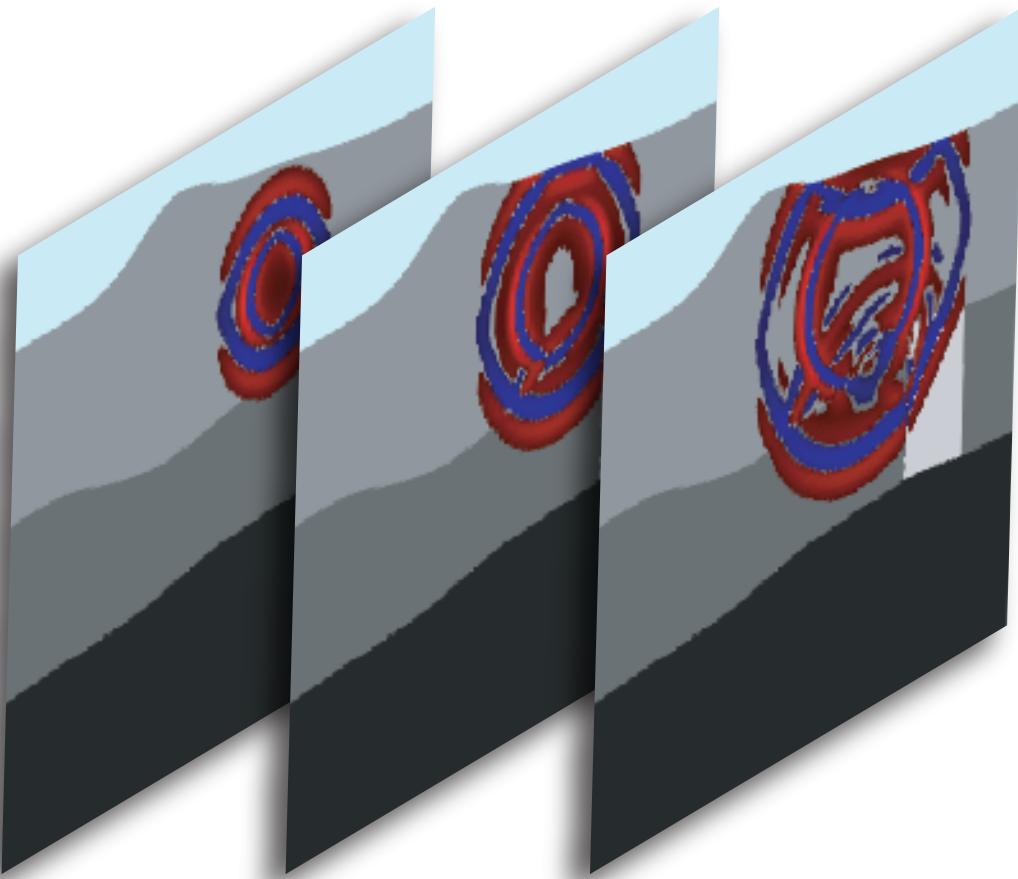


COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)
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SPECFEM 2D

User Manual
Version 7.0



SPECFEM2D

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© CNRS (France) and Princeton University (USA)
Version 7.0

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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, Paul Cristini, Dimitri Komatitsch, Jesús Labarta, Nicolas Le Goff, Pieyre Le Loher, Qinya Liu, Youshan Liu, Roland Martin, René Matzen, Christina Morency, Daniel Peter, Carl Tape, Jeroen Tromp, Jean-Pierre Vilotte, Zhinan Xie.

The code is released open-source under the GNU version 3 license, see the license at the end of this manual.

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



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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 (<http://cubit.sandia.gov>), Gmsh (<http://geuz.org/gmsh>) or GiD (<http://www.gid.cimne.upc.es>). 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.

With version 7.0, the 2D spectral-element solver accommodates Convolution PML absorbing layers and 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 SPECFEM2D (<http://www.geodynamics.org/cig/software/packages/seismo/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 Pitkäraanta, 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. Benjema 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.

