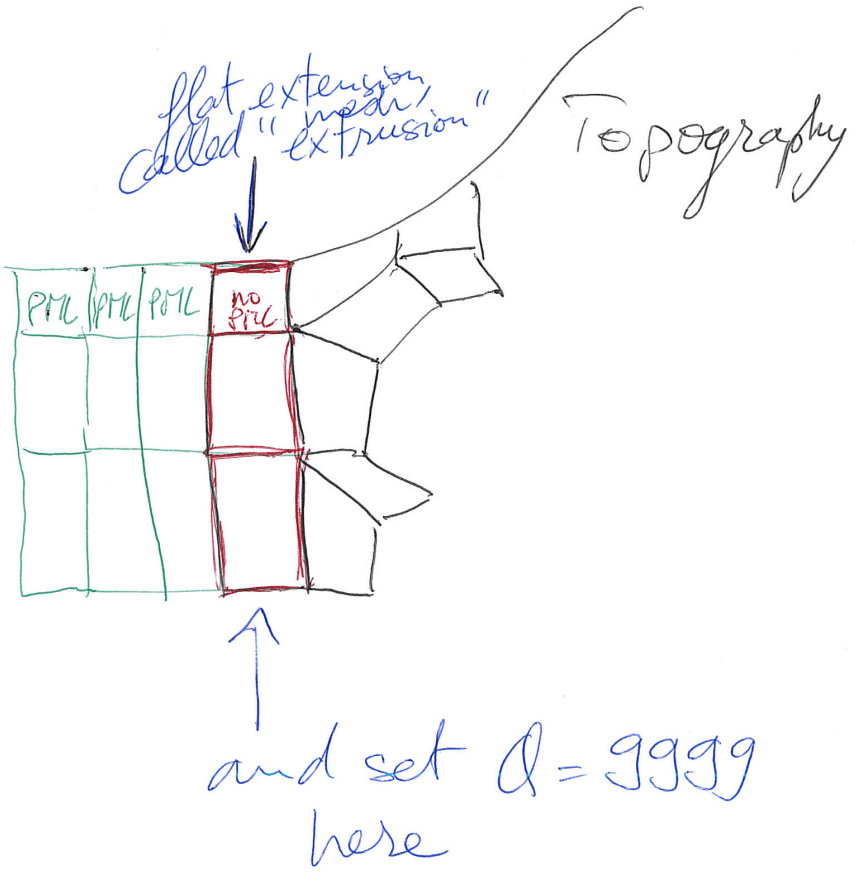


Figure 3.4: Mesh extrusion for PML (green elements) and a non-PML stabilization layer (red elements).

3.5 Controlling the quality of an external mesh

To examine the quality of the elements in your externally build mesh, type

```
./bin/xcheck_quality_external_mesh
```

(and answer "3" to the first question asked). This code will tell you which element in the whole mesh has the worst quality (maximum skewness, i.e. maximum deformation of the element angles) and it should be enough to modify

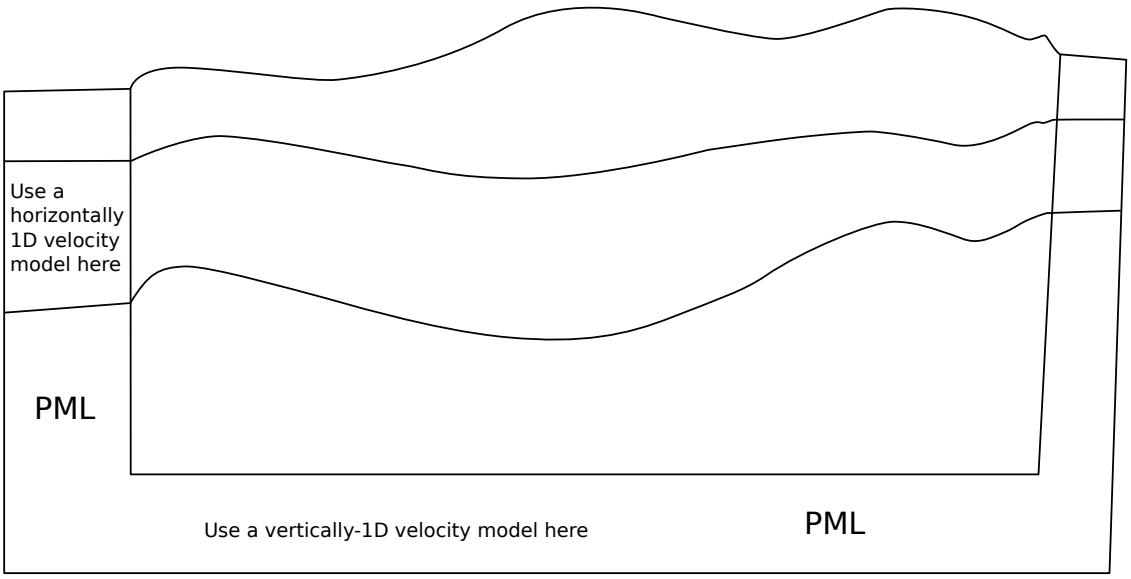


Figure 3.5: How to modify your external 2D velocity and density model in order to use PML. Such a modification is not needed when using Stacey absorbing boundary conditions (but such conditions are significantly less efficient).

this element with the external software package used for the meshing, and to repeat the operation until the maximum skewness of the whole mesh is less or equal to about 0.75 (above is dangerous: from 0.75 to 0.80 could still work, but if there is a single element above 0.80 the mesh should be improved).

The code also shows a histogram of 20 classes of skewness which tells how many element are above the skewness = 0.75, and to which percentage of the total this amounts. To see this histogram, you could type:

```
gnuplot plot_mesh_quality_histogram.gnu
```

This tool is useful to estimate the mesh quality and to see it evolve along the successive corrections.

3.6 Controlling how the mesh samples the wave field

To examine (using Gnuplot) how the mesh samples the wave field, type

```
gnuplot plot_points_per_wavelength_histogram.gnu
```

and also check the following histogram printed on the screen or in the output file:

```
histogram of min number of points per S wavelength (P wavelength in
acoustic regions)
(too small: poor resolution of calculations - too big = wasting
memory and CPU time)
(threshold value is around 4.5 points per wavelength in elastic media
and 5.5 in acoustic media)
```

If you see that you have a significant number of mesh elements below the threshold indicated, then your simulations will not be accurate and you should create a denser mesh. Conversely, if you have a significant number of mesh elements above the threshold indicated, the mesh your created is too dense, it will be extremely accurate but the simulations will be slow; using a coarser mesh would be sufficient and would lead to faster simulations.

Chapter 4

Running the Solver xspecfem2D

To run the solver, type

```
./bin/xspecfem2D
```

from within the main working directory (use `mpirun` or equivalent if you compiled with parallel support). This will output the seismograms and snapshots of the wave fronts at different time steps in directory `OUTPUT_FILES/`.

To visualize snapshot files, type "`gs OUTPUT_FILES/vect*.ps`" to see the Postscript files (in which the wave field is represented with small arrows, fluid/solid matching interfaces with a thick pink line, and absorbing edges with a thick green line) and "`gimp OUTPUT_FILES/image*.gif`" to see the colour snapshot showing a pixelized image of one of the two components of the wave field (or pressure, depending on what you have selected for the output in `DATA/Par_file`).

