COMPUTATIONAL INFRASTRUCTURE FOR GEODYNAMICS (CIG)
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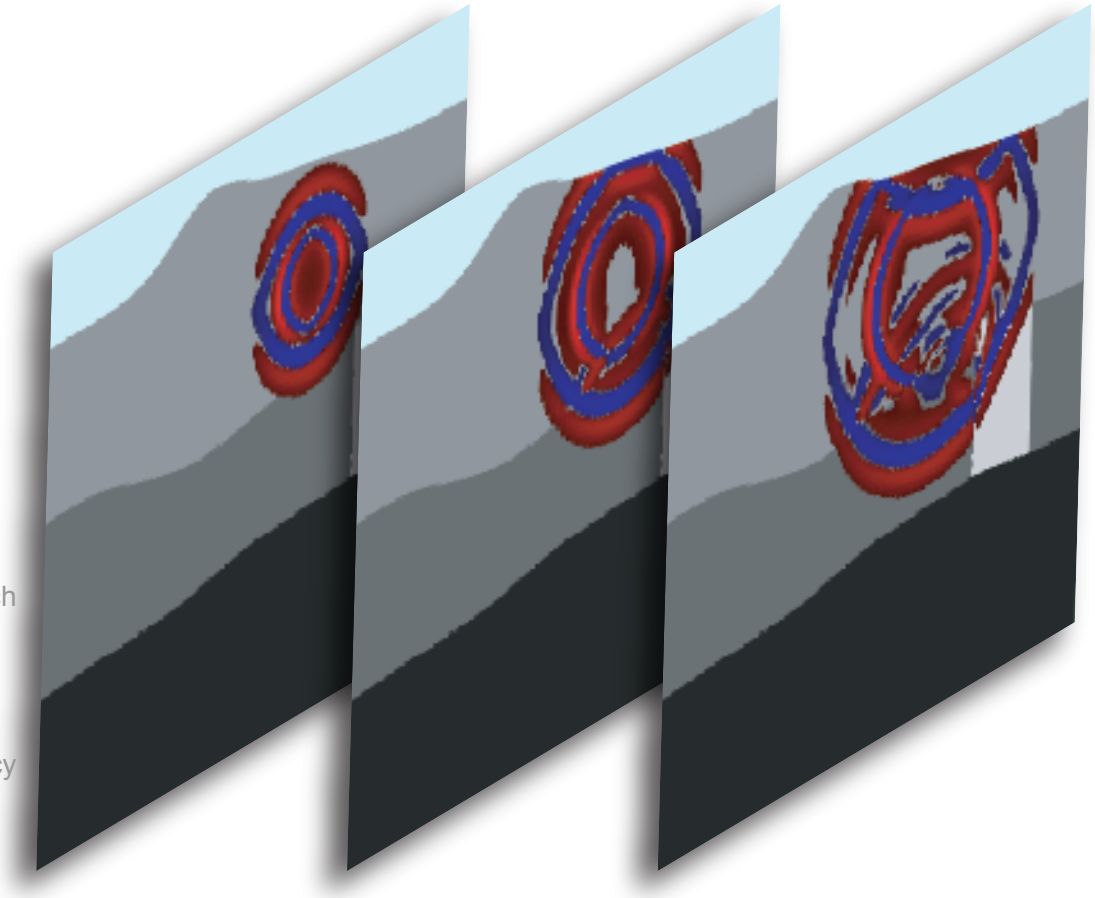
SPECFEM 2D

User Manual
Version 6.2



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Version 6.2

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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 University of Pau (France) from 1998 to 2005.

Since then it has been developed and maintained by a development team: in alphabetical order, Paul Cristini, Dimitri Komatitsch, Jesús Labarta, Nicolas Le Goff, Pieyre Le Loher, Qinya Liu, Roland Martin, Christina Morency, Daniel Peter, Carl Tape, Jeroen Tromp, Zhinan Xie... (add other developers here in the future, several are currently missing).

