Spectral Elements

Introduction

- recalling the elastic wave equation

The spectral-element method: General concept

- domain mapping
- from space-continuous to space-discrete
- time extrapolation
- Gauss-Lobatto-Legendre interpolation and integration

A special flavour of the spectral-element method: SES3D

- programme code description
- computation of synthetic seismograms
- long-wavelength equivalent models

Scope: Understand the principles of the spectral element method and why it is currently maybe the most important method for wave propagation.

This lecture based on notes by Andreas Fichtner.

Elastic wave equation:

$$\mathbf{L}(\mathbf{u}, \rho, \mathbf{C}) = \mathbf{f}$$

$$\mathbf{L}(\mathbf{u}, \rho, \mathbf{C}) = \rho(\mathbf{x})\partial_t^2 \mathbf{u}(\mathbf{x}, t) - \nabla \cdot \int_{-\infty}^{\infty} \dot{\mathbf{C}}(\mathbf{x}, t-\tau) : \nabla \mathbf{u}(\mathbf{x}, t)\, d\tau$$

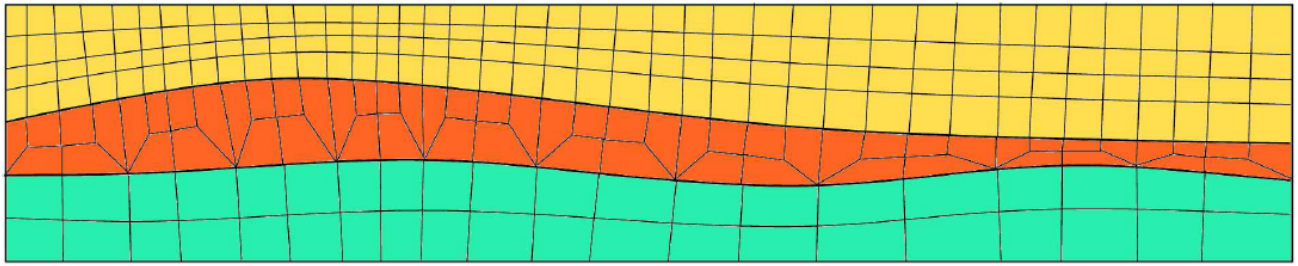
Subsidiary conditions:

$$\mathbf{u}(\mathbf{x}, t)\,|_{t=t_0} = \mathbf{0} \qquad \partial_t \mathbf{u}(\mathbf{x}, t)\,|_{t=t_0} = \mathbf{0} \qquad \mathbf{n} \cdot \int_{-\infty}^{t} \dot{\mathbf{C}}(\mathbf{x}, t-\tau) : \nabla \mathbf{u}(\mathbf{x}, \tau)\, d\tau\,|_{\mathbf{x}\in\Gamma} = \mathbf{0}$$

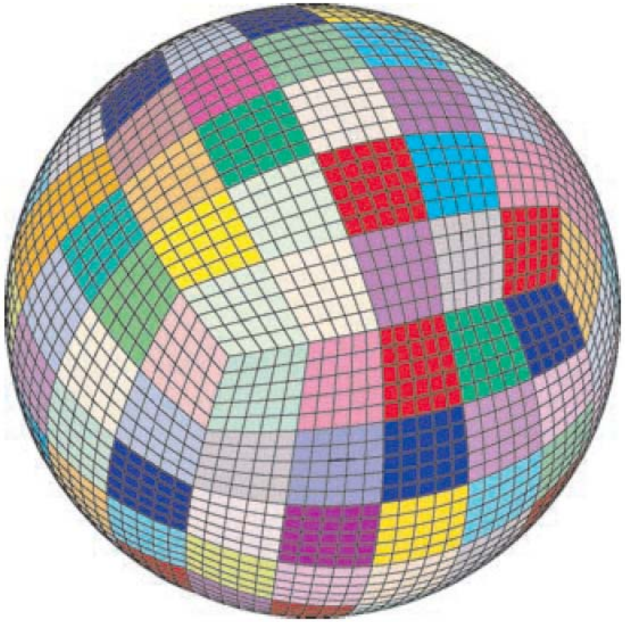
In this formulation **visco-elastic dissipation** is included as well as a general **anisotropic** description of elasticity.

Subdivision of the computational domain into hexahedral elements:

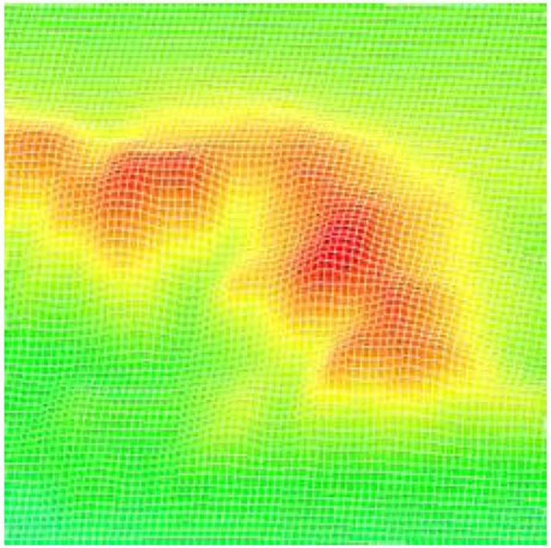
(a) 2D subdivision that honours layer boundaries



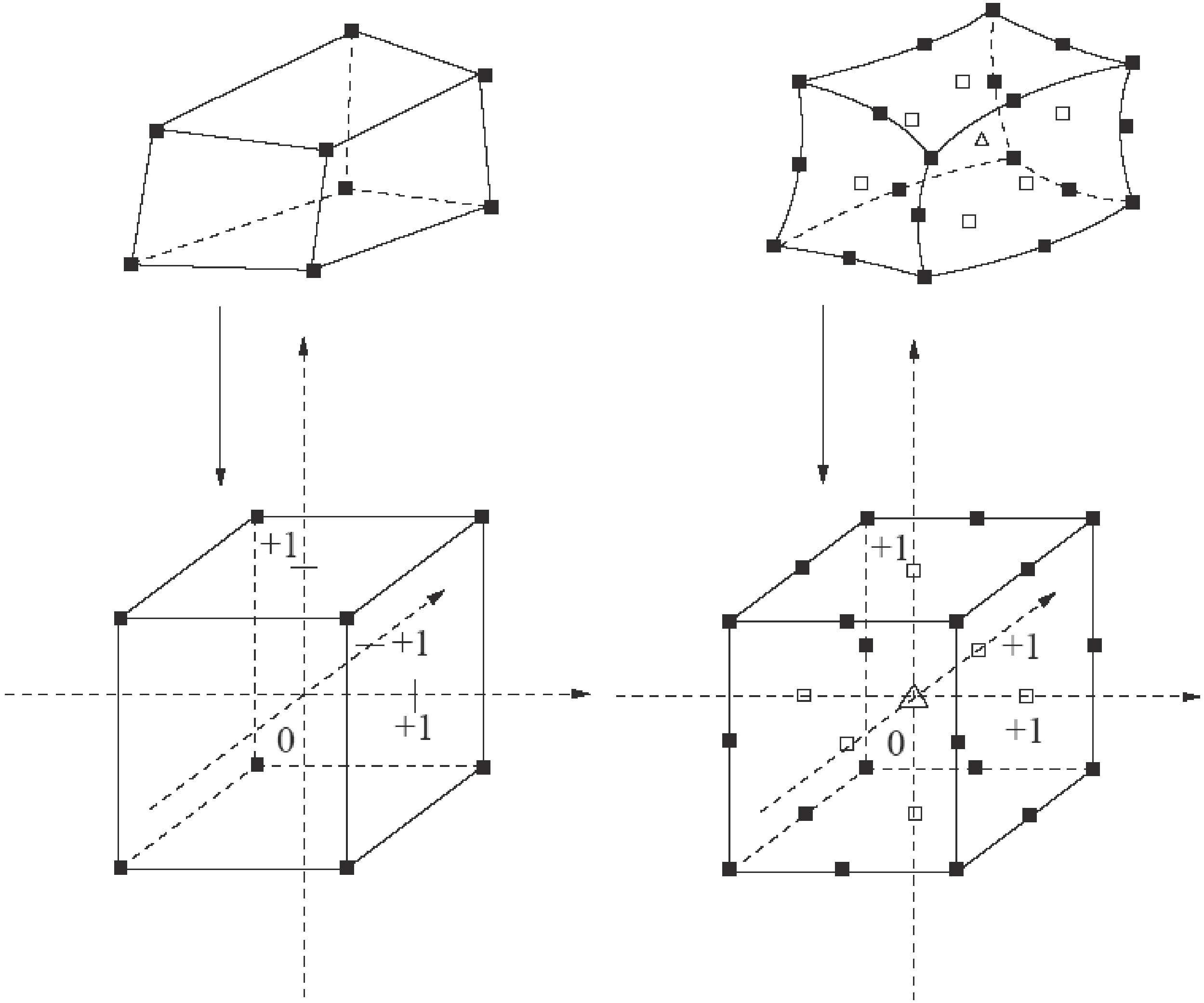
(b) Subdivision of the globe (cubed sphere)



