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PRINCETON UNIVERSITY (USA)
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SPECFEM 2D

User Manual
Version 7.0



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© Princeton University (USA) and CNRS / University of Marseille (France)
Version 7.0

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Authors

The SPECFEM2D package was first developed by Dimitri Komatitsch and Jean-Pierre Vilotte at IPG 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, Paul Cristini, Dimitri Komatitsch, Jesús Labarta, Nicolas Le Goff, Pieyre Le Loher, Qinya 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 CeCILL version 2 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. 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 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. 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].

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].

The next release of the code will include 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

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],
- and/or other articles from <http://komatitsch.free.fr/publications.html>.

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 also cite:

- Martin et al. [2008a].

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 versions dot zero sometimes have bugs or issues that can lead to wrong results when running the code, thus we strongly recommend using versions dot one or above (for instance version 13.1 instead of 13.0, version 14.1 instead of 14.0 and so on).**

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.

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

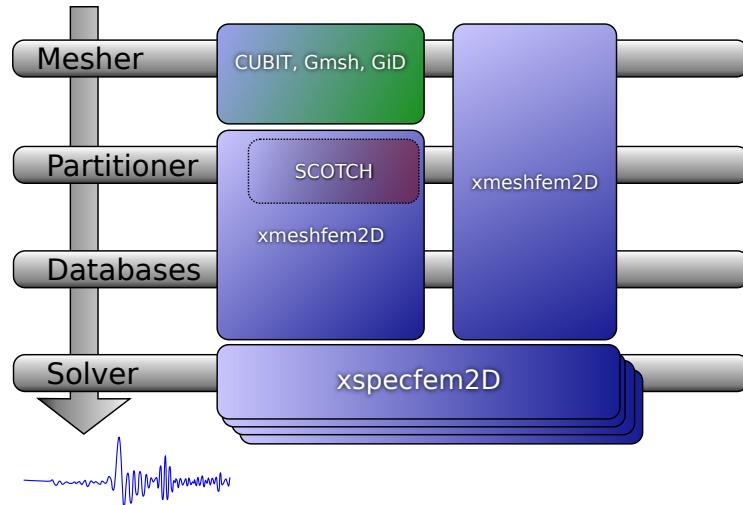


Figure 3.1: Schematic workflow for a SPECFEM2D simulation. The executable `xmeshfem2D` creates the GLL mesh points and assigns specific model parameters. The executable `xspecfem2D` solves the seismic wave propagation.

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.

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??????`, 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 CUBIT/TRELIS or 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/>