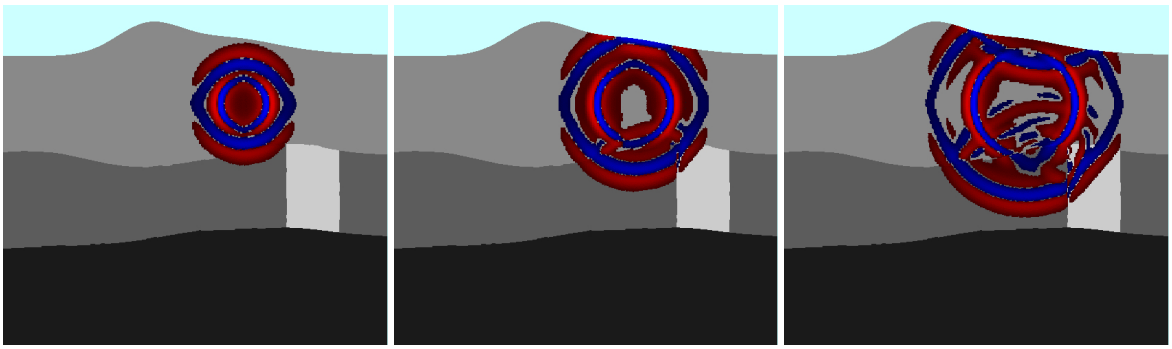


Figure 4.1: Wavefield snapshots of the default example generated by `xspecfem2D` when parameter `output_color_image` is set to `.true.`. To create smaller (subsampled) images you can change double precision parameter `factor_subsample_image = 1.0` to a higher value in file `DATA/Par_file`. This can be useful in the case of very large models. The number of pixels of the image in each direction must be smaller than parameter `NX_NZ_IMAGE_MAX` defined in file `SETUP/constants.h.in`, again to avoid creating huge images in the case of very large models.

Please consider these following points, when running the solver:

- the `DATA/Par_file` given with the code works fine, you can use it without any modification to test the code
- the seismograms `OUTPUT_FILES/*.sem*` are simple ASCII files with two columns: time in the first column and amplitude in the second, therefore they can be visualized with any tool you like, for instance "`gnuplot`"; if you prefer to output binary seismograms in Seismic Unix format (which is a simple binary array dump) you can use parameter `SU_FORMAT`, in which case all the seismograms will be written to a single file with the extension `*.bin`. Depending on your installation of the Seismic Unix package you can use one of these two commands:

```
surange < Uz_file_single.bin
suoldtonew < Uz_file_single.bin | surange
```

to see the header info. Replace `surange` with `suxwigb` to see wiggle plots for the seismograms.

- if flag `MODEL` in `DATA/Par_file` is set to `default`, the velocity and density model is determined using the `nbmodels` and `nbregions` devices. Otherwise, `nbmodels` values are ignored and the velocity and density model is determined from a user supplied file or subroutine.
- when compiling with Intel ifort, use "`-assume byterecl`" option to create binary PNM images displaying the wave field
- there are a few useful scripts and Fortran routines in directory `utils/`.
- you can find a Fortran code to compute the analytical solution for simple media that we use as a reference in benchmarks in many of our articles at EX2DDIR. That code is described in: Berg et al. [1994]

Notes about `DATA/Par_file` parameters

The `DATA/Par_file` contains detailed comments and should be almost self-explanatory. Please see also the corresponding explanations in generating the mesh. Some more detailed informations are listed here for a few parameters affecting the solver:

`ATTENUATION_VISCOELASTIC` or `ATTENUATION_VISCOACOUSTIC` Regarding attenuation (viscoelasticity and viscoacoustic), in the `Par_file` you need to select the number of standard linear solids (N_SLS) to mimic a constant Q quality factor. Using N_SLS = 3 is always safe. If (and only if) you know what you are doing, you can try to reduce that in order to reduce the cost of the simulations. Figure 4.2 shows values that you can consider using (again, if and only if you know what you are doing). That table has been created by Zhinan Xie using a comparison between results obtained with a truly-constant Q and results obtained with its approximation based on N_SLS standard linear solids. The comparison is performed using the time-frequency misfit and goodness-of-fit criteria proposed by Kristeková et al. [2009]. The table is drawn for a dimensionless parameter representing the distance of propagation.

`USE_TRICK_FOR_BETTER_PRESSURE` This option can only be used so far if all the receivers record pressure and are in acoustic elements. Use a trick to increase accuracy of pressure seismograms in fluid (acoustic) elements: use the second derivative of the source for the source time function instead of the source itself, and then record `potential_acoustic()` as pressure seismograms instead of `potential_dot_dot_acoustic()`; this is mathematically equivalent, but numerically significantly more accurate because in the explicit Newmark time scheme acceleration is accurate at zeroth order while displacement is accurate at second order, thus in fluid elements `potential_dot_dot_acoustic()` is accurate at zeroth order while `potential_acoustic()` is accurate at second order and thus contains significantly less numerical noise.

`use_existing_STATIONS` Turn this option on if you have station locations that you want to specify explicitly by an existing `DATA/STATIONS` file. Each line represents one station in the following format:

```
Station Network X-position Z-position Elevation(m) burial(m)
```

Elevation and burial are generally applicable to geographical regions. The code however ignores both, elevation because it uses the mesh topography instead, and burial depth needs to be set to zero because the given X/Z position is used to locate the station. If the option is turned off, the `STATIONS` file will be generated by the mesher using the defined receiver sets in the `Par_file`.

	$x\omega_r/c_r$									
	5 π	10 π	15 π	20 π	25 π	30 π	35 π	40 π	45 π	50 π
$5 \le Q < 10$	3	3	3	3	3	3	3	3	3	4
$10 \le Q < 20$	2	3	3	3	3	3	3	3	3	3
$20 \le Q < 30$	2	2	3	3	3	3	3	3	3	3
$30 \le Q < 40$	2	2	2	3	3	3	3	3	3	3
$40 \le Q < 50$	2	2	2	2	3	3	3	3	3	3
$50 \le Q < 60$	1	2	2	2	2	3	3	3	3	3
$60 \le Q < 70$	1	2	2	2	2	2	3	3	3	3
$70 \le Q < 80$	1	2	2	2	2	2	2	3	3	3
$80 \le Q < 90$	1	2	2	2	2	2	2	2	3	3
$90 \le Q < 100$	1	2	2	2	2	2	2	2	2	3
$100 \le Q < 150$	1	1	2	2	2	2	2	2	2	2
$150 \le Q < 200$	1	1	1	2	2	2	2	2	2	2
$200 \le Q < 250$	1	1	1	1	2	2	2	2	2	2
$250 \le Q < 300$	1	1	1	1	1	2	2	2	2	2
$300 \le Q < 350$	1	1	1	1	1	1	2	2	2	2
$350 \le Q < 400$	1	1	1	1	1	1	1	2	2	2
$400 \le Q < 450$	1	1	1	1	1	1	1	1	2	2
$450 \le Q < 500$	1	1	1	1	1	1	1	1	1	2
$500 \le Q$	1	1	1	1	1	1	1	1	1	1

Figure 4.2: Table showing how you can select a value of N_SLS smaller than 3, if and only if you know what you are doing.