Contents

Chapter 1

Introduction

SPECFEM2D facilitates 2D simulations of acoustic, (an)elastic, and poroelastic seismic wave propagation. With version 6.2, 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.

The solver has adjoint capabilities and can calculate finite-frequency sensitivity kernels 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, which can easily be made discontinous [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, Arnold, 1982, 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]. 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 and Tromp, 2002, Komatitsch et al., 2003, Tsuboi et al., 2003, Komatitsch et al., 2008, Carrington et al., 2008, Komatitsch et al., 2010c] as well as on clusters of GPU accelerating graphics cards [Komatitsch et al., 2009, 2010a, Komatitsch, 2011]. Tensor products inside each element can be optimized to reach very high efficiency [Deville et al., 2002], and mesh point and element numbering can be optimized to reduce processor cache misses and improve cache reuse [Komatitsch et al., 2008]. The SEM can also handle triangular (in 2D) or tetrahedral (in 3D) elements [Wingate and Boyd, 1996, Taylor and Wingate, 2000, Komatitsch et al., 2001, Cohen, 2002, Mercerat et al., 2006] as well as mixed meshes, although with increased cost and reduced accuracy in these elements, as in the discontinuous Galerkin method.

Note that in many geological models in the context of seismic wave propagation studies (except for instance for fault dynamic rupture studies, in which very high frequencies or supershear rupture need to be modeled near the fault, see e.g. Benjemaa et al. [2007, 2009], de la Puente et al. [2009], Tago et al. [2010]) a continuous formulation is

sufficient because material property contrasts are not drastic and thus conforming mesh doubling bricks can efficiently handle mesh size variations [Komatitsch and Tromp, 2002, Komatitsch et al., 2004, Lee et al., 2008, 2009a,b].

For a detailed introduction to the SEM as applied to regional seismic wave propagation, please consult Komatitsch and Vilotte [1998], Komatitsch and Tromp [1999], Chaljub et al. [2007], Tromp et al. [2008] and in particular 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] and Seriani and Oliveira [2007].

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 nondiagonal mass matrix include Seriani and Priolo [1994], Priolo et al. [1994] and Seriani et al. [1995].

All SPECFEM2D software is written in Fortran90 with full portability in mind, and conforms strictly to the Fortran95 standard. It uses no obsolete or obsolescent features of Fortran77. The package uses parallel programming based upon the Message Passing Interface (MPI) [Gropp et al., 1994, Pacheco, 1997].

The next release of the code will include support for GPU graphics card acceleration [Komatitsch et al., 2009, 2010a, Michéa and Komatitsch, 2010, Komatitsch, 2011] as well as Convolutional or Auxiliary Differential Equation Perfectly Matched absorbing Layers (C-PML or ADE-PML) [Komatitsch and Martin, 2007, Martin et al., 2008b,c, Martin and Komatitsch, 2009, Martin et al., 2010].

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] or Vai et al. [1999], Lee et al. [2009a, 2008, 2009b], Komatitsch et al. [2010a,b, 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://web.univ-pau.fr/~dkomati1/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] or 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

The SPECFEM2D software package comes in a gzipped tar ball. In the directory in which you want to install the package, type

```
tar -zxvf SPECFEM2D_6.2.0.tar.gz
```

The directory `SPECFEM2D-6.2.0/` will then contain the source code. In the following, we will refer to this directory as the root directory `SPECFEM2D/`.

To configure the software for your system, run the `configure` shell script. This script will attempt to guess the appropriate configuration values for your system. However, at a minimum, it is recommended that you explicitly specify the appropriate command names for your Fortran90 compiler:

```
./configure FC=ifort
```

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

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

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.

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

`Mac OS` You will probably need to install `XCODE`. In addition, the `clock_gettime` routine, which is used by the `SCOTCH` library that we use, does not exist in Mac OS. You will need to replace it with `clock_get_time` if you want to use `SCOTCH`.

