SPECFEM2D

Mark Asch - ML-PREP

2025

specfem

Program

1. Context and Theoretical Background
2. Download and installation.
3. Preparing the input file.
4. Running simulations.
5. Post-processing:
   (a) animations,
   (b) seismograms,
   (c) spectrograms.

CONTEXT

The Vibrating Planet

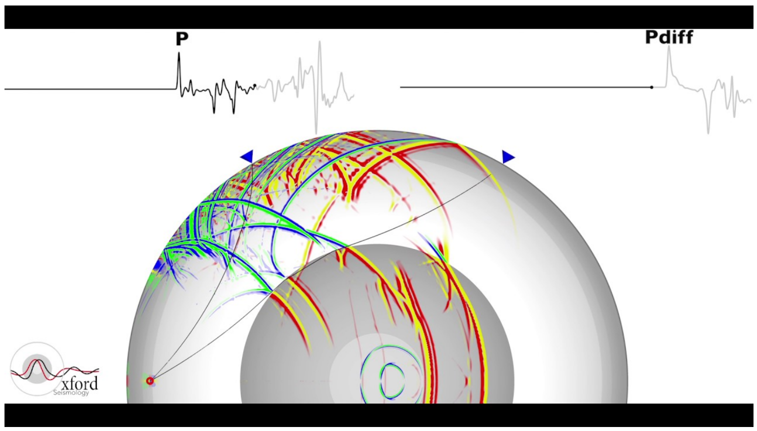
Our planet is permanently vibrating, excited by oceans, atmosphere, earthquakes, or man-made sources. Earth's physical properties are such that these vibrations—elastic waves to be more specific—often propagate to large distances carrying information on the medium they encounter along the way. There are two major challenges:

1. model and simulate this (seismic) wave propagation problem;

2. make an educated guess at the subsurface structure from observations of ground motions.

We call this last problem seismic tomography, inspired by CT scanning in medicine.

Types of Waves



- Primary, P-waves: acoustic, longitudinal, pressure waves.
- Secondary, S-waves: elastic, transversal, shear waves.
- Other waves: Surface, Rayleigh, Stoneley.

Seismology

Seismology is the science based on data from seismograms, records of mechanical vibrations of the Earth, that are caused by earthquakes and volcanic eruptions.

WAVE EQUATIONS

Wave Equation in 1D

The wave equation describes numerous propagation phenomena and is widely used in acoustics, seismics and vibration modeling, in general. It is second-order in both time and space, and in the one-dimensional case is defined by the initial boundary value problem

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - c^2 \dfrac{\partial^2 u}{\partial x^2} = s(x,t), \quad x \in (a,b), \quad 0 < t \leq T, \\ u(x,0) = f(x), \quad \dfrac{\partial u}{\partial t}(x,0) = g(x), \quad x \in (a,b), \\ u(a,t) = 0, \quad u(b,t) = 0, \quad t > 0, \end{cases} \tag{1}$$

- Initial conditions are required on u and $\partial u / \partial t$.
- Boundary conditions can be:

$\Rightarrow$ Dirichlet, where the amplitude u is prescribed.

- ⇒ Neumann, where the normal derivative of u is prescribed.
- ⇒ Mixed, where linear combination of Dirichlet and Neumann, is used.
- ⇒ Absorbing, where the waves can pass straight through the boundaries without any reflections. This is used in practice to limit the size of the computational domain.

Seismic Wave Equation

- Seismic waves are used to infer properties of subsurface geological structures.
- The physical model is a heterogeneous, elastic medium where sound is propagated by small elastic vibrations.
- The general mathematical model for deformations in an elastic medium is based on: Newton's second law and a constitutive law relating stress to displacement.
- We define:
  - ⇒ $\boldsymbol{u} = (u_1, u_2, u_3)^{\mathrm{T}}$ as the displacement in the x-, y- and z-direction,
  - ⇒ λ and μ are the Lamé coefficients,
  - ⇒ ρ is the medium density,
  - ⇒ and $\boldsymbol{f}$ is an initial impulse that represents the acoustic source.

$$
\begin{aligned}
\rho \frac{\partial^2 u_i}{\partial t^2} &= \frac{\partial \sigma_{ij}}{\partial x_j} + f_i \\
\sigma_{ij} &= \lambda \delta_{ij} \epsilon_{kk} + 2\mu \epsilon_{ij} \\
\epsilon_{ij} &= \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)
\end{aligned}
$$