Notes about DATA/SOURCE parameters

The SOURCE file located in the DATA/ directory should be edited in the following way:

source_surf Set this flag to .true. to force the source to be located at the surface of the model, otherwise the sol be placed inside the medium

xs source location x in meters

zs source location z in meters

source_type Set this value equal to 1 for elastic forces or acoustic pressure, set this to 2 for moment tensor sources. For a plane wave including converted and reflected waves at the free surface, P wave = 1, S wave = 2, Rayleigh wave = 3; for a plane wave without converted nor reflected waves at the free surface, i.e. the incident wave only, P wave = 4, S wave = 5. (incident plane waves are turned on by parameter initialfield in DATA/Par_file).

time_function_type Choose a source-time function: set this value to 1 to use a Ricker, i.e. the second derivative of a Gaussian, 2 to use the first derivative of a Gaussian, 3 to use a Gaussian, 4 to use a Dirac or 5 to use a Heaviside source-time function. Note that we use the standard definition of a Ricker, for a dominant frequency f_0: $\text{Ricker}(t) = (1 - 2at^2)e^{-at^2}$, with $a = \pi^2 f_0^2$, whose Fourier transform is thus: $\frac{1}{2}\frac{\sqrt{\pi}\omega^2}{a^{3/2}}e^{-\frac{\omega^2}{4a}}$ This gives the wavelet of Figure 4.3. Note that the Gaussian function (type 3) is defined as the second integral of this

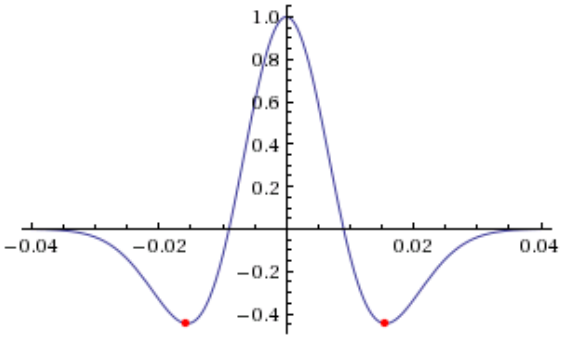


Figure 4.3: We use the standard definition of a Ricker (i.e., second derivative of a Gaussian). Image taken from http://subsurfwiki.org.

Ricker wavelet. This allows the USE_TRICK_FOR_BETTER_PRESSURE feature in DATA/Par_file to compute pressure as second-order accurate solution for acoustic simulations. However, this resulting Gaussian function will have a minus sign in front and thus have values less or equal to zero. Additional source time functions include a normalized Gaussian (type 0; normalized with respect to the integral value), ocean acoustic wavelets (types 6 and 7), an external file (type 8), a Burst wavelet (type 9), a Sinusoidal function (type 10), the Marmousi Ormsby wavelet (type 11), the Brune and smoothed Brune functions (types 12 and 13), and the regularized and integrated regularized Yoffe function (types 14 and 15).

f0 Set this to the dominant frequency of the source. For point-source simulations using a Heaviside source-time function (time_function_type = 5), we recommend setting the source frequency parameter f0 equal to a high value, which corresponds to simulating a step source-time function, i.e., a moment-rate function that is a delta function.

The half duration of a source is obtained by 1/f0. If the code will use a Gaussian source-time function (time_function_type = 3) (i.e., a signal with a shape similar to a 'smoothed triangle', as explained in Komatitsch and Tromp [2002] and shown in Fig 4.4), the source-time function uses a half-width of 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. Komatitsch and Tromp [2002] 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.sh` for this purpose (or alternatively use signal-processing software packages such as SAC). Type

```
make xconvolve_source_timefunction
```

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

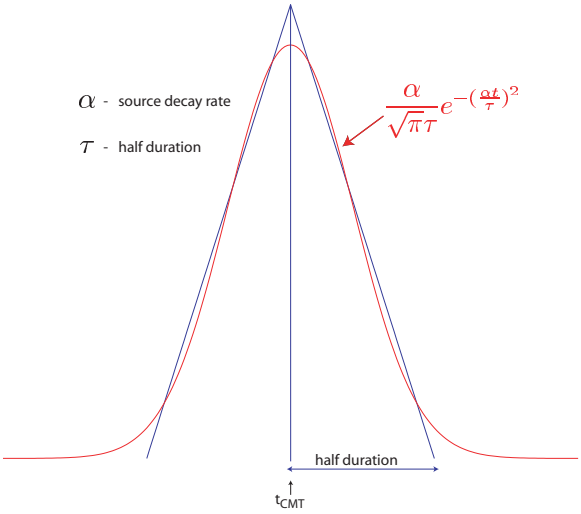


Figure 4.4: Comparison of the shape of a triangle and the Gaussian function actually used.

`t0` For single sources, we recommend to set the time shift parameter `t0` equal to 0.0. The time shift parameter would simply apply an overall time shift to the synthetics (according to the time shift of the first source), something that can be done in the post-processing. This time shift parameter can be non-zero when using multiple sources.

`anglesource` angle of the source (for a force only) given in degrees, measured clockwise from the vertical; for a plane wave, this is the incidence angle. For moment tensor sources this parameter is unused.

`Mxx,Mzz,Mxz` Moment tensor components (valid only for moment tensor sources, `source_type = 2`). Note that the units for the components of a moment tensor source are different in SPECFEM2D and in SPECFEM3D:

- in SPECFEM3D the moment tensor components are in $dyne * cm$
- in SPECFEM2D the moment tensor components are in $N * m$

The conversion factor from $dyne * cm$ to $N * m$ is: $1\, dyne * cm = 10^{-7}\, N * m$. To go from strike / dip / slip to CMTSOLUTION moment-tensor format using the classical formulas (of e.g. Aki and Richards [1980] you can use these two small C programs provided in the SPECFEM3D Globe repository:

```
./utils/scripts/CMTs/strike_dip_rake_to_CMTSOLUTION.c
./utils/scripts/CMTs/CMTSOLUTION_to_AkiRichards.c
```

However, it is another story to make a good 2D approximation of that, because in plain-strain P-SV what you get is the equivalent of a line source in the third direction (orthogonal to the plane) rather than a 3D point source. For more details on this see e.g. Section 7.3 "Two-dimensional point sources" of the book of Pilant [1979]. That book being hard to find, we scanned the related pages in file `discussion_of_2D_sources_and_approximations_from_Pilant_1979.pdf` in the same directory as this users manual. Another very useful reference addressing that is Helmberger and Vidale [1988] and its recent extension [Li et al., 2014].

factor amplification factor

Note, 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 $t = -1.2 * \texttt{half duration} + \texttt{t0}$ (the factor 1.2 is to make sure the moment rate function is very close to zero when starting the simulation; Heaviside functions use a factor 2.0), the half duration is obtained by $1/\texttt{f0}$. If you prefer, you can fix this start time by setting the parameter `USER_T0` in the `constants.h` file to a positive, non-zero value. The simulation in that case would start at a starting time equal to `-USER_T0`.

4.1 How to run elastic wave simulations

For isotropic elastic materials, there are two options:

P-SV: To run a P-SV waves calculation propagating in the x-z plane, set `p_sv = .true.` in the `Par_file`.

SH: To run a SH (membrane) waves calculation travelling in the x-z plane with a y-component of motion, set `p_sv = .false.`

This feature is only implemented for elastic materials and sensitivity kernels can be calculated (see Tape et al. [2007] for details on membrane surface waves).

An optional useful Python script called `SEM_save_dir.py` is provided. It allows one to automatically save all the parameters and results of a given simulation.