The SPECFEM2D software package relies on the SCOTCH library to partition meshes. The SCOTCH library [Pellegrini and Roman, 1996] provides efficent 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/`. It is more recent than METIS, actively maintained and performs better in many cases. A recent version of its source code is provided in directory `scotch_5.1.11/`. In case no SCOTCH libraries can be found on the system, the configuration will bundle this version 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.

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/`.

If you run very large meshes on a relatively small number of processors, the memory size needed on each processor might become greater than 2 gigabytes, which is the upper limit for 32-bit addressing. In this case, on some compilers you may need to add "`-mcmodel=medium`" or "`-mcmodel=medium -shared-intel`" to the compiler options of CFLAGS, FCFLAGS and LDFLAGS otherwise the compiler will display an error message (for instance "`relocation truncated to fit: R_X86_64_PC32 against .bss`" or something similar); on an IBM machine with the `xlf` and `xlc` compilers, using `-q64` is usually sufficient.

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`.

Chapter 3

Mesh Generation

3.1 How to use SPECFEM2D

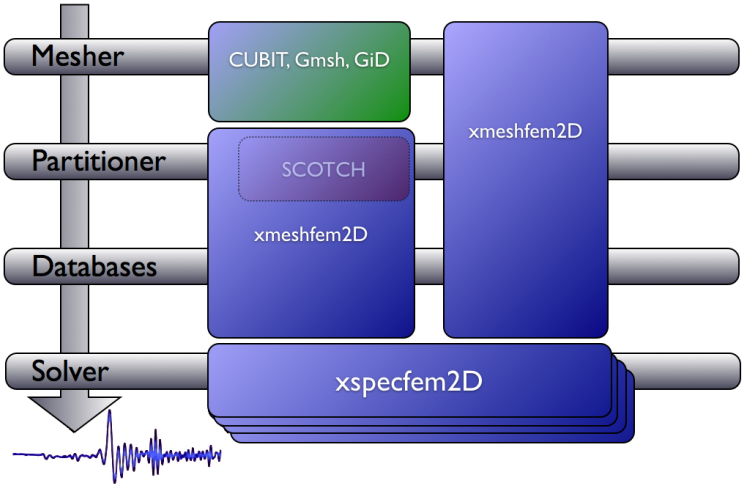

Figure 3.1: Schematic workflow for a SPECFEM2D simulation. The exectable `xmeshfem2D` creates the GLL mesh points and assigns specific model parameters. The executable `xspecfem2D` solves the seismic wave propagation.

To run the mesher, please follow these steps:

- edit the input file `DATA/Par_file` which describes the simulation. It contains comments and should be almost self-explanatory, if you need more details we do not have a manual for the 2D version 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 (`http://geodynamics.org/wsvn/cig/seismo/3D`) in subdirectories `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), 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 nodes : 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 elements : 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 free surface, just put 0 on the first line.

absorbing_surface_file is the file describing the edges forming the absorbing boundaries : the format is the same as the `free_surface_file`.

tangential_detection_curve_file contains points describing the envelope, used for `source_normal_to_surfa` and `rec_normal_to_surface`. Should be fine grained, and ordained 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.

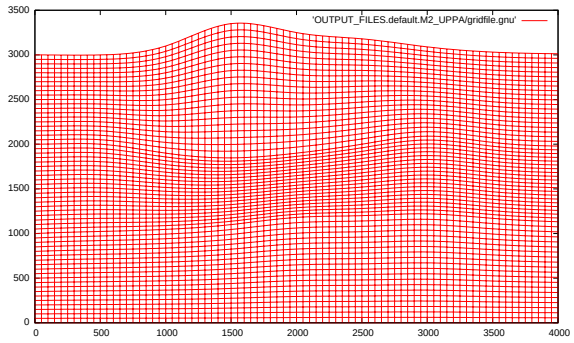

Figure 3.2: Example of a grid file generated by `xmeshfem2D` and visualized with gnuplot (within gnuplot, type ‘`plot "OUTPUT_FILES/gridfile.gnu" w l`‘).

