Ε H F E K M ES3D.inv S Å BSPC Н R RG n N P \cap N P J S C K R R R R G R G F н Т L Y F С S B Α N F R F E Y н ()ΕZ Y R F Х В S Р D D ()()M S F L J R R -ZS Α С Н F \cap L Α

a programme package for seismic waveform modelling and inversion



BASIC CHARACTERISTICS



- seismic wave propagation through spherical sections
- including anisotropy and visco-elastic dissipation
- 3D heterogeneities of all Earth model properties
- inversion of seismic observables for 3D Earth structure

modelling volcanic earthquakes on Iceland





sensitivity analysis: How is my observable affected by Earth structure?

50 s Rayleigh wave



sensitivity analysis: How is my observable affected by Earth structure?

- receiver 2 receiver 1 source 10°E 15°E 20°E 67 35 BU ് 3°S 5°W
 - Cross-correlation measurements for regional scale tomography.
 - Validation of the 2-station method.

by Denise de Vos

sensitivity analysis: How is my observable affected by Earth structure?



by Moritz Bernauer





waveform inversion for 3D Earth structure

Tomography is a 3-stage process:

(1) forward problem

- (2) sensitivities
- (3) optimisation

forward problem		sensitivities		inversion
seismic wave propagation	C	how does an observable	0	finding good obervables
Earth models		Earth model?	0	the inversion grid and kernel vs. gradient
dissipation & anisotropy	C	Fréchet (sensitivity) kernels	0	local minima and the mul
spectral-element disctretisation of the	C	adjoint techniques & time		scale approach
seismic wave equation		i o i o i o i o i	0	regularisation

on non-linear optimisation

forward problem

sensitivities

inversion

- seismic wave propagation through heterogeneous Earth models
- C dissipation & anisotropy
- spectral-element disctretisation of the seismic wave equation

- how does an observable react to changes of the Earth model?
- Fréchet (sensitivity) kernels
- adjoint techniques & time reversal

- finding good obervables
- the inversion grid and kernel vs. gradient
- local minima and the multiscale approach
- regularisation
- on non-linear optimisation

forward problem	sensitivities	inversion
Seismic wave propagation	how does an observable	finding good obervables
through heterogeneous Earth models	react to changes of the Earth model?	the inversion grid and kernel vs. gradient
Galaria dissipation & anisotropy	Fréchet (sensitivity) kernels	local minima and the multi-
Spectral-element disctretisation of the	 adjoint techniques & time reversal 	scale approach
seismic wave equation		regularisation
		non-linear optimisation



Thursday afternoon

Friday morning



PART I

NUMERICAL SOLUTION OF THE SEISMIC WAVE EQUATION

- 1. Introduction
- 2. Spectral-element discretisation
- 3. Practical
- 4. Special topics (dissipation, point sources, absorbing boundaries)

Introduction

Introduction



elastic displacement field

Introduction



elastic displacement field

SES3D.inv

- spectral-elements in a spherical section
- operates in natural spherical coordinates
- visco-elastic dissipation
- radial anisotropy
- absorbing boundaries: PML





Disadvantages

- no poles & no core
- only regular-shaped elements
- elements become smaller with depth

no fluid-solid interaction

SES3D.inv is very efficient for a very specific class of problems:

wave propagation on local to continental scales where topography can be ignored

The SEM origins

- originally developed in fluid dynamics (Patera, 1984)
- migrated to seismology in the early 1990's (Seriani & Priolo, 1991)
- major advantage: accurate modelling of interfaces and the free surface (with topography)



The SEM concept in 1D: Weak form of the wave equation

SEM is based on the weak form of the wave equation

strong form of the wave equation



vibrating string of length L

The SEM concept in 1D: Weak form of the wave equation

SEM is based on the weak form of the wave equation

$$\rho \ddot{u} - \frac{\partial}{\partial x} \left(\mu \frac{\partial}{\partial x} u \right) = f \quad \frac{\partial}{\partial x} u(t,0) = \frac{\partial}{\partial x} u(t,L) = 0$$