4.2 How to run axisymmetric wave simulations

Axisymmetric simulations are possible in SPECFEM2D. For these simulations the 2D domain simulated is physically the meridional 2D shape of an axisymmetric 3D domain. We invite you to read our publication [Bottero et al., 2016] as an introduction. To set the geometry as axisymmetric turn the flag `AXISYM` to `.true.` in the `Par_file`:

```
AXISYM                          = .true.
```

The left border of the model becomes then a symmetry axis. The wavefield calculated is then physically a 3D wavefield obtained by revolution of a 2D wavefield around its left border.

Note about the source:

In axisymmetric geometry the whole model is symmetric with respect to this axis, including the source. Hence if the source is not on the axis it will physically have a circular shape. This is still possible and relevant for some applications as non destructive testing but is most of the time unwanted. This has to be kept in mind. In acoustic medium, as an explosion in a fluid is naturally axisymmetric, the wavefield generated has the correct 3D shape. However, if the source is put in an elastic solid, its 3D radiation pattern will be axisymmetric.

Getting started:

To get started a simple example is available in `EXAMPLES/applications/axisymmetric_examples/axisymmetric_case_AXISYM_option`, we encourage you to read the `README` file you will find there. This example contains an example of the use of `AXISYM` option plus a validation using the semi-analytical code OASES (Schmidt [2004]). In this example the domain studied is a water layer lying above a viscoelastic medium. The source is an explosion in the water and the domain is bounded with PMLs.

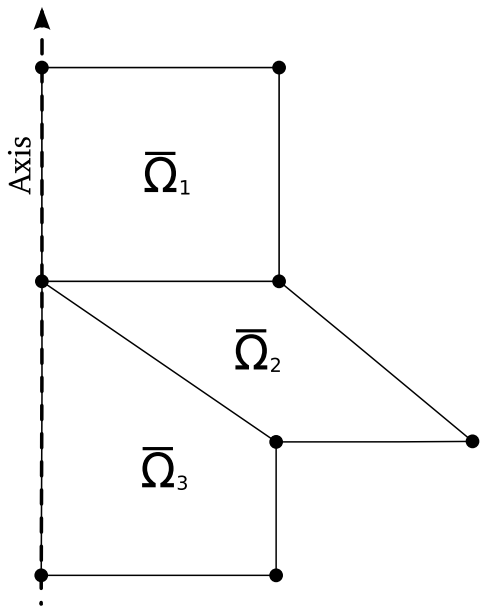


Figure 4.5: For simplicity we exclude cases in which the mesh elements that are in contact with the symmetry axis are in contact with it by a single point instead of by a full edge, such as element $\bar{\Omega}_2$ here. This amounts to imposing that the leftmost layer of elements in the mesh be structured rather than non structured; The rest of the mesh can be non structured.

Note about external meshers:

Using external meshers is possible in axisymmetric geometry. An example is available in `EXAMPLES/reproducible_study/Bottero2016_axisymmetry_example` with the mesher Cubit/Trelis (https://coreform.com). We invite you to check this example and read the previous chapter for more details. The only difference with plane-strain geometry is that SPECFEM2D needs an additional file defining axial elements. The path to this file has to be given in the `Par_file`:

```
axial_elements_file             = /path/to/the/axial_elements_file
```

The axial elements file has the following structure:

```
  48
   1          2       8456       8457
   2          2       8457       8458
   3          2       8458       8459
   4          2       8459       8460
 623          2        171        204
1053          2        172       9512
1054          2        172        173
1055          2        173        174
...
```

Which is similar to free surface files. Hence the first line contains the number of axial elements, then the other lines contain four columns: element id, number of nodes describing an axial element (always 2), first node id, second node id. Note that the axis elements must include the possible (up and/or down) PMLs elements in contact with the axis. For simplicity we assume that the mesh elements that are in contact with the symmetry axis are in contact with it by a full edge rather than by a single point, i.e. we exclude cases as that of Figure 4.5. This amounts to imposing that the left-most layer of elements in the mesh be structured rather than non structured; The rest of the mesh can be non structured.

Note about the resolution:

In axisymmetry a different quadrature is used in the axial elements making the number of points per wavelength necessary a slightly bigger ($\approx 25\%$) than in plane-strain.

Note about a small remaining bug:

It has to be noted that a small bug is still hiding somewhere in the code. Indeed the output signals generated are correct in the whole domain except in the element containing the source. This small bug has not been solved so far but not prevent to use the code.

Note about a demo code to learn:

A simplistic demo code is available in `utils/small_SEM_solver_in_Fortran_without_MPI_to_learn`. This simple code is useful to learn how the spectral-element method works in both plane-strain and axisymmetric geometries. Have a look to it if interested. Once in its directory, type `./make_Fortran_2D_axisymmetric.csh` and then `./xspecfem2D` to compile and run. The bug discussed above is not present in this small code.

4.3 How to run anisotropic wave simulations

Following Carcione et al. [1988a], we use the classical reduced Voigt notation to represent symmetric tensors [Helbig, 1994, Carcione, 2007]:

> The constitutive relation of a heterogeneous anisotropic and elastic solid is expressed by the generalized Hooke's law, which can be written as
>
> $$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}, \qquad i,j,k = 1,\ldots,3,$$
>
> where t is the time, $\mathbf{x}$ is the position vector, $\sigma_{ij}(\mathbf{x},t)$ and $\varepsilon_{ij}(\mathbf{x},t)$ are the Cartesian components of the stress and strain tensors respectively, and $c_{ijkl}(\mathbf{x})$ are the components of a fourth-order tensor called the elasticites of the medium. The Einstein convention for repeated indices is used.
>
> To express the stress-strain relation for a transversely isotropic medium we introduce a shortened matrix notation commonly used in the literature. With this convention, pairs of subscripts concerning the elasticities are replaced by a single number according to the following correspondence:
>
> $$\begin{aligned} (11) &\rightarrow 1, & (22) &\rightarrow 2, & (33) &\rightarrow 3, \\ (23) = (32) &\rightarrow 4, & (31) = (13) &\rightarrow 5, & (12) = (21) &\rightarrow 6. \end{aligned}$$

Thus in the most general 2D case we have the following convention for the stress-strain relationship:

```
! implement anisotropy in 2D
sigma_xx = c11*dux_dx + c13*duz_dz + c15*(duz_dx + dux_dz)
sigma_zz = c13*dux_dx + c33*duz_dz + c35*(duz_dx + dux_dz)
sigma_xz = c15*dux_dx + c35*duz_dz + c55*(duz_dx + dux_dz)

! sigma_yy is not equal to zero in the plane strain formulation
! but is used only in post-processing if needed,
! to compute pressure for display or seismogram recording purposes
sigma_yy = c12*dux_dx + c23*duz_dz + c25*(duz_dx + dux_dz)
```

where the notations are for instance `duz_dx = d(Uz) / dx`.

4.4 How to run poroelastic wave simulations

Check the following new inputs in `Par_file`:

In section **"# Attenuation"**:
`ATTENUATION_PORO_FLUID_PART`, `Q0_poroelastic`, and `freq0_poroelastic` deal with viscous damping in a poroelastic medium. `Q0_poroelastic` is the quality factor set at the central frequency `freq0_poroelastic`. For more details see Morency and Tromp [2008].

In section **"# time step parameters"**:
`SIMULATION_TYPE` defines the type of simulation

(1) forward simulation

(2) UNUSED (purposely, for compatibility with the numbering convention used in our 3D codes)

(3) adjoint method and kernels calculation

In section **"# source parameters"**:
The code now support multiple sources. `NSOURCE` is the number of sources. Parameters of the sources are displayed in the file `SOURCE`, which must be in the directory `DATA/`. The components of a moment tensor source must be given in N.m, not in dyne.cm as in the `DATA/CMTSOLUTION` source file of the 3D version of the code.