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 <http://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/geodynamics/specfem2d.git
```

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.

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.**

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

Mac OS You will probably need to install XCODE.

IBM Blue Gene machines Please refer to the manual of SPECFEM3D_Cartesian, which contains detailed instructions on how to run on Blue Gene.

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://gforge.inria.fr/projects/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 (http://www.labri.fr/perso/pelegrin/scotch/scotch_en.html) . 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 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/Cray_compiler_information` directory.

2.1 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`.

2.2 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 is a robot called BuildBot that is in charge of checking and validating all new contributions and changes), please visit this Web page: <https://github.com/geodynamics/specfem2d/wiki/Using-Hub>.

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`.

Chapter 3

Mesh Generation

3.1 How to use SPECFEM2D

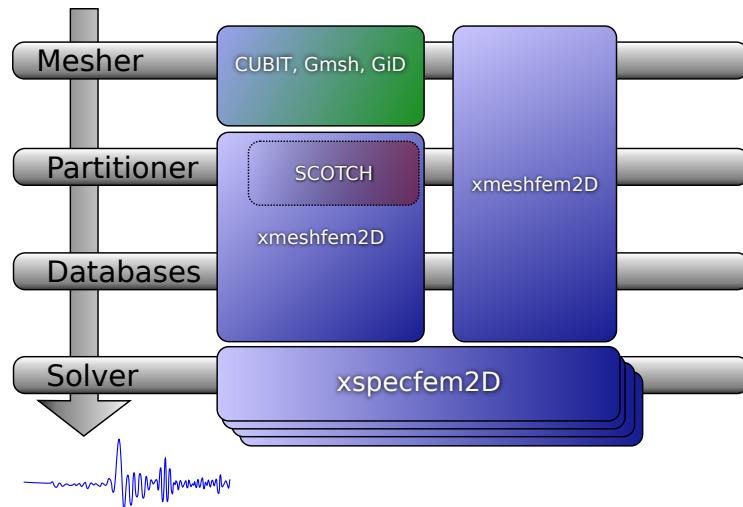


Figure 3.1: Schematic workflow for a SPECFEM2D simulation. The executable `xmeshfem2D` creates the GLL mesh points and assigns specific model parameters. The executable `xspecfem2D` solves the seismic wave propagation.

To run the mesher, please follow these steps:

- edit the input file `DATA/Par_file`, which describes the simulation. **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 (https://github.com/geodynamics/specfem3d/tree/master/doc/USER_MANUAL). 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
- if you are using an external mesher (like GiD or CUBIT / Treliis), you should set `read_external_mesh` to `.true.`:

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.

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.

- if you have compiled with MPI, you must specify the number of processes.

Then type

```
./bin/xmeshfem2D
```

to create the mesh (which will be stored in directory OUTPUT_FILES/). xmeshfem2D is serial; it will output several files called Database?????.bin, one for each process.

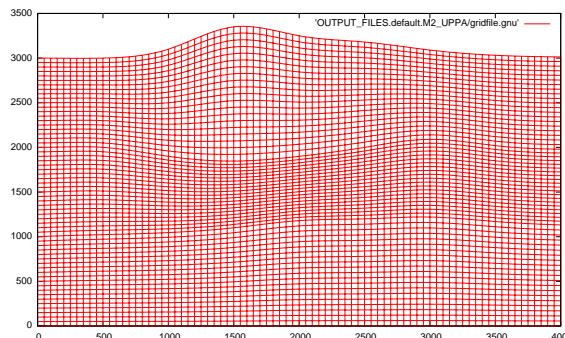


Figure 3.2: Example of a grid file generated by xmeshfem2D and visualized with gnuplot (within gnuplot, type ‘plot “OUTPUT_FILES/gridfile.gnu” w l’).

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