(c) Subdivision with topography



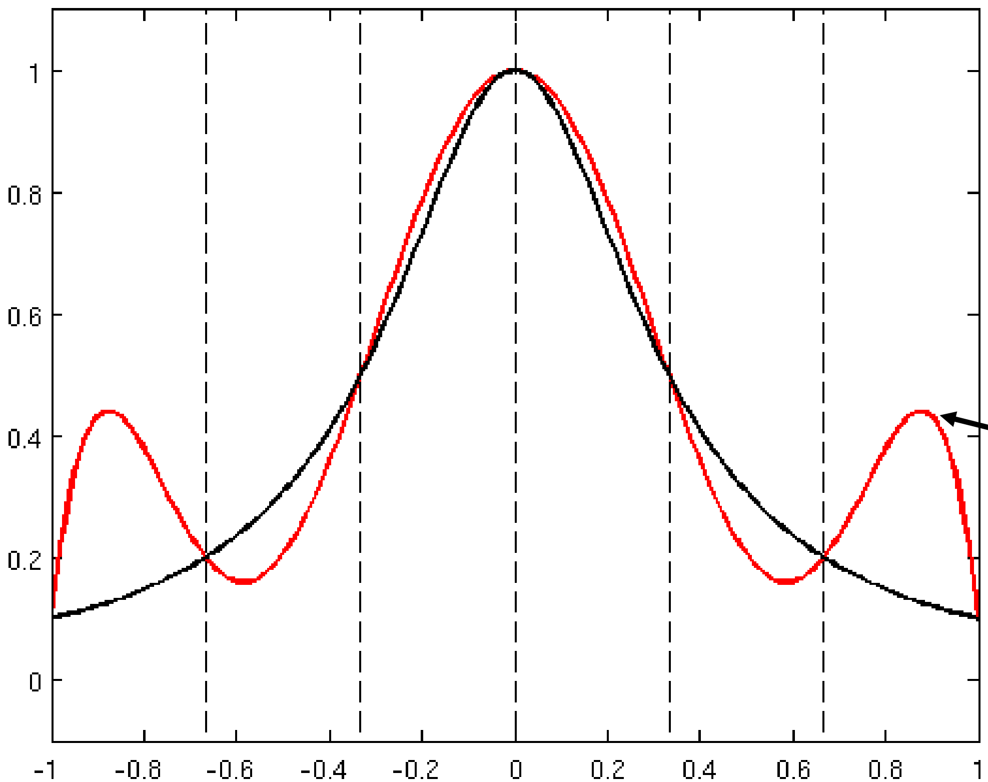
Mapping to the unit cube:



Choice of the collocation points:

Interpolation of Runge's function R(x)

using **6th-order** polynomials and **equidistant** collocation points



$$\mathbf{R}(\mathbf{x}) = \frac{1}{1+\mathbf{ax}^2}$$

interpolant

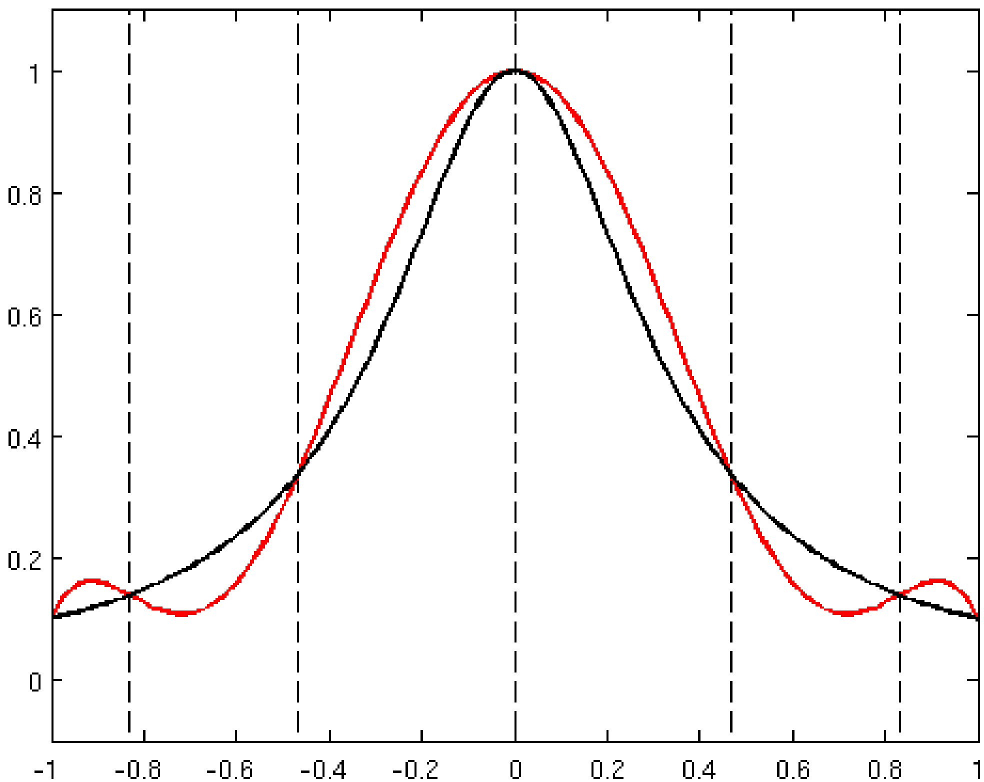
Runge's phenomenon

Choice of the collocation points:

Interpolation of Runge's function R(x)

using **6th-order** polynomials and **Gauss-Lobatto-Legendre** collocation points

[roots of $(1-x^2)Lo_{N-1}$= completed Lobatto polynomial]



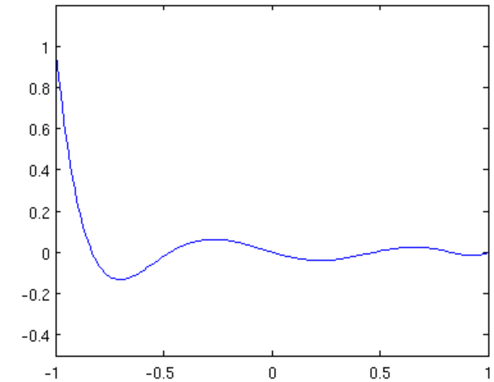
$$\mathbf{R(x)} = \frac{1}{1+\mathbf{ax}^2}$$

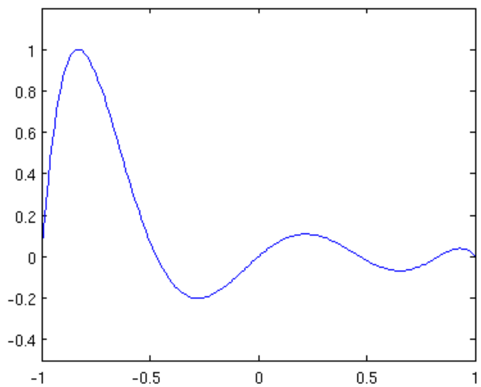
interpolant

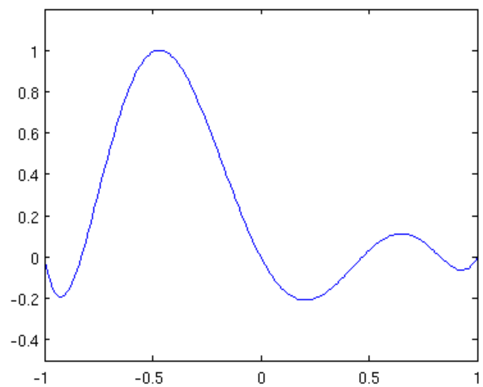
We should use the GLL points as collocation points for the Lagrange polynomials.