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 Gmsh to generate an external mesh

Gmsh[1] is a 3D finite element grid generator which can be used for the generation of quadrangle and hexahedral meshes. It is therefore a good candidate for generating meshes which can be processed by SPECFEM2D. Only two modules of Gmsh are of interest for the SPECFEM2D users : the geometry and the mesh modules. An example is given in directory `EXAMPLES/Gmsh_example` which illustrates the generation of an external mesh using these two modules. The model, which 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`.

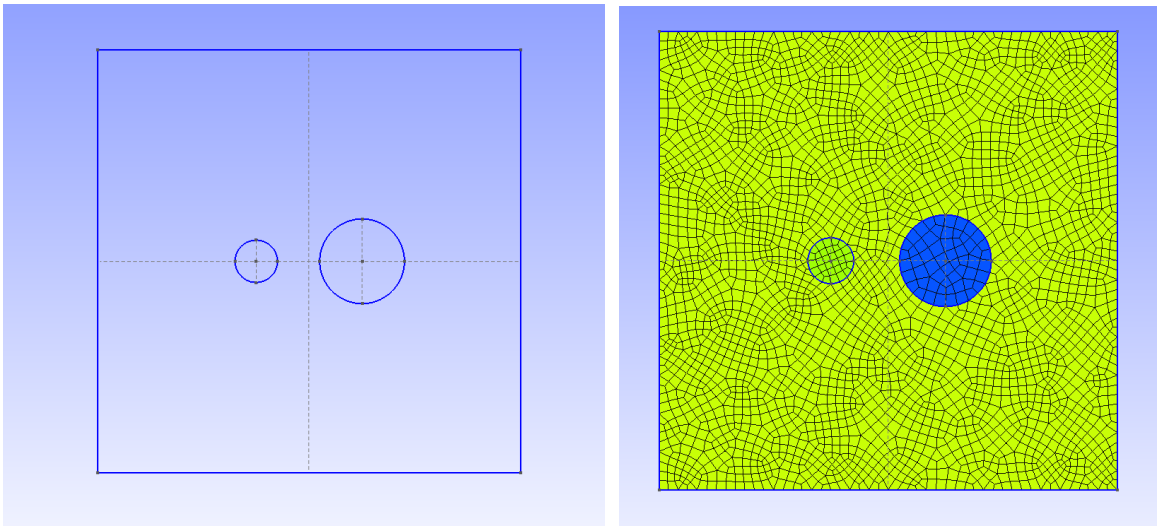

Figure 3.3: Geometry and mesh of the two circle model generated with Gmsh

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

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

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

[1] freely available at the following address : http://www.geuz.org/gmsh/

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

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

3.3 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 element are above the skewness = 0.75, and to which percentage of the total this amounts. To see this histogram, you could type:

```
gnuplot plot_mesh_quality_histogram.gnu
```

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

3.4 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 your created is too dense, it will be extremely accurate but the simulations will be slow; using a coarser mesh would be sufficient and would lead to faster simulations.

Chapter 4

Running the Solver xspecfem2D

To run the solver, type:

```
./bin/xspecfem2D
```

to run the main solver (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 color 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`).