```

4 . . . . 7 . . . . 3
.
.
. eta .
.
. | .
8 9--xi 6
.
.
.
.
1 . . . . 5 . . . . 2

```

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.

3.2 How to use Gmsh to generate an external mesh

Gmsh¹ 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/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
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`.

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**

¹freely available at the following address : <http://www.geuz.org/gmsh/>

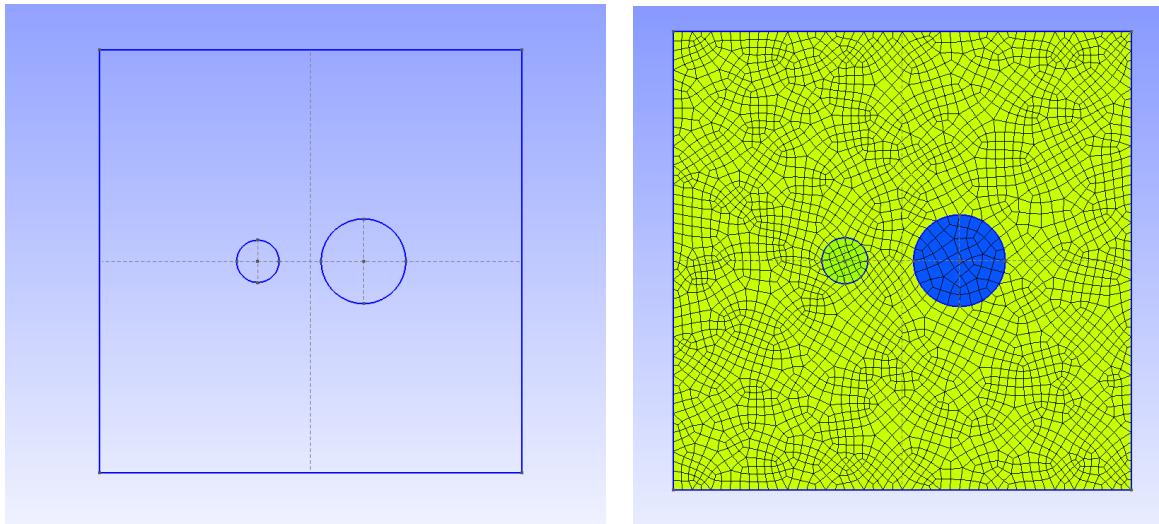


Figure 3.3: Geometry and mesh of the two circle model generated with Gmsh

- 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

Trelis (that was known as Cubit)² is a 2D/3D finite element grid generator distributed by Csimsoft which can be used for the generation of quadrangle and hexahedral meshes. Trelis 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: <http://www.csimsoft.com/tutorials.jsp> 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/paper_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

²available at <http://www.csimsoft.com/>

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 which is not working:

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

- No comments after double dots:

Example which 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! Think about that before getting mad.

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/CPML_absorbing_layers.

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 were 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 `utils/CPML` **should soon (Dimitri: TO DO ONE DAY)** implement that transition layer automatically.

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 `tomography`), 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.