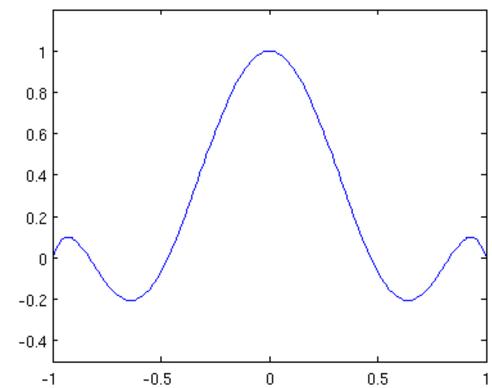
<u>Example:</u> GLL Lagrange polynomials of degree 6

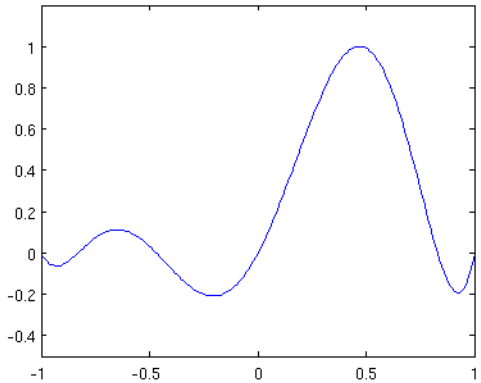
- collocation points = GLL points
- global maxima at the collocation points

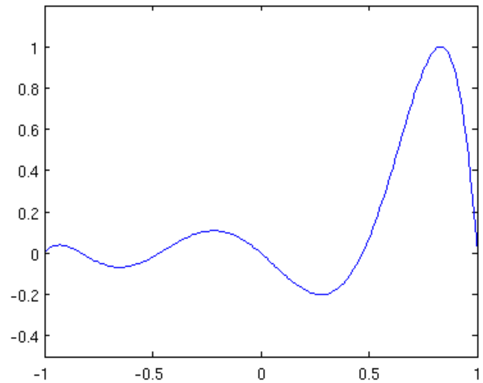


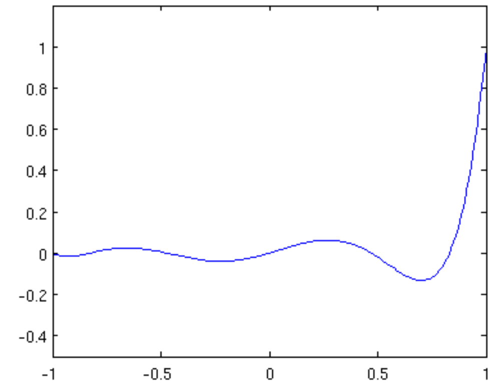












The SE system

$$\sum_{i=1}^{N+1} M_{ji}^e \ddot{u}_i^e(t) + \sum_{i=1}^{N+1} K_{ji}^e u_i^e(t) = f_j^e(t)\,, \quad e = 1, \ldots, n_e\,,$$

Diagonal mass matrix M

$$M_{ji}^e = w_j \rho'(\xi) \frac{dx}{d\xi} \delta_{ij} \Big|_{\xi=\xi_j}\,,$$

$$K_{ji}^e = \sum_{k=1}^{N+1} w_k \mu'(\xi) \dot{\ell}_j(\xi) \dot{\ell}_i(\xi) \left(\frac{d\xi}{dx}\right)^2 \frac{dx}{d\xi} \Big|_{\xi=\xi_k}\,,$$

$$f_j^e(t) = w_j f'(\xi,t) \frac{dx}{d\xi} \Big|_{\xi=\xi_j}\,.$$

Numerical quadrature to determine mass and stiffness matrices:

Quadrature node points = GLL points

→ **The mass matrix is diagonal, i.e., trivial to invert.**

→ **This is THE advantage of the spectral-element method.**

Time extrapolation:

$$\ddot{\mathbf{u}}(\mathbf{t}) \approx \frac{\mathbf{u}(\mathbf{t}+\Delta\mathbf{t}) - 2\mathbf{u}(\mathbf{t}) + \mathbf{u}(\mathbf{t}-\Delta\mathbf{t})}{\Delta\mathbf{t}^2}$$

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

Representation in terms of polynomials:

$$\mathbf{u}(\mathbf{x},\mathbf{t}) \approx \sum_{\mathbf{i}=0}^{\mathbf{N}} \mathbf{u}_{\mathbf{i}}(\mathbf{t})\, \ell_{\mathbf{i}}^{(\mathbf{N})}(\mathbf{x})$$

(within the unit interval [-1 1])

$\ell_{\mathbf{i}}^{(\mathbf{N})}(\mathbf{x})$: N^{th}-degree Lagrange polynomials

→ We can transform the partial differential equation into an ordinary differential equation where we solve for the polynomial coefficients:

$$\mathbf{M}_{\mathbf{ki}}\ddot{\mathbf{u}}_{\mathbf{i}} - \mathbf{K}_{\mathbf{ki}}\mathbf{u}_{\mathbf{i}} = \mathbf{f}_{\mathbf{k}}$$

$\mathbf{M}_{\mathbf{ki}}$: mass matrix

$\mathbf{K}_{\mathbf{ki}}$: stiffness matrix

SES3D: General Concept

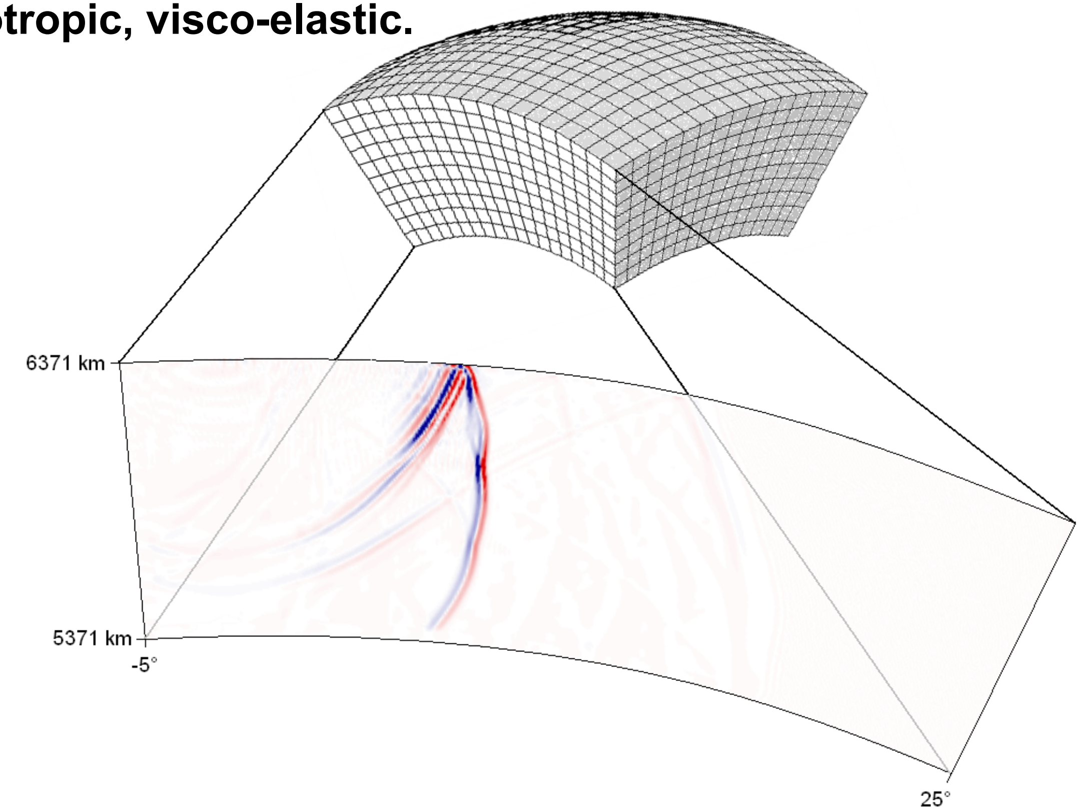
- **Simulation of elastic wave propagation in a spherical section.**
- **Spectral-element discretisation.**
- **Computation of Fréchet kernels using the adjoint method.**