------ PDE ------ PDE ----- B.C. (free surface in 3D) --
$$\int_{0}^{L} \rho w \ddot{u} dx - \int_{0}^{L} w \frac{\partial}{\partial x} \left(\mu \frac{\partial}{\partial x} u \right) dx = \int_{0}^{L} w f dx$$

strong form of the wave equation

multiply with test function w(x) integrate over x from 0 to L

The SEM concept in 1D: Weak form of the wave equation

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$$\rho \ddot{u} - \frac{\partial}{\partial x} \left(\mu \frac{\partial}{\partial x} u \right) = f \quad \frac{\partial}{\partial x} u(t,0) = \frac{\partial}{\partial x} u(t,L) = 0$$

------- PDE ------- PDE ------ B.C. (free surface in 3D) --
$$\int_{0}^{L} \rho w \ddot{u} dx - \int_{0}^{L} w \frac{\partial}{\partial x} \left(\mu \frac{\partial}{\partial x} u \right) dx = \int_{0}^{L} w f dx$$
$$\int_{0}^{L} \rho w \ddot{u} dx + \int_{0}^{L} \mu \left(\frac{\partial}{\partial x} w \right) \left(\frac{\partial}{\partial x} u \right) dx = \int_{0}^{L} w f dx$$

strong form of the wave equation

multiply with test function w(x) integrate over x from 0 to L

integrate by parts use the boundary conditions The SEM concept in 1D: Weak form of the wave equation

Solving the weak form of the wave equation means

to find a displacement field u(x,t) such that

$$\int_{0}^{L} \rho w \ddot{u} dx + \int_{0}^{L} \mu \left(\frac{\partial}{\partial x} w\right) \left(\frac{\partial}{\partial x} u\right) dx = \int_{0}^{L} w f dx$$

is satisfied for any differentiable test function w(x).

The SEM concept in 1D: Weak form of the wave equation

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is satisfied for any differentiable test function w(x).

Basis of element-based methods (e.g. finite elements, spectral elements, discontinuous Galerkin)

Boundary conditions are implicitly satisfied (no additional work required, as in finite-difference methods)

The SEM concept in 1D: Spatial discretisation

- **1.** decompose the computational domain [0, L] into disjoint elements E_i
- 2. consider integral element-wise



$$\int_{E_{i}} \rho w \ddot{u} dx + \int_{E_{i}} \mu \left(\frac{\partial}{\partial x} w\right) \left(\frac{\partial}{\partial x} u\right) dx = \int_{E_{i}} w f dx$$

$$E_{i}$$

The SEM concept in 1D: Spatial discretisation

3. map each element to the reference interval [-1, 1]



$$\int_{E_{i}} \rho w \ddot{u} dx + \int_{E_{i}} \mu \left(\frac{\partial}{\partial x} w\right) \left(\frac{\partial}{\partial x} u\right) dx = \int_{E_{i}} w f dx$$

$$E_{i}$$



-1

The SEM concept in 1D: Spatial discretisation



The SEM concept in 1D: Spatial discretisation





The SEM concept in 1D: Spatial discretisation

4. Approximate u by interpolating polynomials.



exact wave field approximation (interpolant)

degree 6

7 collocation points



The SEM concept in 1D: Spatial discretisation

- 4. Approximate u by Lagrange polynomials of degree N collocated at the GLL points
- 5. choose Lagrange polynomials also for the test function w



M=mass matrix

The SEM concept in 1D: Spatial discretisation

- 4. Approximate u by Lagrange polynomials of degree N collocated at the GLL points
- 5. choose Lagrange polynomials also for the test function w
- 6. The integral is approximated using Gauss-Lobatto-Legendre (GLL) quadrature.
 - Mass matrix is diagonal !!!
 - Integration exact for polynomials up to degree 2N-1



M=mass matrix

The SEM concept in 1D: Spatial discretisation

$$\int_{E_i} \rho w \ddot{u} dx + \int_{E_i} \mu \left(\frac{\partial}{\partial x} w \right) \left(\frac{\partial}{\partial x} u \right) dx = \int_{E_i} w f dx$$

weak form, element-wise

- 1. mapping to the reference interval [-1,1]
- 2. polynomial approximation (GLL points)
- 3. numerical integration (GLL quadrature)



The SEM concept in 1D: Spatial discretisation

$$\int_{E_{i}} \rho w \ddot{u} dx + \int_{E_{i}} \mu \left(\frac{\partial}{\partial x} w \right) \left(\frac{\partial}{\partial x} u \right) dx = \int_{E_{i}} w f dx$$
reported to the second s

weak form, element-wise

repeat this for the remaining two terms ...