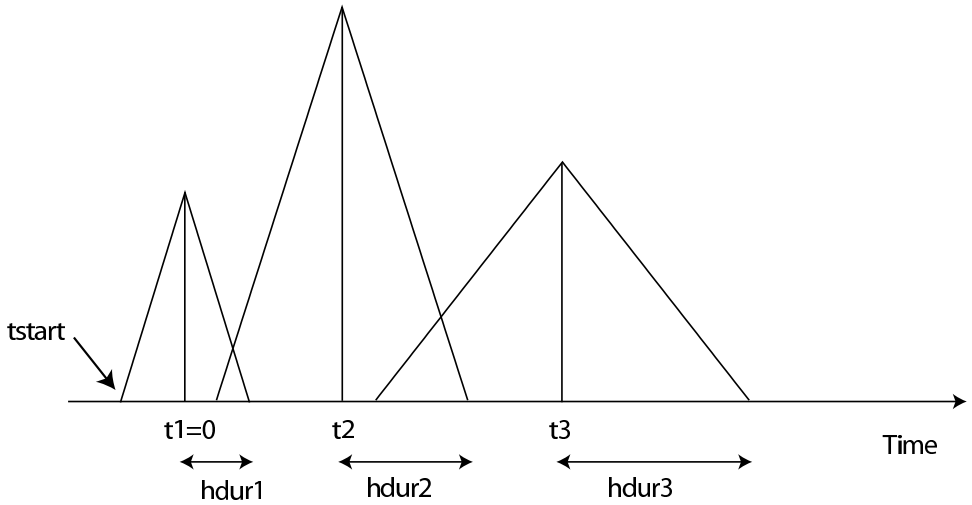


Figure 4.6: Example of timing for three sources. The center of the first source triangle is defined to be time zero. Note that this is NOT in general the hypocentral time, or the start time of the source (marked as `tstart`). The time shift parameter `t0` in the `SOURCE` file would be $t1(=0)$, $t2$, $t3$ in this case, and the half-duration parameter, `f0`, would be $\texttt{hdur1} = 1/\texttt{f0}_1$, $\texttt{hdur2} = 1/\texttt{f0}_2$, $\texttt{hdur3} = 1/\texttt{f0}_3$ for the sources 1, 2, 3 respectively.

In section **"# receiver line parameters for seismograms"**:
`SAVE_FORWARD` determines if the last frame of a forward simulation is saved (`.true.`) or not (`.false`)

In section **"# define models...."**:
There are three possible types of models for seismic wave propagation:

I: (`model_number 1 rho Vp Vs 0 0 QKappa Qmu 0 0 0 0 0 0`) or

II: (`model_number 2 rho c11 c13 c15 c33 c35 c55 c12 c23 c25 0 0 0`) or

III: (`model_number 3 rhos rhof phi c kxx kxz kzz Ks Kf Kfr etaf mufr Qmu`).

For isotropic elastic/acoustic material use `I` and set `Vs` to zero to make a given model acoustic, for anisotropic elastic use `II`, and for isotropic poroelastic material use `III`. The mesh can contain acoustic, elastic, and poroelastic models simultaneously.

For anisotropic elastic media the last three parameters, `c12 c23 c25`, are used only when the user asks the code to compute pressure for display or seismogram recording purposes. Thus, if you do not know these parameters for your anisotropic material and/or if you do not plan to display or record pressure you can ignore them and set them to zero. When pressure is used these three parameters are needed because the code needs to compute σ_{yy}, which is not equal to zero in the plane strain formulation.

`rho_s` = solid density

`rho_f` = fluid density

`phi` = porosity

`tort` = tortuosity

`permxx` = xx component of permeability tensor

`permxz` = xz,zx components of permeability tensor

`permzz` = zz component of permeability tensor

`kappa_s` = solid bulk modulus

`kappa_f` = fluid bulk modulus

`kappa_fr` = frame bulk modulus

`eta_f` = fluid viscosity

`mu_fr` = frame shear modulus

`Qmu` = shear quality factor

Note: for the poroelastic case, `mu_s` is irrelevant. For details on the poroelastic theory see Morency and Tromp [2008].

`get_poroelastic_velocities.f90` allows to compute cpI, cpII, and cs function of the source dominant frequency. Notice that for this calculation we use `permxx` and the dominant frequency of the first source, f0(1). Caution if you use several sources with different frequencies and if you consider anistropic permeability.

4.5 How to run electromagnetic wave simulations

For more details on the electromagetic (EM) wave propagation in SPECFEM, please refer to Morency [2020]. Check the following new inputs in `Par_file`:

In section **"# Attenuation"**:
`ATTENUATION_PERMITTIVITY`, `ATTENUATION_CONDUCTIVITY`, and `f0_electromagnetic` deal with dispersive and attenuating EM media. For more details see section 2.2 in Morency [2020].

In section **"# time step parameters"**:
`SIMULATION_TYPE` defines the type of simulation

(1) forward simulation

(2) UNUSED (purposely, for compatibility with the numbering convention used in our 3D codes)

(3) adjoint method and kernels calculation – **TO DO**

In section **"# define models...."**:
There are three possible types of models for seismic wave propagation and one for EM wave propagation:

`I:` (`model_number 1 rho Vp Vs 0 0 QKappa Qmu 0 0 0 0 0 0`) or

`II:` (`model_number 2 rho c11 c13 c15 c33 c35 c55 c12 c23 c25 0 0 0`) or

III: (model_number 3 rhos rhof phi c kxx kxz kzz Ks Kf Kfr etaf mufr Qmu) or
IV: (model_number 4 mu0 e0 e11 e33 sig11 sig33 Qe11 Qe33 Qs11 Qs33 0 0 0).

For isotropic EM material use IV, where

mu_0 = magnetic permeability

e_0 = vacuum dielectric permittivity

e_11 = xx component of relative dielectric permittivity

e_33 = zz component of relative dielectric permittivity

sig_11 = xx component of conductivity

sig_33 = zz component of conductivity

Qe_11 = quality factor of xx component of permittivity

Qe_33 = quality factor of zz component of permittivity

Qs_11 = quality factor of xx component of conductivity

Qs_33 = quality factor of zz component of conductivity

get_electromagnetic_velocities.f90 allows to compute the anisotropic EM wavespeeds as a function of the source dominant frequency. Notice that for this calculation we use the dominant frequency of the first source, f0(1). Caution if you use several sources with different frequencies.

Finally, 2-D transverse electric (TE) mode, more suitable for crosshole and vertical radar profiling applications, and transverse magnetic (TM) mode, suitable for surface based reflection ground penetration radar type of applications, can be handled using the P-SV/SH flag in Par_file:

P-SV (EM TE): To run a EM waves calculation propagating in the x-z plane, set p_sv = .true.

SH (EM TM): To run EM waves calculation travelling in the x-z plane with a y-component of electric field, set p_sv = .false.

4.6 Coupled simulations

The code supports acoustic/elastic, acoustic/poroelastic, elastic/poroelastic, and acoustic, elastic/poroelastic simulations. Elastic/poroelastic coupling supports anisotropy, but not attenuation for the elastic material.