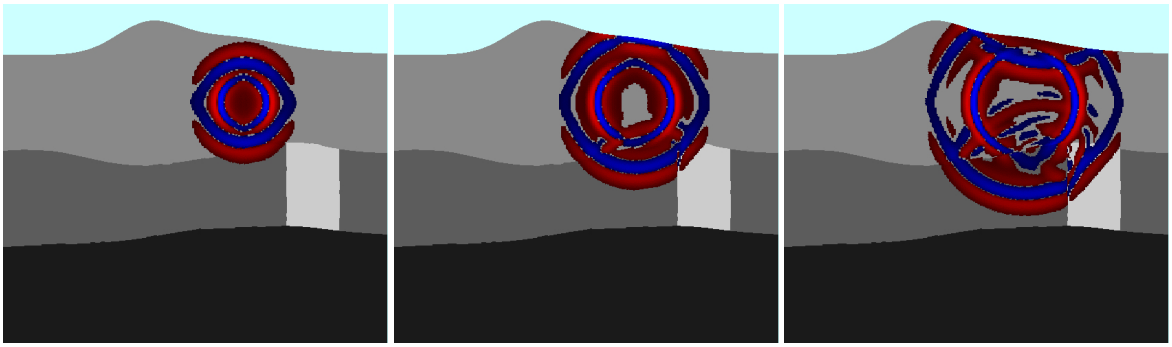

Figure 4.1: Wavefield snapshots of the default example generated by `xspecfem2D` when parameter `output_color_image` is set to `.true.`. To create smaller (subsampled) images you can change parameter `factor_subsample_image = 1` to a higher value in file `setup/constants.h` and recompile the whole code using `make all`. This can be useful 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 colum and amplitude in the second, therefore they can be visualized with any tool you like, for instance "`gnuplot`"
- if you set flag `assign_external_model` to `.true.` in `DATA/Par_file`, the velocity and density model that is given at the end of `DATA/Par_file` is then ignored and overwritten by the external velocity and density model that you define yourself in `define_external_model.f90`
- when compiling with Intel ifort, use "`-assume byterecl`" option to create binary PNM images displaying the wave field

- we do not have PML absorbing conditions implemented in the fluid/solid code yet. We use (older and less efficient) paraxial Clayton-Engquist or Sommerfeld equations instead. This is only by lack of time, we have a developer who is currently implementing PML but the code is not fully ready. For now, since the paraxial conditions are less efficient, please use a larger model
- there are a few useful scripts and Fortran routines in directory `UTILS/`.
- if you find bugs (or if you have comments or suggestions) please send an email to cig-seismo AT geodynamics.org and the developers will try to fix them and send you an updated version
- 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]

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.

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/f0`. If the code will use a Gaussian source-time function (time_function_type "3") (i.e., a signal with a shape similar to a 'smoothed triangle', as explained in Komatitsch and Tromp [2002] and shown in Fig 4.2), 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.csh` for this purpose, or alternatively use signal-processing software packages such as SAC (`www.llnl.gov/sac`). Type

```
make convolve_source_timefunction
```

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

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.

angleforce Angle of the source (for a force only)

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

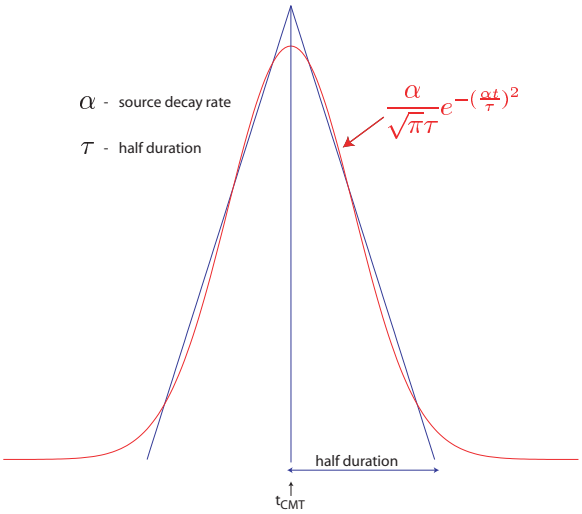

Figure 4.2: Comparison of the shape of a triangle and the Gaussian function actually used.

SPECFEM2D: in SPECFEM2D the moment tensor components are in N*m

factor amplification factor

Note, the zero time of the simulation corresponds to the center of the triangle/Gaussian, or the centroid time of the earthquake. The start time of the simulation is $t = -1.2 * \texttt{half duration} + \texttt{t0}$ (the factor 1.2 is to make sure the moment rate function is very close to zero when starting the simulation; Heaviside functions use a factor 2.0), the half duration is obtained by 1/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`.