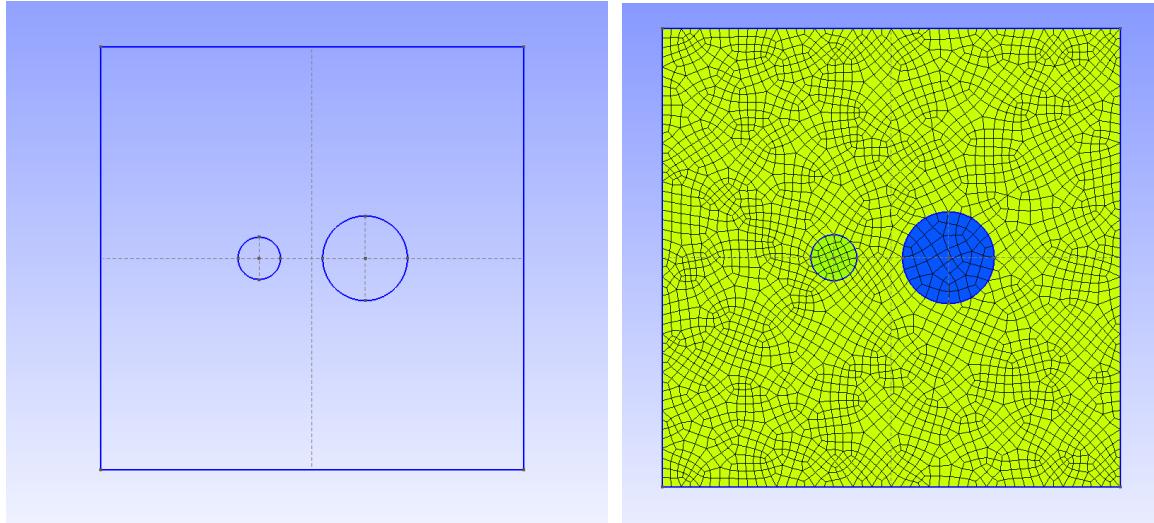


Figure 3.3: Geometry and mesh of the two circle model generated with Gmsh

- 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.

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 X_{\min} or in X_{\max})
2	element belongs to a Y CPML layer only (either in Y_{\min} or in Y_{\max})
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 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 3.4. 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.

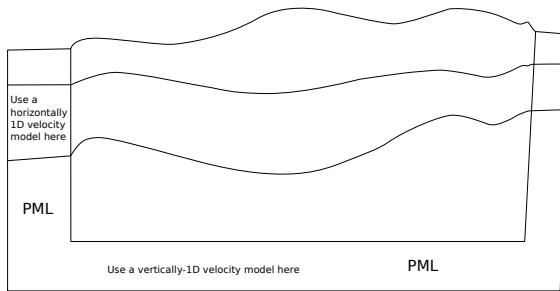


Figure 3.4: How to modify your external 2D velocity and density model in order to use PML. Such a modification is not needed when using Stacey absorbing boundary conditions (but such conditions are significantly less efficient).

3.3 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

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.

3.4 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`).

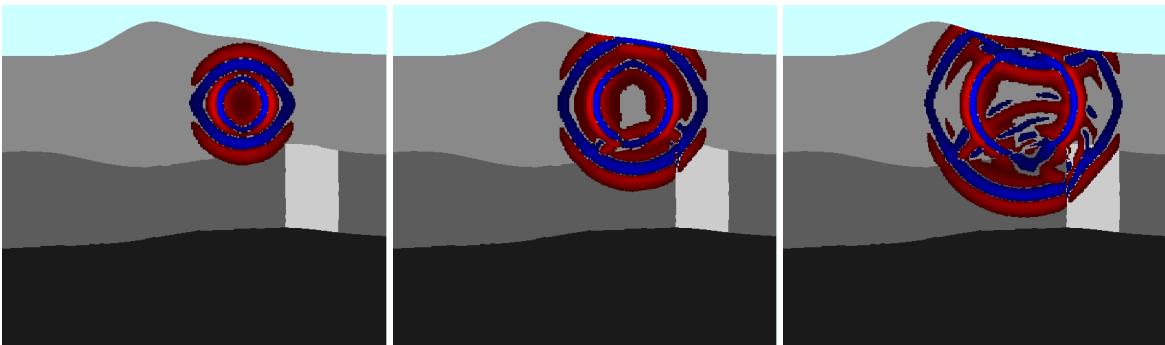


Figure 4.1: Wavefield snapshots of the default example generated by `xspecfem2D` when parameter `output_color_image` is set to `.true.`. To create smaller (subsampled) images you can change double precision parameter `factor_subsample_image = 1.0` to a higher value in file `DATA/Par_file`. This can be 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 II and make Vs be nonzero. See Section 4.1 for more details.

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

To make a given region poroelastic, use IV. 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 .

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

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, 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 4.2), 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.

anglereource 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

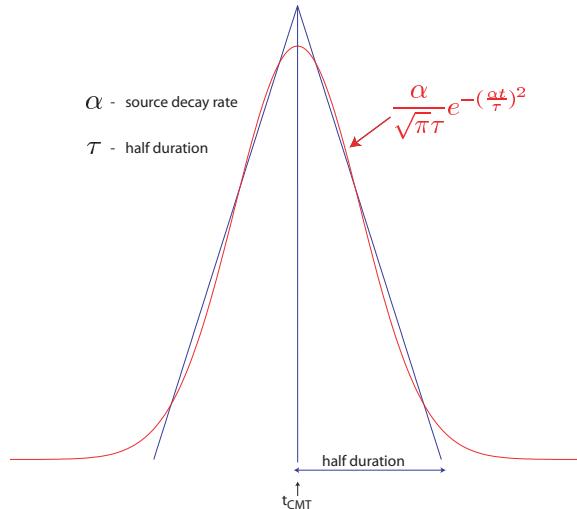


Figure 4.2: Comparison of the shape of a triangle and the Gaussian function actually used.