The SEM concept in 1D: Spatial discretisation

$$\int_{E_i} \rho w \ddot{u} dx + \int_{E_i} \mu \left(\frac{\partial}{\partial x} w \right) \left(\frac{\partial}{\partial x} u \right) dx = \int_{E_i} w f dx$$

weak form, element-wise

enforce continuity between elements

weak form, global

$$\ddot{\mathbf{u}} = \mathbf{M}^{-1} \cdot \left(\mathbf{f} - \mathbf{K} \cdot \mathbf{u} \right)$$



The SEM concept in 3D

accurate solutions: discontinuities need to coincide with element boundaries



low velocities: short wavelength \rightarrow small elements

high velocities: long wavelength \rightarrow large elements

many small elements \rightarrow high computational costs !!!
Spectral-element discretisation

The SEM concept in 3D

Realistic example: The Grenoble valley



The SEM concept in 3D

Essentially the same as in 1D:

$$\rho \ddot{u}_{i} - \frac{\partial}{\partial x_{j}} \left(C_{ijkl} * \frac{\partial}{\partial x_{k}} u_{l} \right) = f_{i}$$

- 1. mapping to the reference cube $[-1, 1]^3$
- 2. polynomial approximation (GLL points)
- 3. numerical integration (GLL quadrature)



deformed element

reference cube

Spectral-element discretisation

The SEM concept in 3D: SES3D discretisation

- Discretisation of a spherical section without poles and core.
- Each element is a small spherical subsection.



- Speeds up the calculations.
- Simplifies the programme code.
- Reduces flexibility.

- 1. SES3D file structure
- 2. Input files
- 3. Model generation
- 4. Forward simulation: wiggly lines at last!



MATLAB

MODELS

File structure OUTPUT seismograms, snapshots, kernels

 DATA
 COORDINATES
 files with collocation point coordinates

 LOGFILES
 logfiles written during runtime

 INPUT
 simulation parameters, source time function, receivers

 SOURCE
 FORTRAN source code

MAIN executables and scripts for parallel jobs

MAIN

SOURCE

collection of Matlab (plotting) tools

Earth model properties (density, elastic parameters, ...)

executables for model generation

source code for model generation

Example

- regional-scale wave propagation
- 1 processor (not parallel)







0

Input files: Par file

File Edit View Terminal Go Help SIMULATION PARAMETERS ==== 500 ! nt, number of time steps 0.75 ! dt in sec, time increment SOURCE 90.00 ! xxs, theta-coord. 2.50 ! yys, phi-coord. 30000.0 ! zzs, source depth in (m) 10 ! srctype, 1:f_x, 2:f_y, 3:f_z, 10:M_ij 0.00e19 ! M_theta_theta 0.00e19 ! M_phi_phi 0.00e19 ! M_r_r 0.00e19 ! M_theta_phi 0.00e19 ! M_theta_r 1.00e19 ! M_phi_r MODEL == 82.50 source characteristics 97.50 source type: 1,2,3=single forces, 10=moment tensor -5.0 moment tensor components in Nm 20.0 5371000.0 Mtt, Mpp, Mrr, Mtp, Mtr, Mpr 6371000.0

ļ	is_aniso
ł	is_diss
ł	model type



MODEL ===== 82.50	<pre></pre>								
97.50	! theta max (colatitude) in degrees								
-5.0 20.0 5371000.0 6371000.0	 radial anisotropy switched on (=1) or off (=0) visco-elastic dissipation switched on (=1) or off (=1) structural model (2=PREM) 								
0	! is_aniso								
0	! is_diss								
2	! model_type								
COMPUTATION	AL SETUP (PARALLELISATION) ====================================								
15	! nx_global								
25	! ny_global								
10	! nz_global								
4	! lpd, LAGRANGE polynomial degree								
1	<pre>! px, processors in theta direction</pre>								
1	! py, processors in phi direction								
1	<pre>! pz, processors in r direction</pre>								
OUTPUT DIRE	CTORY ====================================								