Caution

See file `todo_list_please_dont_remove.txt` for a list of known bugs, problems, or missing options.

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.

4.1 How to run P-SV or SH (membrane) wave simulations

For elastic materials, you have these additional 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 traveling 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 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 homogenous model need to be set. No additional body or boundary forces are required. To set up this senario:

`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)

4.3 How to use Poroelasticity

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 simulations
(1) forward simulation
(2) adjoint method and kernels calculation

In section **"# source parameters"**:
The code now support multi sources. `NSOURCE` is the number of source. 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`)

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 0 0 0 0 0 0) or
`III`: (model_number 3 rhos rhof phi c kxx kxz kzz Ks Kf Kfr etaf mufr Qmu).

For istropic 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. 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

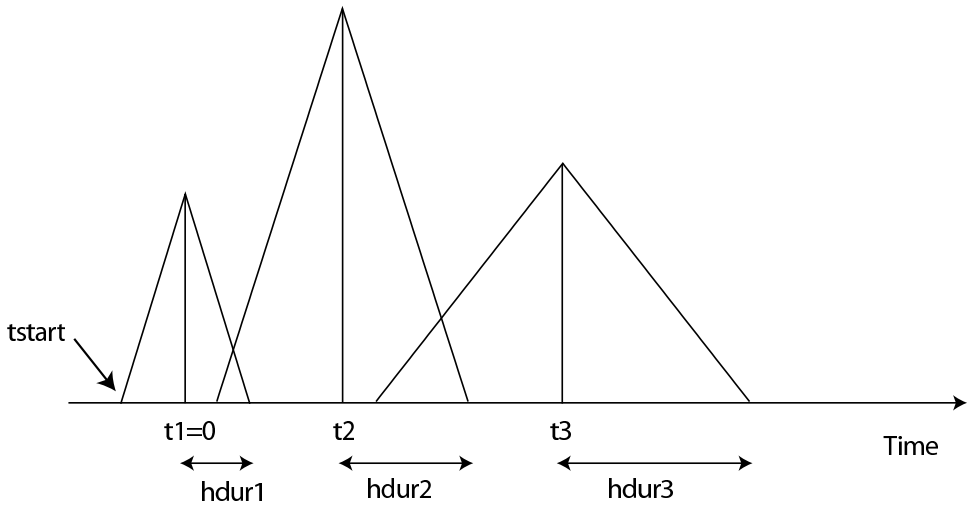

Figure 4.3: Example of timing for three sources. The center of the first source triangle is defined to be time zero. Note that this is NOT in general the hypocentral time, or the start time of the source (marked as tstart). The time shift parameter `t0` in the `SOURCE` file would be t1(=0), t2, t3 in this case, and the half-duration parameter, resp. `f0`, would be hdur1=1/f0_1, hdur2=1/f0_2, hdur3=1/f0_3 for the sources 1, 2, 3 respectively.

kappa_s = solid bulk modulus
kappa_f= fluid bulk modulus
kappa_fr= frame bulk modulus
eta_f = fluid viscosity
mu_fr = frame shear modulus
Qmu = shear quality factor

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

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

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 ouput 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 pic 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 ouput 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 = 2`
   => `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)".

Remarks about adjoint runs and solving inverse problems

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

The algorithm is simple:

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

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

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

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 6

Oil and gas industry simulations

The SPECFEM2D package provides compatibilities in industrial (oil and gas industry) types of simulations. These features include importing Seismic Unix (SU) format wavespeed models into SPECFEM2D, outputing seismograms also 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 previsouly defined). The new definition is critical when there are adjoint sources (in other words, receivers) in the acoustic domain, and is the direct consequence of the optimization problem.

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

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

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

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Appendix A

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`