4.7 How to choose the time step

Three different explicit conditionally-stable time schemes can be used for elastic, acoustic (fluid) or coupled elastic/acoustic media: the Newmark method, the low-dissipation and low-dispersion fourth-order six-stage Runge-Kutta method (LDDRK4-6) presented in Berland et al. [2006], and the classical fourth-order four-stage Runge-Kutta (RK4) method. Currently the last two methods are not implemented for poroelastic media. According to De Basabe and Sen [2010] and Berland et al. [2006], with different degrees $N = NGLLX - 1$ of the GLL basis functions the CFL bounds are given in the following tables. Note that by default the SPECFEM solver uses $NGLLX = 5$ and thus a degree $N = 4$, which is thus the value you should use in most cases in the following tables. You can directly compare these values with the value given in sentence 'Max stability for P wave velocity' in file output_solver.txt to see whether you set the correct Δt in Par_file or not. For elastic simulation, the CFL value given in output_solver.txt does not consider the V_p/V_s ratio, but the CFL limit slight decreases when V_p/V_s increases. In viscoelastic simulations the CFL limit does not change compared to the elastic case because we use a rational approximation of a constant quality factor Q, which has no attenuation effect on zero-frequency waves. Additionally, if you use C-PML absorbing layers in your simulations, which are implemented for the Newmark and LDDRK4-6 techniques but not for the classical RK4), the CFL upper limit decreases to approximately 95% of the limit without absorbing layers in the case of Newmark and to 85% in the case of LDDRK4-6.

Table 4.1: CFL upper bound for an acoustic (fluid) simulation.

Degree N	Newmark	LDDRK4-6	RK4
1	0.709	1.349	1.003
2	0.577	1.098	0.816
3	0.593	1.129	0.839
4	**0.604**	**1.150**	**0.854**
5	0.608	1.157	0.860
6	0.608	1.157	0.860
7	0.608	1.157	0.860
8	0.607	1.155	0.858
9	0.607	1.155	0.858
10	0.607	1.155	0.858

Table 4.2: CFL upper bound for an elastic simulation with $V_p/V_s = \sqrt{2}$.

Degree N	Newmark	LDDRK4-6	RK4
1	0.816	1.553	1.154
2	0.666	1.268	0.942
3	0.684	1.302	0.967
4	**0.697**	**1.327**	**0.986**
5	0.700	1.332	0.990
6	0.700	1.332	0.990
7	0.700	1.332	0.990
8	0.699	1.330	0.989
9	0.698	1.328	0.987
10	0.698	1.328	0.987

4.8 How to set plane waves as initial conditions

To simulate the propagation of incoming plane waves in the simulation domain, initial conditions based on analytical formulae of plane waves in a homogeneous model need to be set. No additional body or boundary forces are required. To set up this scenario:

`Par_file`:

- switch on `initialfield = .true.`
- at this point setting `add_bielak_condition` does not seem to help with absorbing boundaries, therefore, it should be turned off.

`SOURCE`:

- `zs` has to be the same as the height of the simulation domain defined in `interfacesfile`.
- `xs` is the x-coordinate of the intersection of the initial plane wave front with the free surface.
- `source_type` = 1 for a plane P wave, 2 for a plane SV wave, 3 for a Rayleigh wave.
- `angleforce` can be negative to indicate a plane wave incident from the right (instead of the left)

4.9 Note on the viscoelastic model used

The model used is a constant Q, thus with no dependence on frequency ($Q(f)$ = constant). See e.g. Blanc et al. [2016].

However in practice for technical reasons it is approximated based on the sum of different Generalized Zener body mechanisms and thus the code outputs the band in which the approximation is very good, outside of that range it can be less accurate. The logarithmic center of that frequency band is the `f0` parameter defined (in Hz) in input file `DATA/SOURCE`.

4.10 Note on viscoelasticity in the 2D plane strain approximation

In 2D plane strain, one spatial dimension is much greater than the others (see for example: `http://www.engineering.ucsb.edu/~hpscicom/projects/stress/introge.pdf`) and thus $\kappa = \lambda + \mu$ in 2D plane strain (instead of $\kappa = \lambda + \frac{2}{3}\mu$ in 3D). See for example Carcione et al. [1988b] equation (A9), and equation 6 in `http://cherrypit.princeton.edu/papers/paper-99.pdf`.

In 2D axisymmetric the 2/3 coefficient is probably OK, but it would be worth doublechecking.

Chapter 5

Adjoint Simulations

5.1 How to obtain finite sensitivity kernels

1. Run a forward simulation:

   - `SIMULATION_TYPE = 1`
   - `SAVE_FORWARD = .true.`
   - `seismotype = 1` (we need to save the displacement fields to later on derive the adjoint source. Note: if the user forgets it, the program corrects it when reading the proper `SIMULATION_TYPE` and `SAVE_FORWARD` combination and a warning message appears in the output file)

   Important output files (for example, for the elastic case, P-SV waves):

   - `absorb_elastic_bottom*****.bin`
   - `absorb_elastic_left*****.bin`
   - `absorb_elastic_right*****.bin`
   - `absorb_elastic_top*****.bin`
   - `lastframe_elastic*****.bin`
   - `AA.S****.BXX.semd`
   - `AA.S****.BXZ.semd`

2. Define the adjoint source:

   - Use `adj_seismogram.f90`
   - Edit to update `NSTEP`, `nrec`, `t0`, `deltat`, and the position of the cut to pick any given phase if needed (`tstart`,`tend`), add the right number of stations, and put one component of the source to zero if needed.
   - The output files of `adj_seismogram.f90` are `AA.S****.BXX.adj` and `AA.S****.BXZ.adj`, for P-SV waves (and `AA.S****.BXY.adj`, for SH (membrane) waves). Note that you will need these three files (`AA.S****.BXX.adj`, `AA.S****.BXY.adj` and `AA.S****.BXZ.adj`) to be present in the `SEM/` directory together with the `absorb_elastic_****.bin` and `lastframe_elastic.bin` files to be read when running the adjoint simulation.

3. Run the adjoint simulation:

   - Make sure that the adjoint source files absorbing boundaries and last frame files are in the `OUTPUT_FILES/` directory.
   - `SIMULATION_TYPE = 3`
   - `SAVE_FORWARD = .false.`

Output files (for example for the elastic case):

- `snapshot_rho_kappa_mu*****`
- `snapshot_rhop_alpha_beta*****`

which are the primary moduli kernels and the phase velocities kernels respectively, in ascii format and at the local level, that is as "`kernels(i,j,ispec)`".

5.2 Remarks about adjoint runs and solving inverse problems

SPECFEM2D can produce the gradient of the misfit function for a tomographic inversion, but options for using the gradient within an iterative inversion are left to the user (e.g., conjugate-gradient, steepest descent). The plan is to include some examples in the future.

The algorithm is simple:

1. calculate the forward wave field $\mathbf{s}(x,t)$
2. calculate the adjoint wave field $\mathbf{s}^\dagger(x,t)$
3. calculate their interaction $\mathbf{s}(x,t) \cdot \mathbf{s}^\dagger(x, T-t)$ (these symbolic, temporal and spatial derivatives should be included)
4. integrate the interactions, which is summation in the code.

That is all. Step 3 has some tricks in implementation, but which can be skipped by regular users.

If you look into SPECFEM2D, besides "`rhop_ac_kl`" and "`rho_ac_kl`", there are more variables such as "`kappa_ac_kl`" and "`rho_el_kl`" etc. "`rho`" denotes density ρ ("`kappa`" for bulk modulus κ etc.), "`ac`" denotes acoustic ("`el`" for elastic), "`kl`" means kernel (and you may find "`k`" as well, which is the interaction at each time step, i.e., before doing time integration).