MODEL =									
82.50	! theta_min (colatitude) in degrees								
97.50	! theta_max (colatitude) in degrees								
-5.0	Spatial discretisation								
20.0	• number of elements in theta (colatitude) direction (15)								
5371000	number of elements in theta (colatitude) direction (15)								
6371000	number of elements in phi (longitude) direction (25)								
0	number of elements in vertical direction (10)								
0	Lagrange polynomial degree								
2									
COMPUTA	TIONAL SETUP (PARALLELISATION) ====================================								
15	! nx_global								
25	! ny_global								
10	! nz_global								
4	! lpd, LAGRANGE polynomial degree								
1	<pre>! px, processors in theta direction</pre>								
1	<pre>! py, processors in phi direction</pre>								
1	<pre>! pz, processors in r direction</pre>								
OUTPUT 1	DIRECTORY ====================================								
/DATA	/output/1/								



MODEL ==	
82.50	! theta_min (colatitude) in degrees
97.50	! theta_max (colatitude) in degrees
-5.0	! phi_min (longitude) in degrees
20.0	! phi_max (longitude) in degrees
5371000	.0 ! z_min (radius) in m
6371000	.0 ! z_max (radius) in m
0	! is_aniso
0	! is_diss
2	Parallelisation
COMPUTA	number of processors in theta (colatitude) direction (1)
15	• Humber of processors in theta (colatitude) direction (1)
25	number of processors in phi (longitude) direction (1)
10	number of processors in vertical direction (1)
4	: Ipa, LAGRANGE polynomial degree
1	<pre>! px, processors in theta direction</pre>
1	! py, processors in phi direction
1	<pre>! pz, processors in r direction</pre>
OUTPUT I	DIRECTORY ====================================
/DATA	/OUTPUT/1/

Input files: Par file

MODEL ==========	
82.50	! theta_min (colatitude) in degrees
97.50	! theta_max (colatitude) in degrees
-5.0	! phi_min (longitude) in degrees
20.0	! phi_max (longitude) in degrees
5371000.0	! z_min (radius) in m
6371000.0	! z_max (radius) in m
0	! is_aniso
0	! is_diss
2	! model_type
COMPUTATIONAL SETUP ((PARALLELISATION) ====================================
15	! nx_global
25	! ny_global
10	! nz_global
4	! lpd, LAGRANGE polynomial degree
1	! px, processors in theta direction
1	! py, processors in phi direction
1	<pre>! pz, processors in r direction</pre>
OUTPUT DIRECTORY ===	
	directory where the output (e.g. seismograms) is writte

./DATA/OUTPUT/I/

anectory where the output (e.g. seismograms) is written





Input files: source time function (stf)

- Heaviside function, bandpass-filtered between 60 s and 500 s
- Iower cutoff period (60 s) dictated by the size of the elements
- upper cutoff (500 s) ensures that the stf returns to zero
- always use bandlimited stf's



Input files: source time function (stf)

- Heaviside function, bandpass-filtered between 60 s and 500 s
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<u>F</u> ile	<u>E</u> dit	<u>V</u> iew	<u>T</u> erminal	<u>G</u> o	<u>H</u> elp
1.68	008e-	17			A.
1.17	534e-	07			
1.90	214e-	06			
1.04	616e-	05			
3.60	694e-	05			
9.52	114e-	05			
0.00	02111	55			
0.00	04141	13			
0.00	07410	76			
0.00	12353	7			
0.00	19459	8			
0.00	29267	4			
0.00	42353	8			
0.00	59324	6			

stf: plain ASCII list of numbers

Input files: receiver configuration (recfile)

<u>F</u> ile	<u>E</u> dit	<u>V</u> iew	<u>T</u> erminal	<u>G</u> o	<u>H</u> elp			
2 xx01 90.00 xx02	7.5	0 0.0	number first st station secon	er of tatior cola d sta	receive n name atitude (ation na	rs (2) (XX01) 90.0°), Ion me (XX02)	gitude)	e (7.5°), depth (0.0 m)
90.00	12.	50 0.0						
~					1,1	Command	-	







1 file for each model parameter (lambda, mu, 1/rho) ...