- **Operates in natural spherical coordinates!**

- **3D heterogeneous, radially anisotropic, visco-elastic.**
- **PML as absorbing boundaries.**

Programme philosophy:

- **Puritanism** [easy to modify and
- adapt to different problems, easy
- implementation of 3D models,
- simple code]



SES3D: Example

Southern Greece

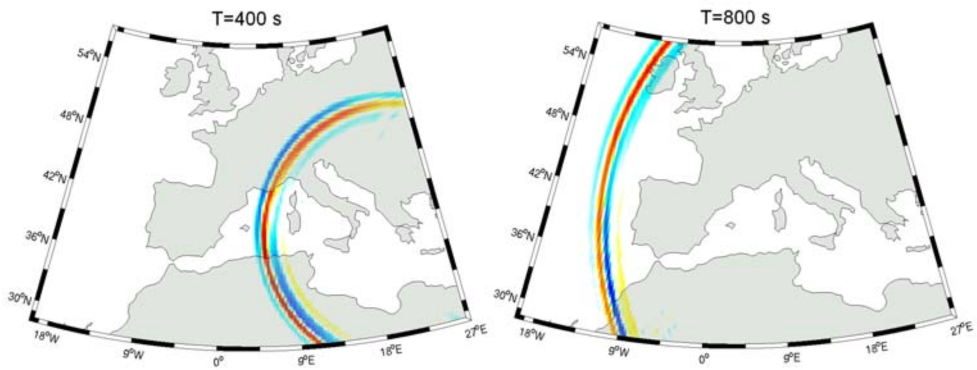
8 June, 2008

M_w=6.3

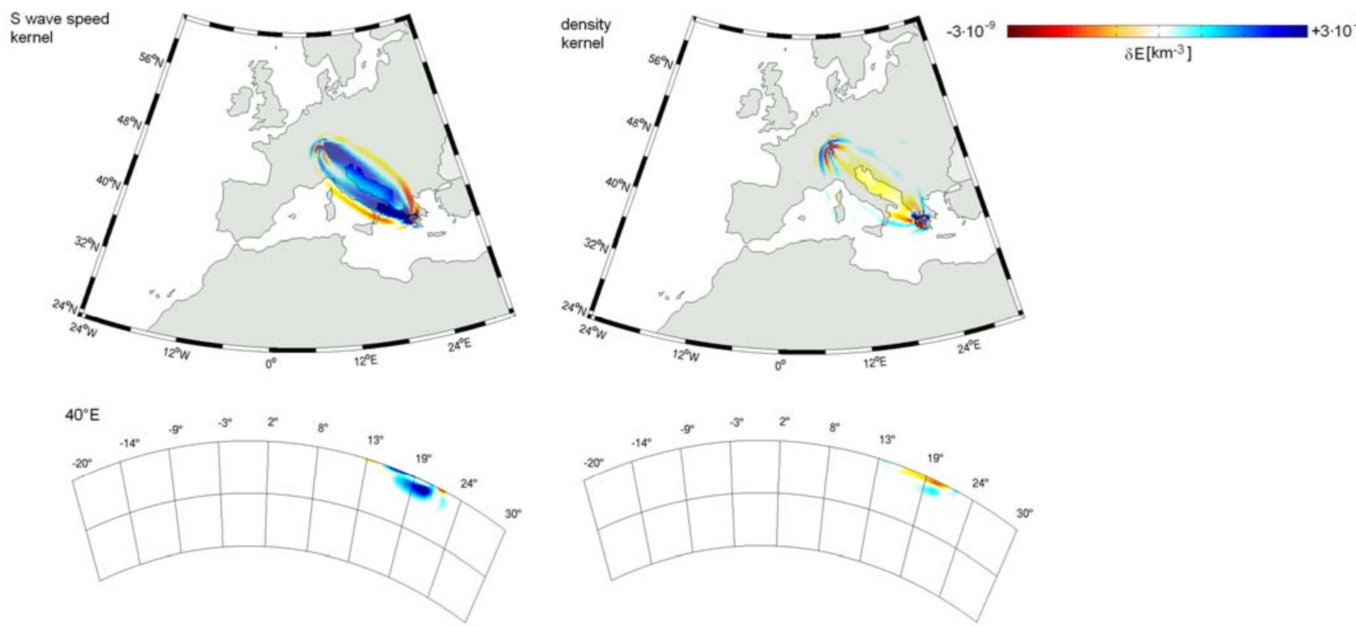
latitude: 37.93°,
longitude: 21.63°,
depth: 24.7 km,

$$M_{rr} = -0.289 \cdot 10^{18} \text{ Nm},$$
$$M_{ss} = 3.870 \cdot 10^{18} \text{ Nm},$$
$$M_{ee} = -3.580 \cdot 10^{18} \text{ Nm},$$
$$M_{rs} = -1.390 \cdot 10^{18} \text{ Nm},$$
$$M_{re} = -0.790 \cdot 10^{18} \text{ Nm},$$
$$M_{se} = 2.160 \cdot 10^{18} \text{ Nm}.$$

1. **Input files** [geometric setup, source, receivers, Earth model]
2. **Forward simulation** [wavefield snapshots and seismograms]



3. **Adjoint simulation** [adjoint source, Fréchet kernels]