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 this element with the external software package used for the meshing, and to repeat the operation until the maximum

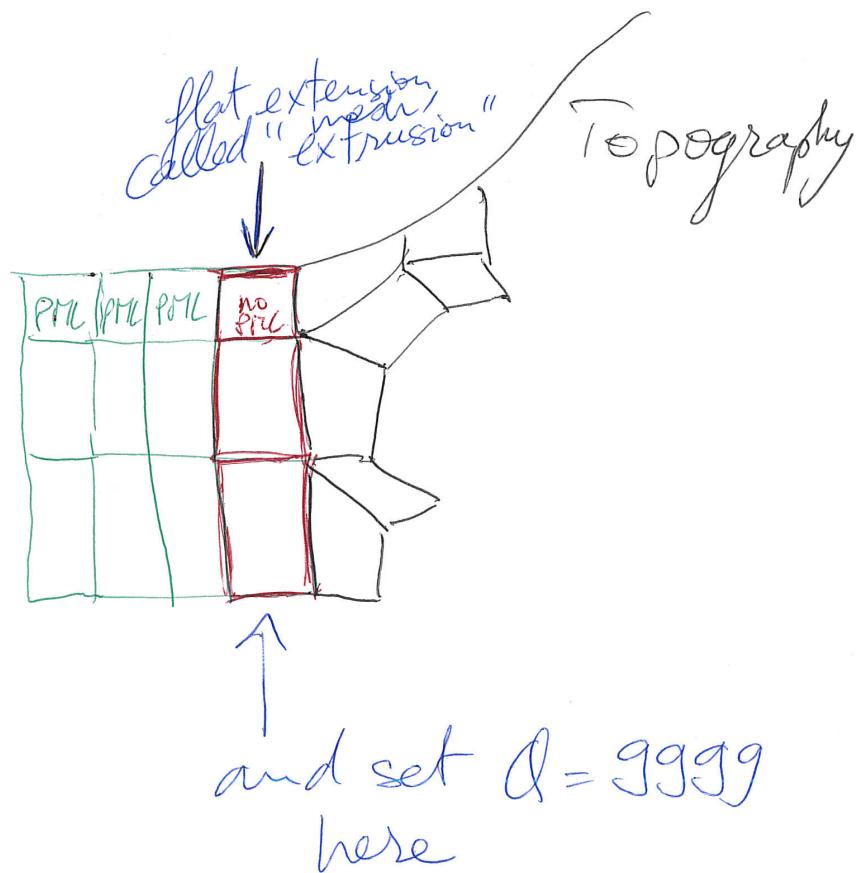


Figure 3.4: Mesh extrusion for PML (green elements) and a non-PML stabilization layer (red elements).

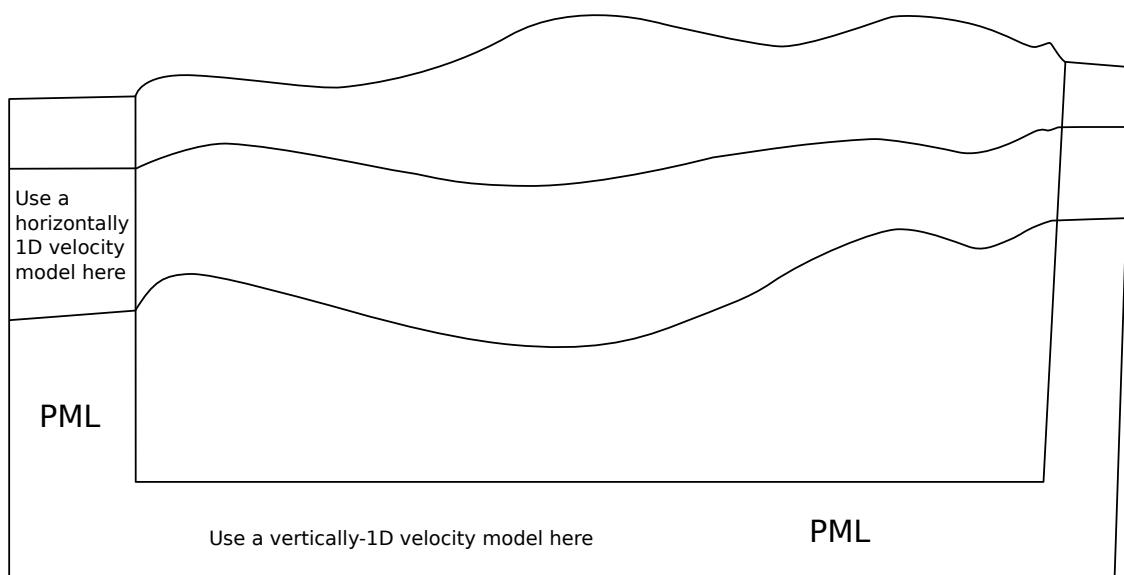


Figure 3.5: How to modify your external 2D velocity and density model in order to use PML. Such a modification is not needed when using Stacey absorbing boundary conditions (but such conditions are significantly less efficient).

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 elements 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 you 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 them, 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`).

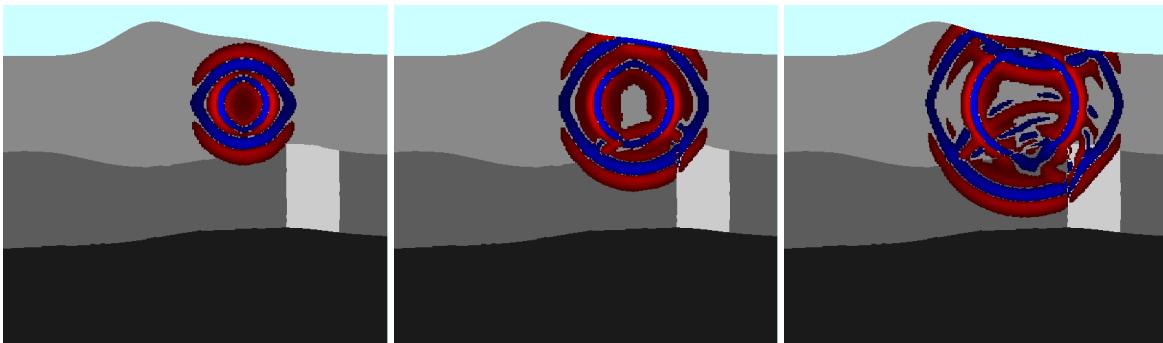


Figure 4.1: Wavefield snapshots of the default example generated by `xspecfem2D` when parameter `output_color_image` is set to `.true.`. To create smaller (subsampled) images you can change double precision parameter `factor_subsample_image = 1.0` to a higher value in file `DATA/Par_file`. This can be 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 (<http://www.spice-rtn.org/library/software/EX2DDIR>). That code is described in: Berg et al. [1994]

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).

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.

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. We may want to change this and impose that the values read are those for a given frequency (here f0_attenuation). (when we do this, velocities will then slightly decrease and waves will thus slightly slow down)

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