- The pressure (primary) and shear (secondary) wave speeds are related to the Lamé coefficients, λ and μ (the shear modulus) and the density ρ,

$$
c_p^2 = \frac{\lambda + 2\mu}{\rho} \qquad \text{and} \qquad c_s^2 = \frac{\mu}{\rho},
$$

- Non-isotropic rheologies are important for realistic applications:

  $\Rightarrow$ viscoelastic material,
  $\Rightarrow$ anisotropic material, and
  $\Rightarrow$ poro-elasticity.

- Seismic sources: in addition to the structural parameters of the Earth model, the physical description of the seismic source parameters will affect the resulting wavefield.

  $\Rightarrow$ Forces and moments.

  $\Rightarrow$ Point sources.

NUMERICAL METHODS

Categories

- Finite differences (seen above): for researchers who are interested in understanding partial differential equations, the finite-difference method offers an efficient and fast way to develop numerical approximations that allow the investigation of some of the main characteristics of the underlying modeled problem. Finite differences are always used for the time-discretization. For the spatial interpolation problem, there is an additional class of methods.

- Finite elements:

  $\Rightarrow$ classical - low-order, continuous across element boundaries.

  $\Rightarrow$ **spectral** - combination of Lagrange polynomials as interpolants and an integration scheme based on Gauss quadrature defined on the GLL points for the elastic wave equation. This leads to a diagonal mass matrix that can be trivially inverted.

$\Rightarrow$ discontinuous Galerkin - combines spectral with finite volume flux scheme.

SPECTRAL FINITE ELEMENTS

Background and Motivation

- The spectral finite element method uses high-order piecewise polynomial approximations of Lagrange type, usually of order four to nine, in the weak formulation of time-evolution problems.

- When coupled with Gauss-Lobatto-Legendre quadrature rules for evaluation of the integrals, and hexahedral elements, the resulting mass matrix, M, is diagonal and thus trivial to invert.

- A further advantage is that the mesh size can be larger than what is normally required, in particular when the number of mesh points per wavelength is critical in wave propagation problems of high frequency signals.

- There is, however, much more computational work at the element level.

Formulation

Consider the 1D elastic wave equation in a domain $\Omega \times (0, T]$,

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(\mu \frac{\partial u}{\partial x}\right) + f, \tag{2}$$

where

- displacement u, external force f, mass density ρ, shear modulus μ depend on x
- u and f depend on t also.
- boundary conditions are:

  $\Rightarrow$ stress-free condition on the Earth's surface

  $$\sigma_{ij} n_j = 0,$$

  where σ_{ij} is the symmetric stress tensor and n_j is the unit normal vector in direction x_j

$\Rightarrow$ spatial boundary conditions on the boundary $\partial\Omega$, either of Neumann type

$$\left| \mu \frac{\partial u}{\partial x} \right|_{x=0,L} = 0,$$

or an absorbing (transparent) condition.

Formulation - steps

1. Formulate the weak form of the wave equation (2) and its boundary conditions.

2. Transform the weak equation to the element level, using a Jacobian.

3. The discretization of our system comes with the approximation of the unknown function u using Lagrange polynomials as interpolants.

4. The formulation also requires the evaluation of the first derivatives of the Lagrange polynomials, the calculation of which requires the Legendre polynomials.

5. The numerical integration scheme based on GLL quadrature allows us to calculate all system matrices at elemental level.

6. Assemble in a final step to obtain the global system of equations that is integrated over time using a simple finite-difference scheme.

Formulation - system

- This is the well-known equation for time-dependent finite-element problems, which can be rewritten in matrix-vector notation as

$$M\ddot{\mathbf{u}}(t) + K\mathbf{u}(t) = \mathbf{f}(t)$$

- The mass matrix , M, is diagonal (thanks to the Lagrange polynomial basis), thus its inversion is trivial.

- The stiffness matrix, K, has a banded structure in this case with the bandwidth depending on the number of basis functions that are required inside each element.