5.3 Caution

Please note that:

- at the moment, adjoint simulations do not support anisotropy, attenuation, and viscous damping.
- you will need `AA.S****.BXX.adj`, `AA.S****.BXY.adj` and `AA.S****.BXZ.adj` to be present in directory `SEM/` even if you are just running an acoustic or poroelastic adjoint simulation.
  - `AA.S****.BXX.adj` is the only relevant component for an acoustic case.
  - `AA.S****.BXX.adj` and `AA.S****.BXZ.adj` are the only relevant components for a poroelastic case.

Chapter 6

Doing tomography, i.e., updating the model based on the sensitivity kernels obtained

The process is described in the same chapter of the manual of SPECFEM3D Cartesian. Please refer to it.

Chapter 7

Oil and gas industry simulations

The SPECFEM2D package provides compatibility with industrial (oil and gas industry) types of simulations. These features include importing Seismic Unix (SU) format wavespeed models into SPECFEM2D, output of seismograms in SU format with a few key parameters defined in the trace headers and reading adjoint sources in SU format etc. There is one example given in `EXAMPLES/real_world/Industrial_Format_SEP`, which you can follow.

We also changed the relationship between adjoint potential and adjoint displacement in fluid region (the relationship between forward potential and forward displacement remains the same as previously defined). The new definition is critical when there are adjoint sources (in other words, receivers) in the acoustic domain, and is the direct consequence of the optimization problem.

$$\begin{aligned} \mathbf{s} &\equiv \frac{1}{\rho}\,\nabla\phi \\ p &\equiv -\kappa\,(\nabla\cdot\mathbf{s}) = -\partial_t^2\phi \end{aligned}$$

$$\begin{aligned} \partial_t^2\mathbf{s}^\dagger &\equiv -\frac{1}{\rho}\,\nabla\phi^\dagger \\ p^\dagger &\equiv -\kappa\left(\nabla\cdot\mathbf{s}^\dagger\right) = \phi^\dagger \end{aligned}$$

Chapter 8

Information for developers of the code, and for people who want to learn how the technique works

You can get a very simple 1D version of a demo code (there is one in Fortran and one in Python):

```
git clone --recursive https://github.com/SPECFEM/specfem1d.git
```

We also have simple 3D demo source codes that implement the SEM in a single, small program, in directory `utils/small_SEM_solvers_in_Fortran_and_C_without_MPI_to_learn` of the SPECFEM3D Cartesian package. They are useful to learn how the spectral-element method works, and how to write or modify a code to implement it. Also useful to test new ideas by modifying these simple codes to run some tests. We also have a similar, even simpler, demo source code for the 2D case in directory `utils/small_SEM_solver_in_Fortran_without_MPI_to_learn` of the specfem2d package.

For information on how to contribute to the code, i.e., for how to make your modifications, additions or improvements part of the official package, see https://github.com/SPECFEM/specfem3d/wiki .

Simulation features supported in SPECFEM2D

The following lists all available features for a SPECFEM2D simulation, where *CPU* and *CUDA* denote the code versions for CPU-only simulations and CUDA hardware support, respectively.

Feature		*CPU*	*CUDA*
Physics	P-SV waves	X	X
	SH/membrane waves	X	X
	Acoustic	X	X
	Elastic	X	X
	Poroelastic	X	-
	Electromagnetic	X	-
	Anisotropy	X	X
	Attenuation	X	X
Simulation Setup	Axisymmetric (2.5D) simulations	X	-
	Noise simulations	X	X
	initial field	X	X
	C-PML	X	-
	Periodic boundaries	X	-
	Simultaneous runs	X	X
Meshing	in-house mesher	X	-
	external (CUBIT/Trelis,Gmsh)	X	-
	SCOTCH/Metis/Analytical partitioning	X	-
Sensitivity kernels	Undoing of attenuation	X	X
	Anisotropic kernels	X	X
	Isotropic kernels	X	X
	Approximate Hessian	X	X
Time schemes	Newmark	X	X
	LDDRK	X	-
	RK4	X	-
	symplectic PEFRL	X	-
Visualization	JPEG images	X	X
	Postscript snapshots	X	X
	Wavefield dumps	X	X
Seismogram formats	Ascii	X	X
	Binary	X	X
	SU	X	X
	down-sampling	X	X

Notes & Acknowledgments

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Please provide your feedback, questions, comments, and suggestions through the github repository.

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Main historical authors: Dimitri Komatitsch and Jeroen Tromp
CNRS, France and Princeton University, USA

Evolution of the code:

version 8.1, Hom Nath Gharti, Daniel Peter, Eduardo Valero Cano, December 2023:
adds support for Q values in tomographic models; updates GPU support, OpenMP and test workflows; various code updates and improvements (noise simulations)

version 8.0, Etienne Bachmann, Alexis Bottero, Bryant Chow, Paul Cristini, Rene Gassmoeller, Michael Gineste, Felix Halpaap, Dimitri Komatitsch, Matthieu Lefebvre, Qiancheng Liu, Qinya Liu, Zhaolun Liu, David Luet, Ryan Modrak, Christina Morency, Daniel Peter, Eric Rosenkrantz, Herurisa Rusmanugroho, Elliott Sales de Andrade, Eduardo Valero Cano, Zhendong Zhang, Xie Zhinan, December 2022:
various code improvements; GPU support; axisymmetric 2.5D simulations

version 7.0, Dimitri Komatitsch, Zhinan Xie, Paul Cristini, Roland Martin and Rene Matzen, July 2012:
added support for Convolution PML absorbing layers; added higher-order time schemes (4th order Runge-Kutta and LDDRK4-6); many small or moderate bug fixes

version 6.2, many developers, April 2011:
restructured package source code into separate src/ directories; added configure & Makefile scripts and a PDF manual in doc/; added user examples in EXAMPLES/; added a USER_T0 parameter to fix the onset time in simulation

version 6.1, Christina Morency and Pieyre Le Loher, March 2010:
added SH (membrane) waves calculation for elastic media; added support for external fully anisotropic media; fixed some bugs in acoustic kernels

version 6.0, Christina Morency and Yang Luo, August 2009:
support for poroelastic media; adjoint method for acoustic/elastic/poroelastic

version 5.2, Dimitri Komatitsch, Nicolas Le Goff and Roland Martin, February 2008:
support for CUBIT and GiD meshes; MPI implementation of the code based on domain decomposition with METIS or SCOTCH; general fluid/solid implementation with any number, shape and orientation of matching edges; fluid potential of density $*$ displacement instead of displacement; absorbing edges with any normal vector; general numbering of absorbing and acoustic free surface edges; cleaned implementation of attenuation as in Carcione (1993); merged loops in the solver for efficiency; simplified input of external model; added CPU time information; translated many

comments from French to English

version 5.1, Dimitri Komatitsch, January 2005:
more general mesher with any number of curved layers; Dirac and Gaussian time sources and corresponding convolution routine; option for acoustic medium instead of elastic; receivers at any location, not only grid points; moment-tensor source at any location, not only a grid point; color snapshots; more flexible DATA/Par_file with any number of comment lines; Xsu scripts for seismograms; subtract t0 from seismograms; seismograms and snapshots in pressure in addition to vector field

version 5.0, Dimitri Komatitsch, May 2004:
got rid of useless routines, suppressed commons etc.; weak formulation based explicitly on stress tensor; implementation of full anisotropy; implementation of attenuation based on memory variables

based on SPECFEM2D version 4.2, June 1998
(c) by Dimitri Komatitsch, Harvard University, USA and Jean-Pierre Vilotte, Institut de Physique du Globe de Paris, France
itself based on SPECFEM2D version 1.0, 1995
(c) by Dimitri Komatitsch and Jean-Pierre Vilotte, Institut de Physique du Globe de Paris, France

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Appendix A

Reference Frame Convention

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

- the x axis points right (i.e., East)
- the z axis points up (i.e., North).