```
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 0 0
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
```

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.

To make a given region anisotropic, use II. See Section 4.2 for more details.

To make a given region poroelastic, use III. See Section 4.3 for more details.

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 above 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_Qp.py.

nbregions With MODEL = default chosen, a variety of simple layered model configurations can be specified using the nbregions device.

Regarding attenuation (viscoelasticity), in the Par_file you need to select the number of standard linear solids (N_SLS) to use 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.

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

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 source will 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, 2 the first derivative, 3 a Gaussian, 4 a Dirac or 5 a Heaviside source-time function.

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 $1/f_0$. 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 4.3), 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 (www.llnl.gov/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.

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); 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:

SPECFEM3D: in SPECFEM3D the moment tensor components are in dyne*cm

SPECFEM2D: in SPECFEM2D the moment tensor components are in 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 from SPECFEM3D_GLOBE:

```
./utils/strike_dip_rake_to_CMTSOLUTION.c
./utils/CMTSOLUTION_to_AkiRichards.c
```

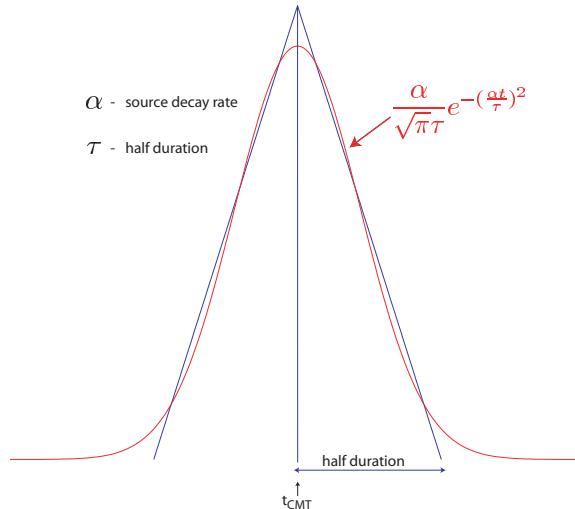


Figure 4.3: Comparison of the shape of a triangle and the Gaussian function actually used.

but then 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 $t = -1.2 * \text{half duration} + t0$ (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 $1/f0$. 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/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.

Note about external meshers:

Using external meshers is possible in axisymmetric geometry. An example is available in EXAMPLES/paper_axisymmetry_example with the mesher Cubit/Trelis (<http://www.csimsoft.com/trelis>). 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 4.4. 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.

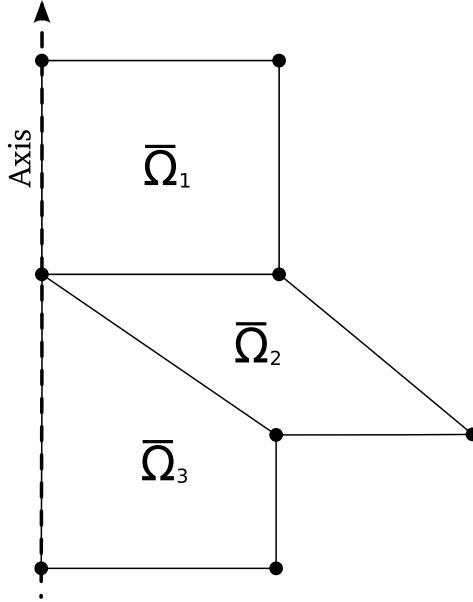


Figure 4.4: For simplicity we exclude cases in which the mesh elements that are in contact with the symmetry axis are in contact with it by a single point instead of by a full edge, such as element $\bar{\Omega}_2$ here. This amounts to imposing that the leftmost layer of elements in the mesh be structured rather than non structured; The rest of the mesh can be non structured.

Note about 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

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}, \quad i, j, k = 1, \dots, 3,$$

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 elasticities 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 $\text{duz}_\text{dx} = \frac{d(\text{Uz})}{dx}$.

4.4 How to run poroelastic wave simulations

Check the following new inputs in `Par_file`:

In section "# geometry of model and mesh description":

`TURN_VISCATTENUATION_ON`, `Q0`, and `FREQ0` deal with viscous damping in a poroelastic medium. `Q0` is the quality factor set at the central frequency `FREQ0`. 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.