- A simple centred finite-difference approximation of the second derivative in time gives the time-stepping scheme

$$\mathbf{u}^{n+1} = (\Delta t)^2 \left[M^{-1}\left(\mathbf{f} - K\mathbf{u}^n\right)\right] + 2\mathbf{u}^n - \mathbf{u}^{n-1}$$

- In SPECFEM, a Newmark time-stepping scheme is used.

SPECFEM

The SPECFEM Family

- SPECFEM2D simulates forward and adjoint seismic wave propagation in two-dimensional acoustic, (an)elastic, poroelastic or coupled acoustic-(an)elastic-poroelastic media, with Convolution PML absorbing conditions.

- SPECFEM3D_Cartesian, SPECFEM3D_GLOBE simulate acoustic (fluid), elastic (solid), coupled acoustic/elastic, poroelastic or seismic wave propagation in any type of conforming mesh of hexahedra (structured or not) on global and regional (continental-scale) scale (GLOBE).

- SPECFEM++ unifies the solver capabilities of the suite of SPECFEM packages (SPECFEM2D, SPECFEM3D and SPECFEM3D_GLOBE) under a single interface.

SPECFEM2D Installation

- Requires a Unix/Linux environment.
- Download using the command

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

- This creates a complete directory structure.
- Go into the specfem2d directory, check for and configure the Fortran and C++ compilers. Typically:

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

- Compile:

```
make all
```

- Test the default example:

```
./bin/xmeshfem2D
./bin/xspecfem2D
```

- Results are saved in the OUTPUT_FILES directory—see below.

SPECFEM2D Input Files

- All input is placed in the file DATA/Par_file which contains the following sections:
  - ⇒ Simulation input parameters
  - ⇒ Mesh
  - ⇒ Attenuation
  - ⇒ Sources
  - ⇒ Receivers
  - ⇒ Boundary conditions
  - ⇒ Parameters for internal meshing
  - ⇒ Display parameters
  - ⇒ Movies/images/snaphots visualizations

- Start from the EXAMPLES and find one that is somewhat similar. Many parameters have default values, and do not need to be set.

SPECFEM2D Simulations

There are several options for the simulation:

- single CPU
- multiple CPU, parallel using MPI
- GPU accelerated

SPECFEM2D Post-Processing

- All output files are saved in the OUTPUT_FILES directory
  - ⇒ image snapshots of the displacement wavefield et preselected times - forward_image*.jpg
  - ⇒ seismograms at each receiver as a function of time - - AA*.semd (displacement), *.semv (velocity)
  - ⇒ mesh geometry files
  - ⇒ vector image snapshots of wavefield at prescribed timesteps - vect*.ps

- Python scripts can then be written/used to
  - ⇒ generate animations of the wavefields
  - ⇒ plot seismogram traces
  - ⇒ compute and plot spectrograms
  - ⇒ plot potential energy

SPECFEM2D Post-Processing (contd.)

- To create an animation from the image snapshot:
  - ⇒ use ffmpeg: ffmpeg -framerate 9 -pattern_type glob -i "forward_image*.jpg" out.mp4
  - ⇒ alternatively, write a python script that does the same thing

- To display seismograms:
  - ⇒ install the python package obspy
  - ⇒ create a stream: st = obspy.Stream(traces)
  - ⇒ display: st.plot()

- To compute and display spectrograms:
  - ⇒ st[0].spectrogram(log=True)

Seismograms and Spectrograms

- Seismograms are records of the shear and pressure wave amplitudes as a function of time, as recorded at each receiver station.
  - ⇒ AA.S0001.BXX.semd contains the times and amplitudes of the XX (horizontal/pressure) wave measured at receiver 1
  - ⇒ AA.S0001.BXZ.semd contains the times and amplitudes of the XZ (vertical/shear) wave measured at receiver 1
  - ⇒ etc.

- Spectrograms are a 3D representation of the frequency content and amplitude as a function of time, for each receiver.
  - ⇒ The spectrogram is the square magnitude of the STFT (short-time Fourier transform).
  - ⇒ This gives us a 2D representation of how the power of the different frequencies in the signal varies with time.

$\Rightarrow$ Each point in the spectrogram corresponds to a specific time and frequency, and its value corresponds to the power of the signal at that frequency and time.