Seismogram outputs

The seismogram output directions are given in Cartesian x/z directions. They can be rotated (from the direction of positive z, i.e. from the North) if needed using a flag defined in the `Par_file`.

For the labeling of the seismogram channels, see Appendix B. Additionally, we add labels to the synthetics using the following convention: For a receiver station located in an

elastic domain:

- `semd` for the displacement vector
- `semv` for the velocity vector
- `sema` for the acceleration vector

acoustic domain:

(please note that receiver stations in acoustic domains must be buried. This is due to the free surface condition which enforces a zero pressure at the surface.)

- `semd` for the displacement vector
- `semv` for the velocity vector
- `sema` for pressure which will be stored in the vertical component `Z`. Note that pressure in the acoustic media is isotropic and thus the pressure record would be the same in the other two component directions. We therefore use the other two seismogram components to store the acoustic potential in component `X` (or `N`) and the first time derivative of the acoustic potential in component `Y` (or `E`).

The seismograms are by default written out in ASCII-format to the `OUTPUT_FILES/` subdirectory by each parallel process.

Appendix B

Channel Codes of Seismograms

Seismic networks, such as the Global Seismographic Network (GSN), generally involve various types of instruments with different bandwidths, sampling properties and component configurations. There are standards to name channel codes depending on instrument properties. IRIS (http://www.iris.edu) uses SEED format for channel codes, which are represented by three letters, such as LHN, BHZ, etc. In older versions of the SPECFEM3D Cartesian package, a common format was used for the channel codes of all seismograms, which was BHE/BHN/BHZ for three components. To avoid confusion when comparison are made to observed data, we are now using the FDSN convention (http://www.fdsn.org/) for SEM seismograms. In the following, we give a brief explanation of the FDSN convention used by IRIS, and how it is adopted in SEM seismograms. Please visit http://www.iris.edu/manuals/SEED_appA.htm for further information.

Band code: The first letter in the channel code denotes the band code of seismograms, which depends on the response band and the sampling rate of instruments. The list of band codes used by IRIS is shown in Figure B.1. The sampling rate of SEM synthetics is controlled by the resolution of simulations rather than instrument properties. However, for consistency, we follow the FDSN convention for SEM seismograms governed by their sampling rate. For SEM synthetics, we consider band codes for which $dt \leq 1$ s. IRIS also considers the response band of instruments. For instance, short-period and broad-band seismograms with the same sampling rate correspond to different band codes, such as S and B, respectively. In such cases, we consider SEM seismograms as broad band, ignoring the corner period (≥ 10 s) of the response band of instruments (note that at these resolutions, the minimum period in the SEM synthetics will be less than 10 s). Accordingly, when you run a simulation the band code will be chosen depending on the resolution of the synthetics, and channel codes of SEM seismograms will start with either L, M, B, H, C or F, shown by red color in the figure.

Instrument code: The second letter in the channel code corresponds to instrument codes, which specify the family to which the sensor belongs. For instance, H and L are used for high-gain and low-gain seismometers, respectively. The instrument code of SEM seismograms will always be X, as assigned by FDSN for synthetic seismograms.

Orientation code: The third letter in channel codes is an orientation code, which generally describes the physical configuration of the components of instrument packages. SPECFEM3D Cartesian uses the traditional orientation code E/N/Z (East-West, North-South, Vertical) for three components when a UTM projection is used. If the UTM conversion is suppressed, i.e. the flag SUPPRESS_UTM_PROJECTION is set to .true., then the three components are labelled X/Y/Z according to the Cartesian reference frame.

EXAMPLE: The sampling rate is given by DT in the main parameter file Par_file located in the DATA/ subdirectory. Depending on the resolution of your simulations, if you choose a sampling rate greater than 0.01 s and less than 1 s, a seismogram recording displacements on the vertical component of a station ASBS (network AZ) will be named AZ.ASBS.MXZ.semd.sac, whereas it will be AZ.ASBS.BXZ.semd.sac, if the sampling rate is greater than 0.0125 and less equal to 0.1 s.

Band code	Band type	Sampling rate (sec)	Corner period (sec)
F	...	> 0.0002 to <= 0.001	≥ 10 sec
G	...	> 0.0002 to <= 0.001	< 10 sec
D	...	> 0.001 to <= 0.004	< 10 sec
C	...	> 0.001 to <= 0.004	≥ 10 sec
E	Extremely Short Period	<= 0.0125	< 10 sec
S	Short Period	<= 0.1 to > 0.0125	< 10 sec
H	High Broad Band	<= 0.0125	>= 10 sec
B	Broad Band	<= 0.1 to > 0.0125	>= 10 sec
M	Mid Period	< 1 to > 0.1	
L	Long Period	1	
V	Very Long Period	10	
U	Ultra Long Period	100	
R	Extremely Long Period	1000	
P	On the order of 0.1 to 1 day	<= 100000 to > 10000	
T	On the order of 1 to 10 days	<= 1000000 to > 100000	
Q	Greater than 10 days	> 1000000	
A	Administrative Instrument Channel	variable	NA
O	Opaque Instrument Channel	variable	NA

Figure B.1: The band code convention is based on the sampling rate and the response band of instruments. Please visit http://www.iris.edu/manuals/SEED_appA.htm for further information. Grey rows show the relative band-code range in SPECFEM3D Cartesian, and the band codes used to name SEM seismograms are denoted in red.

Appendix C

Troubleshooting

FAQ

Regarding the structure of some of the database files

Question: Can anyone tell me what the columns of the SPECFEM2D boundary condition files in `SPECFEM2D/DATA/Mesh_canyon` are?

```
SPECFEM2D/DATA/Mesh_canyon/canyon_absorbing_surface_file
SPECFEM2D/DATA/Mesh_canyon/canyon_free_surface_file
```

Answer: `canyon_absorbing_surface_file` refers to parameters related to the absorbing conditions: The first number (180) is the number of absorbing elements (nelemabs in the code). Then the columns are:

column 1: the element number

column 2: the number of nodes of this element that form the absorbing surface

column 3: the first node

column 4: the second node

`canyon_free_surface_file` refers to the elements of the free surface (relevant for enforcing free surface condition for acoustic media): The first number (160) is the number of elements of the free surface. Then the columns are (similar to the absorbing case):

column 1: the element number

column 2: the number of nodes of this element that form the absorbing surface

column 3: the first node

column 4: the second node

Concerning the free surface description file, nodes/edges pertaining to elastic elements are discarded when the file is read (if for whatever reason it was simpler to include all the nodes/edges on one side of a studied area and that there are among them some elements that are elastic elements, only the nodes/edges of acoustic elements are kept).

These files are opened and read in `meshfem2D.F90` using subroutines `read_abs_surface()` and `read_acoustic_surface()`, which are in `part_unstruct.F90`

Appendix D

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