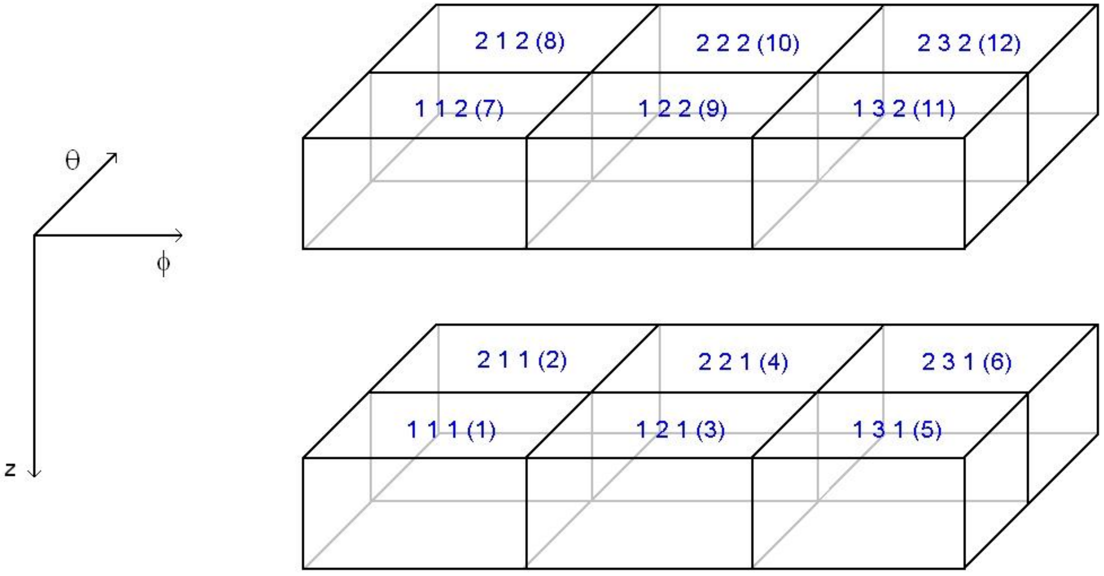
Spectral element method

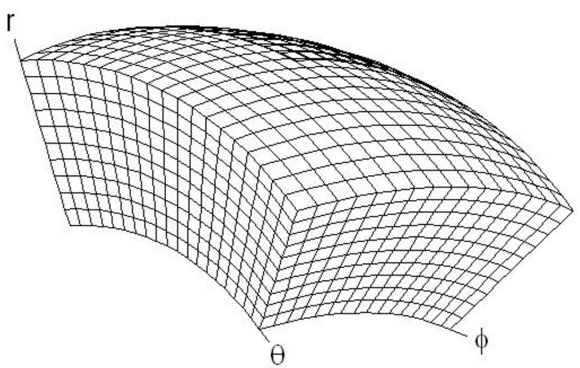
SES3D: Input files

- **Par:**
  - Numerical simulation parameters
  - Geometrical setup
  - Seismic Source
  - Parallelisation
- **stf:**
  - Source time function
- **recfile:**
  - Receiver positions

SES3D: Parallelisation

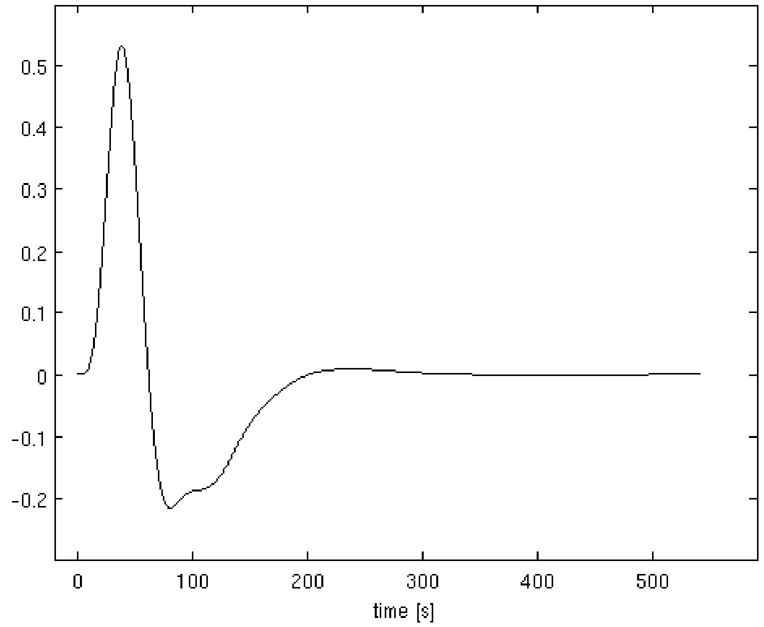
- **Spherical section subdivided into equal-sized subsections**
- **Each subsection is assigned to one processor.**
- **Communication: MPI**





Source time function

- time step and length agree with the simulation parameters
- PMLs work best with bandpass filtered source time functions
- Example: bandpass [50 s to 200 s]



Simulating delta functions?

$$1 = \int_{G_e} \bar{\delta}(\mathbf{x} - \mathbf{x}^s)\, d^3\mathbf{x}\,.$$

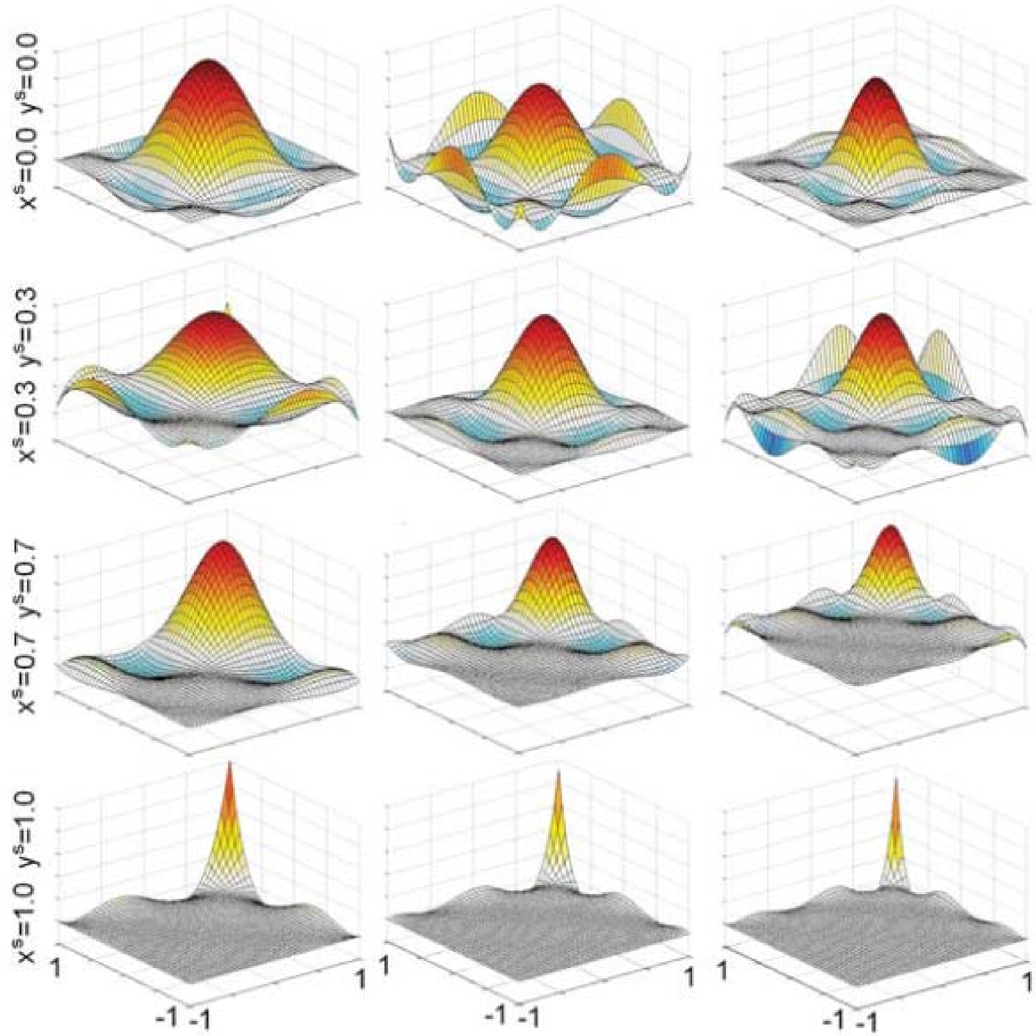
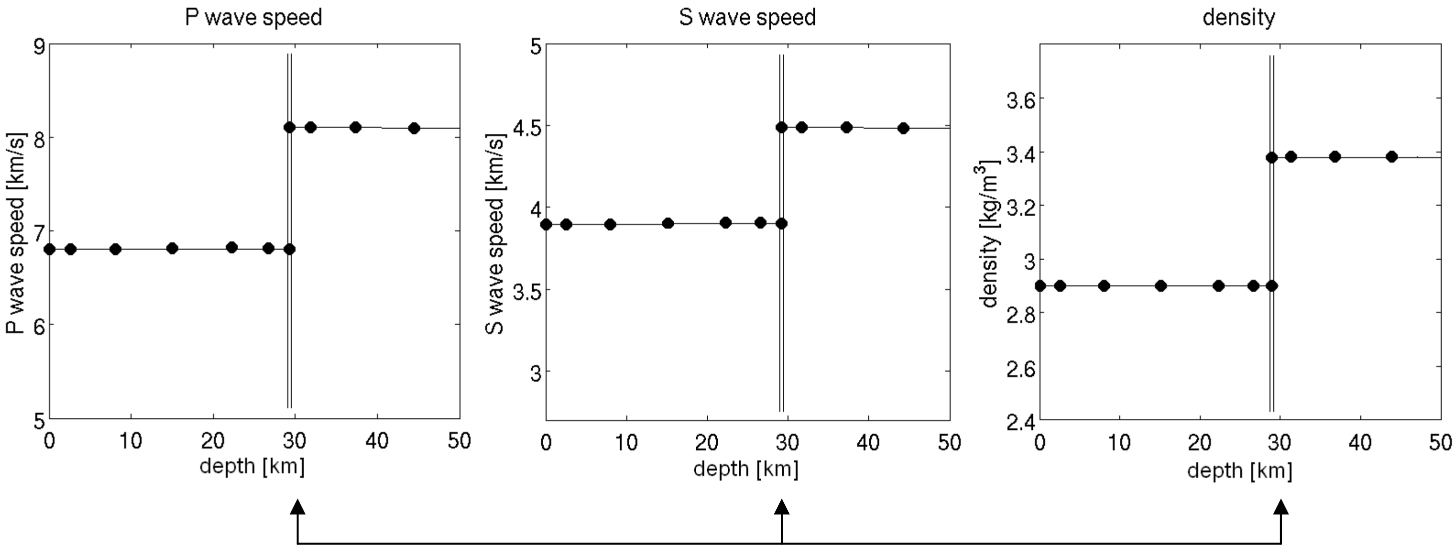