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
```

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).

A useful Python script called `SEM_save_dir.py`, written by Paul Cristini from Laboratoire de Mecanique et d'Acoustique, CNRS, Marseille, France, is provided. It allows one to automatically save all the parameters and results of a given simulation.

4.2 How to run anisotropic wave simulations

Following Carcione et al. [1988], 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 $\text{duz}_\text{dx} = \frac{d(U_z)}{dx}$.

4.3 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`, Q_0 , and `FREQ0` deal with viscous damping in a poroelastic medium. Q_0 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.

In section "# receiver line parameters for seismograms":

`SAVE_FORWARD` determines if the last frame of a forward simulation is saved (`.true.`) or not (`.false.`)

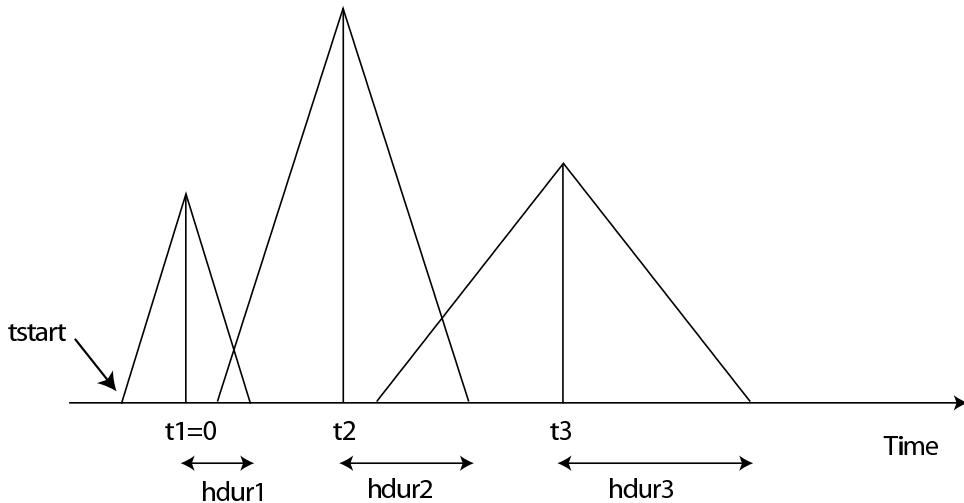


Figure 4.3: Example of timing for three sources. The center of the first source triangle is defined to be time zero. Note that this is NOT in general the hypocentral time, or the start time of the source (marked as `tstart`). The time shift parameter `t0` in the `SOURCE` file would be $t1(= 0)$, $t2$, $t3$ in this case, and the half-duration parameter, f_0 , would be $hdur1 = 1/f_{01}$, $hdur2 = 1/f_{02}$, $hdur3 = 1/f_{03}$ for the sources 1, 2, 3 respectively.

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.

4.4 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.

4.5 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

4.6 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)

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

Chapter 5

Note on the SPECFEM acoustic formulation

Note from Quentin Brissaud, Dimitri Komatitsch and Raphaël Garcia, October 2015

5.1 About the potential formulation used in SPECFEM for pure acoustic waves (i.e. in the absence of gravity terms)

In SPECFEM, when considering purely acoustic waves (neglecting gravity acceleration and viscosity) in fluid regions one uses a potential formulation to represent the "density times displacement" perturbation Chaljub et al. [2007]:

$$\rho \mathbf{u} = \nabla \chi \quad (5.1)$$

where \mathbf{u} is the displacement perturbation, ρ the background density and χ is the scalar potential.

This formulation has two great advantages: it reduces the number of unknowns from three to one, and it also automatically removes artefacts in finite-element methods (FEM) caused by the displacement formulation Hamdi et al. [1978]. This is crucial since it is the main reason for which a displacement formulation cannot be used in fluid regions in a FEM.

However, this formulation assumes that the density is spatially constant, or locally slowly varying (e.g. inside a given spectral element), because the use of a potential for acoustic waves is justified by the fact that acoustic displacements are irrotational. In the cases for which the background density has strong local variations, that formulation is not valid any more. Indeed, taking the rotational of (5.1)

$$\nabla \times (\rho \mathbf{u}) = \nabla \times \nabla \chi$$

Since for any scalar χ , $\nabla \times \nabla \chi = 0$, this yields

$$\begin{aligned} \nabla \rho \times \mathbf{u} + \rho \nabla \times \mathbf{u} &= \mathbf{0} \\ \nabla \times \mathbf{u} &= -(1/\rho) \nabla \rho \times \mathbf{u} \end{aligned}$$