ADVANCED SPECFEM

- To go (much) further:

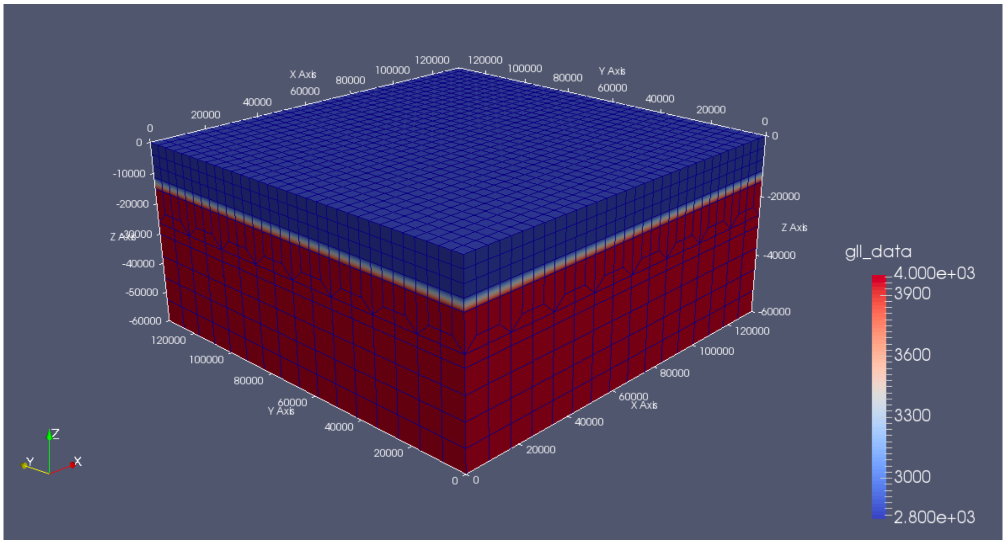
  ⇒ Specfem3D
  ⇒ Adjoint and Inverse simulations

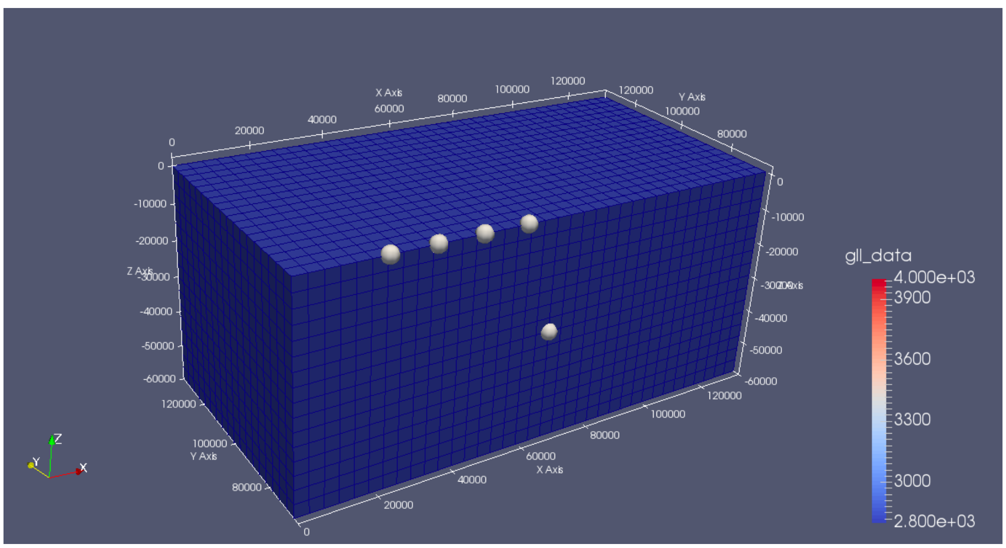
- Steps (see this link)

  ⇒ start docker
  ⇒ download docker image
  ⇒ run the container
  ⇒ open jupyterlab
  ⇒ navigate to workshops

- Docker container enables:

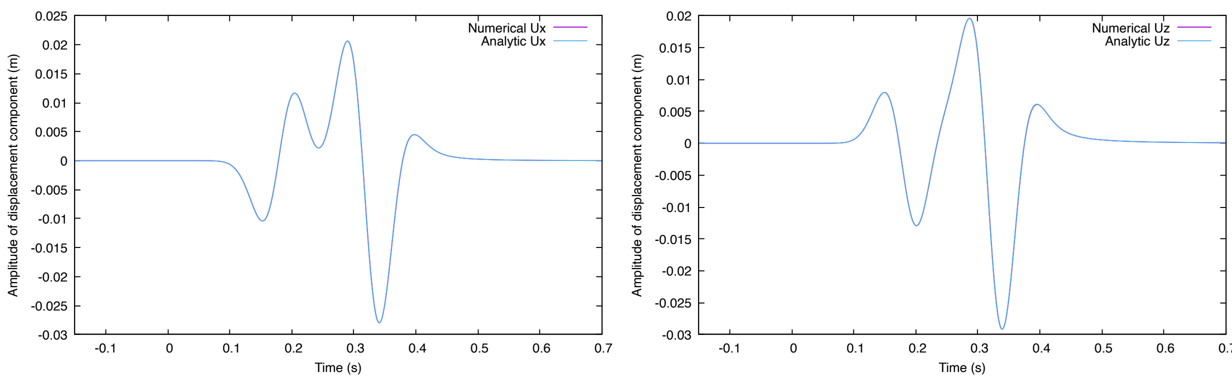
  ⇒ parallel execution with MPI
  ⇒ 3D simulations
  ⇒ inverse problem solutions...


X Axis
Y Axis
Z Axis
gll_data
4.000e+03
3900
3600
3300
3000
2.800e+03


X Axis
Y Axis
Z Axis
gll_data
4.000e+03
3900
3600
3300
3000
2.800e+03

Example: semi-infinite homogeneous

- simplest example with an analytical solution
- seismogram measured at single station
- use gnuplot to compare analytical and numerical solutions—see plot_compare_to_analytical_solution.gnu

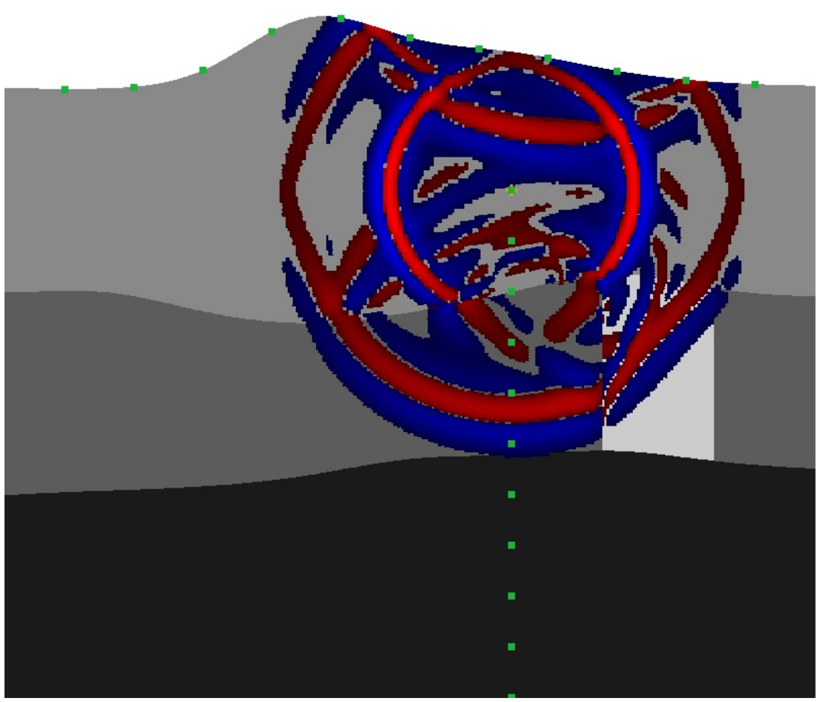


Example: 4-layer with topography

- more realistic situation with 4 layers having different material properties (ρ, v_s, v_p) and varying topography

- one layer is liquid, with $v_s = 0$ with a high velocity column

- 22 stations



Other Examples

- to be defined based on PHIVOLCS data

References

1. H.P. Langtangen. *Finite Difference Computing with PDEs: A Modern Software Approach.* Springer Cham. 2017. Download pdf

2. H. Igel. *Computational Seismology: A Practical Introduction.* Oxford University Press, 2017. website

3. SPECFEM2D

4. SPECFEM3D