... and for each processor.





run main.exe and wait ...









Simulation

$v \approx \frac{2\frac{3}{4} \text{ elements}}{75 \text{ s}} \approx \frac{305 \text{ km}}{75 \text{ s}} \approx 4.1 \text{ km/s}$

→ fundamental-mode Rayleigh wave @ 60 s period



Results: Synthetic seismograms

- prominent Rayleigh wave
- no displacement on the N-S component
- pollution by reflections because absorbing boundaries are switched off



- 1. Visco-elastic dissipation
- 2. Point sources
- 3. Absorbing boundaries

Dissipation

- Again, the concept in 1D:
- The Earth is assumed to have a visco-elastic rheology defined as:

$$\sigma(t) = (C * \dot{\varepsilon})(t) = \int_{-\infty}^{t} C(t - t') \dot{\varepsilon}(t') dt'$$

This convolution is very inconvenient in time-domain wave propagation!

Dissipation

- Again, the concept in 1D:
- The Earth is assumed to have a visco-elastic rheology defined as:

$$\boldsymbol{\sigma}(t) = (C \ast \dot{\boldsymbol{\varepsilon}})(t) = \int_{-\infty}^{t} C(t - t') \dot{\boldsymbol{\varepsilon}}(t') dt'$$

For the stress-relaxation function C(t) one assumes a superposition of standardlinear solids:

$$C(t) = C_r \left[1 + \frac{\tau}{N} \sum_{n=1}^{N} e^{-t/\tau_n} \right] H(t)$$

- C(t) describes the stress that occurs in response to a unit step strain.
- The parameters of C(t) are chosen such that the corresponding Q(ω) takes a specific form.

Dissipation

$$C(t) = C_r \left[1 + \frac{\tau}{N} \sum_{n=1}^{N} e^{-t/\tau_n} \right] H(t)$$

Example for N=3:



Dissipation

The example was designed to have Q=100=const within a frequency range from 0.02 Hz to 0.2 Hz.



More mechanisms increase the quality of the Q-const approximation and also the computational costs.

Point sources

There are generally two ways of implementing a point source – each with its advantages and disadvantages:

Point sources

There are generally two ways of implementing a point source – each with its advantages and disadvantages:

1. Grid point implementation

Force acts at the grid point that is closest to the true point source location.

- easy to implement
- correct near field
- numerical error when the true location of the point force is too far from the nearest grid point


Point sources

There are generally two ways of implementing a point source – each with its advantages and disadvantages:

2. Lowpass filtered δ-function (implemented in SES3D)

The δ -function is approximated by a polynomial (degree and collocation points as in the spatial discretisation)

- correct solution in the far field for any source position
- implementation more difficult
- near-field inaccurate (within ≈ 2 elements around the source)



Fig.: Polynomial approximation of the δ -function (degree 4) within one 2D element, for different source positions (x^s, y^s).

Absorbing boundaries

Methods to avoid reflections from unphysical boundaries fall into 2 categories:

1. Absorbing boundary conditions

Boundary conditions that prevent the popagation of energy into the medium.

- easy and elegant implementation
- highly inefficient for large angles of incidence
- can be unstable

2. Absorbing boundary layers (implemented in SES3D)

Boundary layers where the amplitudes of incoming waves decay rapidly

- efficient for all angles of incidence
- implementation more involved
- can be unstable

Absorbing boundaries

2. Absorbing boundary layers (implemented in SES3D)

- Perfectly Matched Layers (PML) are the most popular and efficient absorbing technique.
- Wave equation is modified within the boundary region so that incoming waves decay exponentially:



Fig.: SES3D wavefield snapshots, illustrating the absorption of energy within the PML region.

Absorbing boundaries

2. Absorbing boundary layers (implemented in SES3D)

- Perfectly Matched Layers (PML) are the most popular and efficient absorbing technique.
- Wave equation is modified within the boundary region so that incoming waves decay exponentially:



Fig.: Total kinetic energy within the model as a function of time. The energy decreases rapidly but does not reach 0 due to imprefect absorption.