Then, one notices that in the case of strong density gradients the rotational of \mathbf{u} is no longer zero. Thus, the potential formulation (5.1) is no more valid. It is valid only when $(1/\rho) \nabla \rho \times \mathbf{u}$ can be considered negligible, i.e. when both the gradient of density and the value of displacement are small, or if the displacement is parallel or quasi-parallel to the gradient of density, in which case their rotational is also close to zero.

Another approach exists for acoustic waves, based on a displacement potential instead of a potential of $\rho \mathbf{u}$:

$$\mathbf{u} = \nabla \chi, \quad (5.2)$$

which gives $\nabla \times \mathbf{u} = \mathbf{0}$. But in this case the gradient of density is neglected in the Eulerian momentum equation in order to identify gradient terms. Indeed, from the Eulerian momentum equation for inviscid acoustic waves only

$$\begin{aligned} \rho \partial_t^2 \mathbf{u} &= -\nabla p \\ \nabla(\partial_t^2 \chi) &= -(1/\rho) \nabla p. \end{aligned}$$

When $\nabla\rho \gg 0$ strictly speaking one cannot identify $\partial_t^2\chi$ with p .

The solution to this is to work with pressure as the scalar unknown (Godin [2011], equation 23), or even better with the time integral (the primitive) of pressure (see e.g. Everstine [1981]); this was the approach that was originally implemented in SPECFEM until 10 years ago or so, but Chaljub et al. [2003] showed that switching to a displacement potential or to a potential of $\rho\mathbf{u}$ enables one to couple the fluid and solid regions without iterating on the coupling condition in the time scheme, thus resulting in much easier and cheaper implementation; since at that time SPECFEM users were not studying media with strong local variations of density (in solid Earth geophysics such large local variations in fluid regions never happen), the SPECFEM developers permanently switched to such a displacement-based potential formulation. However, for media with strong local variations of density in a fluid region we should reconsider the issue and consider trying the pressure-based formulation again.

Cases in which this can be problematic may include e.g. upper atmosphere studies: the density there is very small but displacements can become very large; in 1D atmosphere models $\frac{\nabla\rho}{\rho}$ is approximately constant and equal to $-1/H$, where H is the scaling height, which leads to $\frac{\nabla\rho}{\rho} \simeq 3.42*1e-5$, i.e. very small; however displacements there can be large and thus it is not clear if $(1/\rho)\nabla\rho \times \mathbf{u}$ can be considered negligible there.

Chapter 6

Adjoint Simulations

6.1 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
- S****.AA.BXX.semd
- S****.AA.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 S****.AA.BXX.adj and S****.AA.BXZ.adj, for P-SV waves (and S****.AA.BXY.adj, for SH (membrane) waves). Note that you will need these three files (S****.AA.BXX.adj, S****.AA.BXY.adj and S****.AA.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)`”.

6.2 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).

6.3 Caution

Please note that:

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

Chapter 7

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 8

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 9

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>.

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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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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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Version 2.0 dated 2006-09-05.