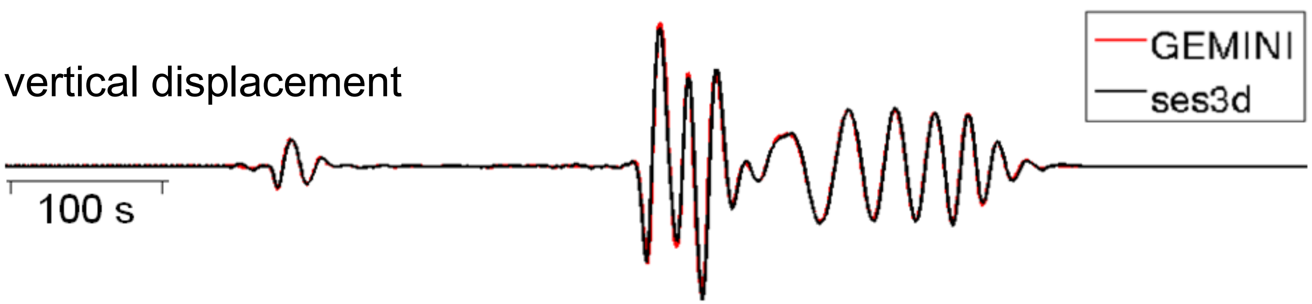
Fig. 4.6 Polynomial approximations of the $\delta-$function for different polynomial degrees and different point source localisations inside the reference cube.

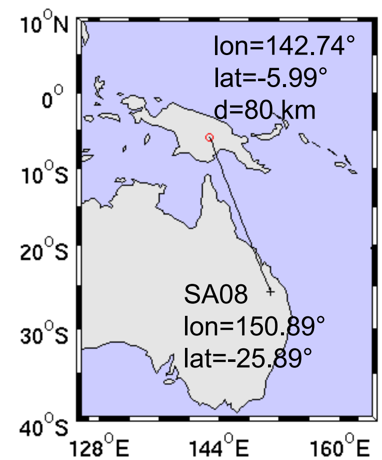


Single-layered crust that coincides with **the upper layer of elements** …

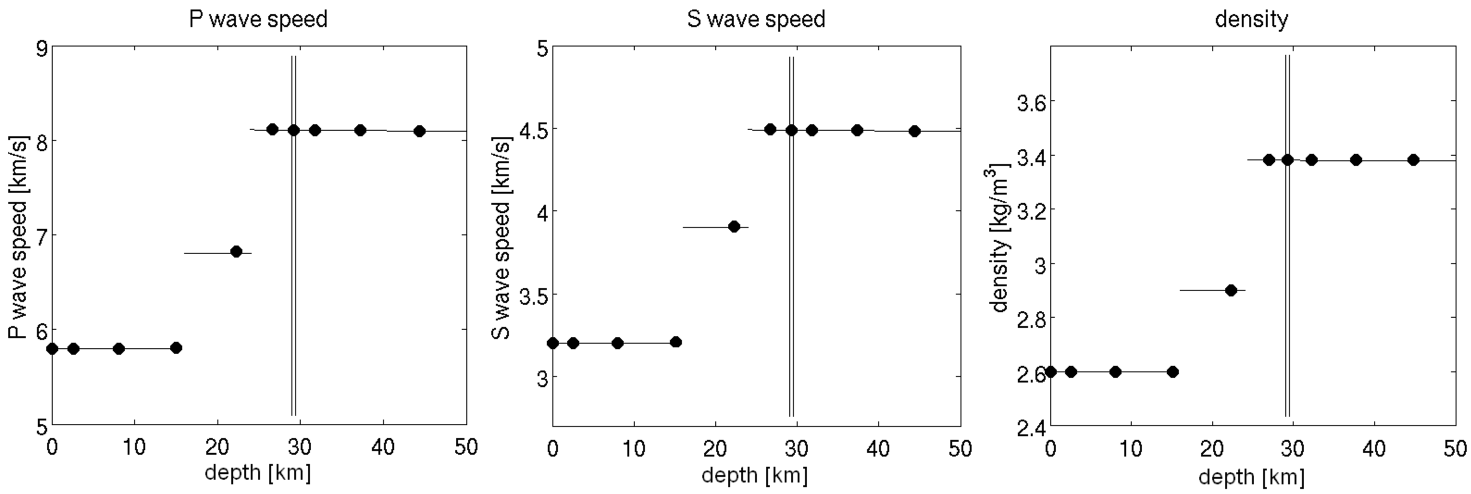
… and PREM below

boundary between the upper 2 layers of elements





Dalkolmo & Friederich, 1995. *Complete synthetic seismograms for a spherically symmetric Earth …*, GJI, 122, 537-550

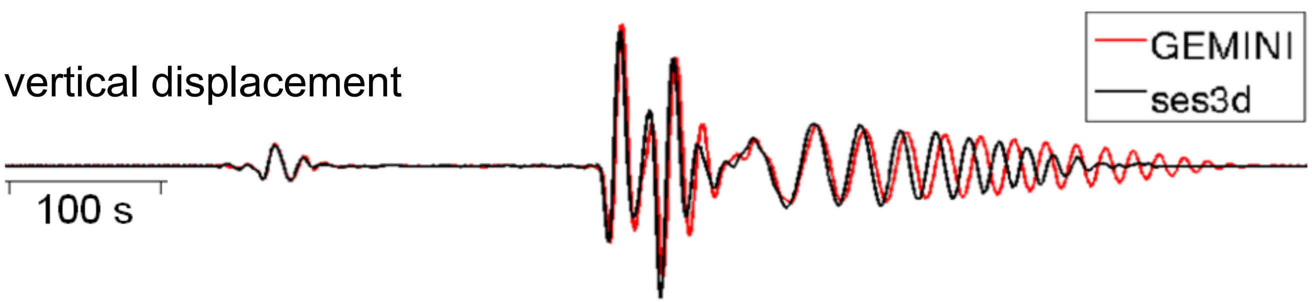


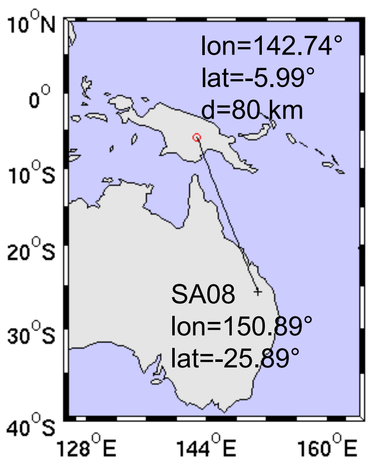
2-layered crust that does not coincide with **a layer of elements** …