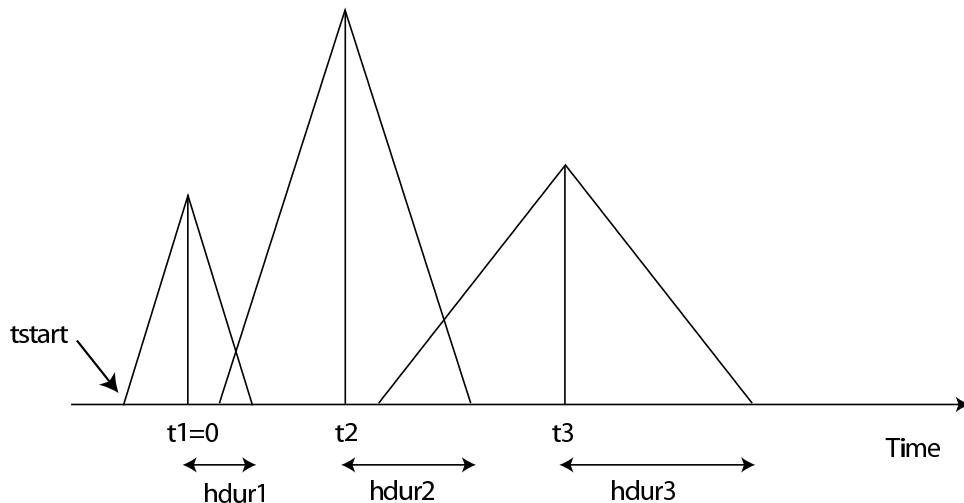


Figure 4.5: Example of timing for three sources. The center of the first source triangle is defined to be time zero. Note that this is NOT in general the hypocentral time, or the start time of the source (marked as `tstart`). The time shift parameter `t0` in the `SOURCE` file would be $t1(= 0)$, $t2$, $t3$ in this case, and the half-duration parameter, `f0`, would be $\text{hdur1} = 1/f_01$, $\text{hdur2} = 1/f_02$, $\text{hdur3} = 1/f_03$ 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:

`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 anisotropic permeability.

4.5 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.

4.6 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

4.7 How to set plane waves as initial conditions

To simulate propagation of incoming plane waves in the simulation domain, initial conditions based on analytical formulae of plane waves in 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)

4.8 Note on the viscoelastic model used

The model used is a constant Q , thus with no dependence on frequency ($Q(f) = \text{constant}$). 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.

4.9 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 I think the 2/3 coefficient is 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_k1`” and “`rho_ac_k1`”, there are more variables such as “`kappa_ac_k1`” and “`rho_el_k1`” etc. “`rho`” denotes density ρ (“`kappa`” for bulk modulus κ etc.), “`ac`” denotes acoustic (“`el`” for elastic), “`k1`” 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. 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/INDUSTRIAL_FORMAT, 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.

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

$$\partial_t^2 \mathbf{s}^\dagger \equiv -\frac{1}{\rho} \nabla \phi^\dagger$$
$$p^\dagger \equiv -\kappa (\nabla \cdot \mathbf{s}^\dagger) = \phi^\dagger$$

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/geodynamics/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` 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/geodynamics/specfem3d/wiki>.

Notes & Acknowledgments

The Gauss-Lobatto-Legendre subroutines in `gll_library.f90` are based in part on software libraries from the Massachusetts Institute of Technology, Department of Mechanical Engineering (Cambridge, Massachusetts, USA). The non-structured global numbering software was provided by Paul F. Fischer (Brown University, Providence, Rhode Island, USA, now at Argonne National Laboratory, USA).

Please e-mail your feedback, bug reports, questions, comments, and suggestions to the CIG Computational Seismology Mailing List (cig-seismo@geodynamics.org).

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This program is free software; you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation (see Appendix B).

Please note that by contributing to this code, the developer understands and agrees that this project and contribution are public and fall under the open source license mentioned above.

Evolution of the code:

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:

CHAPTER 8. INFORMATION FOR DEVELOPERS OF THE CODE, AND FOR PEOPLE WHO WANT TO LEARN HOW THE TEC

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

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Appendix A

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 B

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