… and PREM below

boundary between the upper 2 layers of elements

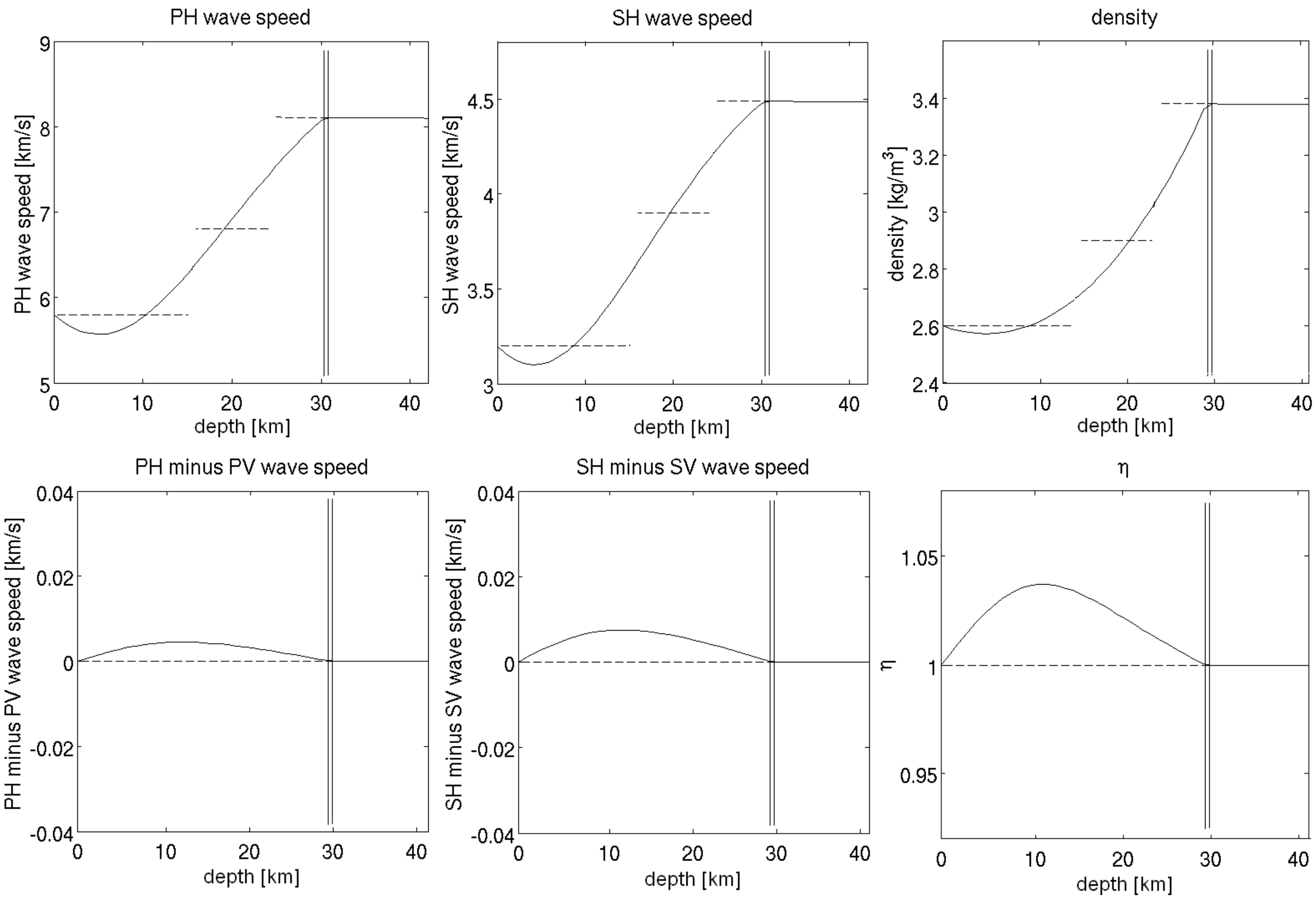
vertical displacement





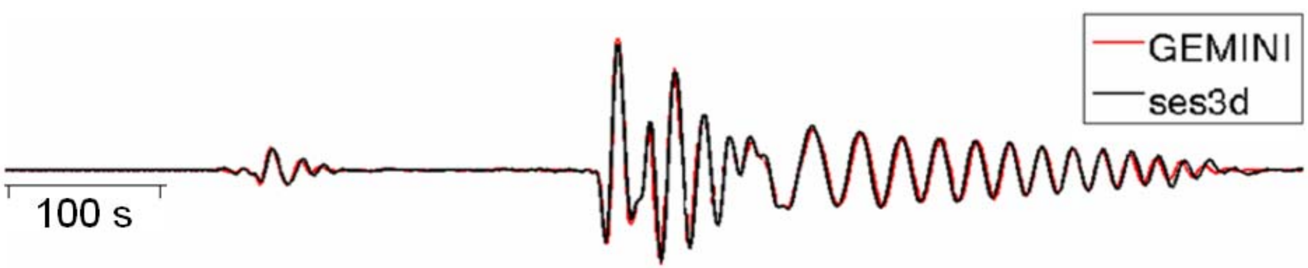
Dalkolmo & Friederich, 1995. *Complete synthetic seismograms for a spherically symmetric Earth …*, GJI, 122, 537-550

LONG WAVELENGTH EQUIVALENT MODELS



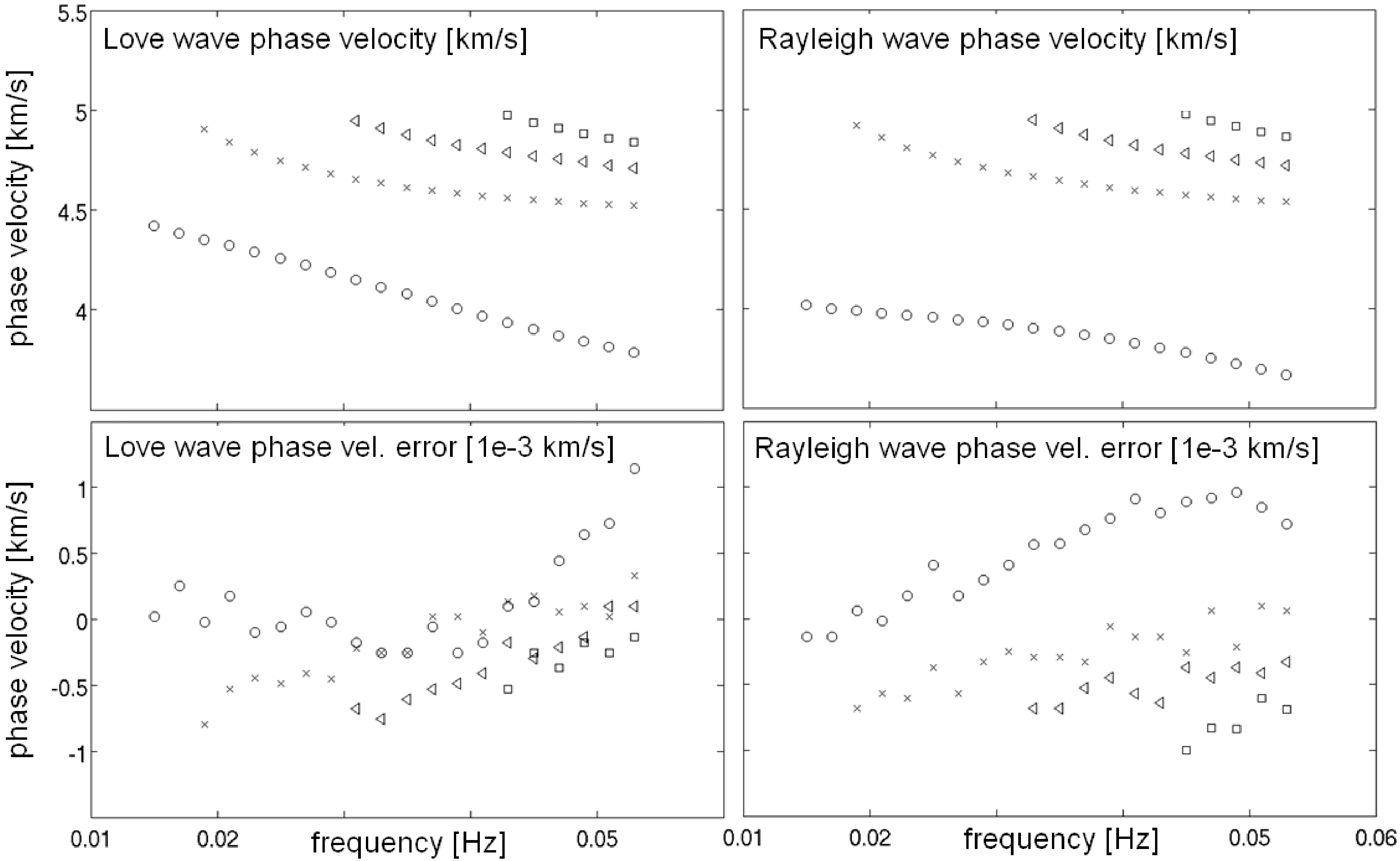
- Replace original crustal model by a **long-wavelength equivalent model** …
- … which is **transversely isotropic** [*Backus, 1962*].

- The optimal smooth model is found by **dispersion curve matching**.



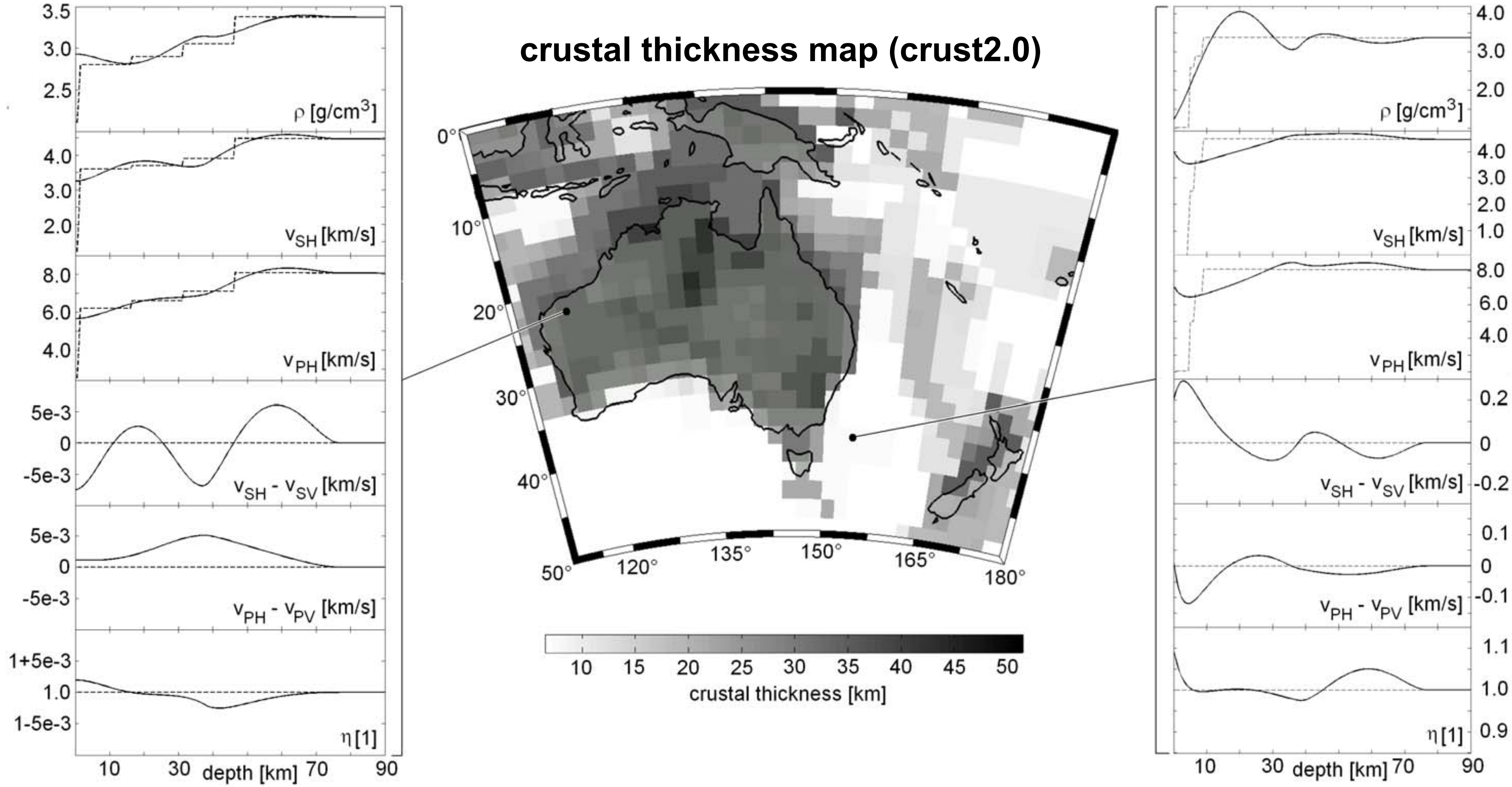
Fichtner & Igel, 2008. *Efficient numerical surface wave propagation through the optimisation of discrete crustal models*, GJI.

LONG WAVELENGTH EQUIVALENT MODELS



Minimisation of the phase velocity differences for the fundamental and higher modes in the frequency range of interest **through simulated annealing.**

LONG WAVELENGTH EQUIVALENT MODELS



- **3D solution:** interpolation of long wavelength equivalent profiles to obtain 3D crustal model.
- **Problem 1:** crustal structure not well constrained (receiver function non-uniqueness)
- **Problem 2:** abrupt changes in crustal structure (not captured by pointwise RF studies)

SES3D: Calls to caution!

1. **Long-term instability of PMLs**

   - All PML variants are long-term unstable!
   - SES3D monitors the total kinetic energy E_{total}.
   - When E_{total} increases quickly, the PMLs are switched off and …
   - … absorbing boundaries are replaced by less efficient multiplication by small numbers.

2. **The poles and the core**

   - Elements become infinitesimally small at the poles and the core.
   - SES3D is efficient only when the computational domain is sufficiently far from the poles and the core.

3. **Seismic discontinuities and the crust**

   - SEM is very accurate only when discontinuities coincide with element boundaries.
   - SES3D‘s static grid may not always achieve this.
   - It is up to the user to assess the numerical accuracy in cases where discontinuities run through elements. [Implement long-wavelength equivalent models.]
   - Generally no problem for the 410 km and 660 km discontinuities.

Spectral elements: summary

- Spectral elements (SE) are a special form of the finite element method.
- The key difference is the choice of the basis (form) functions inside the elements, with which the fields are described.
- **It is the Lagrange polynomials with Gauss-Lobato-Legendre (GLL) collocation points that make the mass matrix diagonal**
- This leads to a fully explicit scheme without the need to perform a (sparse) matrix inverse inversion
- Material parameters can vary at each point inside the elements
- SE works primarily on hexahedral grids
- The hexahedra can be curvilinear and adapt to complex geometries (cubed sphere, reservoir models)

Two open-source codes are available here:

- www.geodynamics.org (specfem3d) – regional and global scale
- www.geophysik.uni-muenchen.de/Members/fichtner (ses3d) - regional scale