Seismic Modelling

Spectral Element Method

Thomas Bohlen, Geophysical Institute, KIT-Faculty of Physics

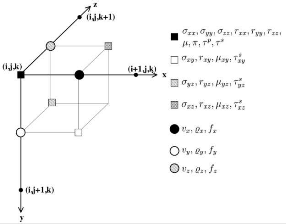
Wave equations

$$p_{ij} = \lambda\theta\delta_{ij} + 2\mu\epsilon_{ij}$$

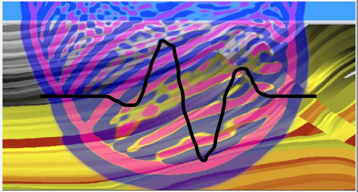
$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

$$\rho\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial p_{ij}}{\partial x_j} + f_i$$

Discretization



Solutions



Agenda

Agenda

Review: Finite Elements (FE)

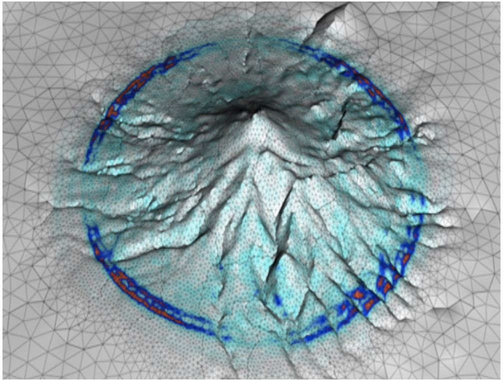


Figure 1: Simulation of waves in the presence of strong surface topography.

- FE methods allow for the flexible space discretization by using finite elements.
- The weak formulation of the wave equation inside of each element is solved.
- The inner wavefield is approximated by basis functions.
- At the edges boundary conditions are applied.
- Geological interfaces must be aligned with the edges of the finite-elements. This may require sophisticated meshing.

Literature

- Most of the material describing the methodology of the SEM presented in this lecture is copied 1:1 from the book of Heiner Igel, which you find in the references (Igel 2016).
- This book also includes many other seismic modelling approaches that could not be discussed in our lecture, such as Finite Volumes and Discontinuous Galerkin Methods.
- This book is therefore recommended for further studies on the subject seismic modelling.

Review: Finite Elements (FE)

1. We approximate u by an expansion of space dependent time-invariant basis functions $\varphi_i(x)$.

$$u(x,t) \approx \bar{u}(x,t) = \sum_{i=1}^{N} u_i(t)\varphi_i(x) \tag{1}$$

   The coefficients $u_i(t)$ are time dependent only.

2. We solve the discrete weak formulation of the wave equation which becomes a system of j linear equations

$$\sum_{i=1}^{N} \partial_t^2 u_i(t) \int_D \rho\varphi_i\varphi_j dx + \sum_{i=1}^{N} u_i(t) \int_D \mu\partial_x\varphi_i\partial_x\varphi_j dx = \int_D \varphi_j f dx \tag{2}$$

Global Finite Element formulation

We re-formulate it using matrix-vector notation

$$\boxed{\boldsymbol{M}^T \partial_t^2 \boldsymbol{u} + \boldsymbol{K}^T \boldsymbol{u} = \boldsymbol{f}} \tag{3}$$

$$\begin{aligned}
\text{displacement} \quad \boldsymbol{u}(t) \quad &\rightarrow \quad u_i(t) \\
\text{mass matrix} \quad \boldsymbol{M}(x) \quad &\rightarrow \quad M_{ij} = \int_D \rho \varphi_i \varphi_j dx \\
\text{stiffness matrix} \quad \boldsymbol{K}(x) \quad &\rightarrow \quad K_{ij} = \int_D \mu \partial_x \varphi_i \partial_x \varphi_j dx \\
\text{force} \quad \boldsymbol{f}(x) \quad &\rightarrow \quad f_j(x) = \int_D \varphi_j f dx
\end{aligned}$$

which is integrated over time by an explicit FD scheme

$$\boxed{\boldsymbol{u}(t+dt) = dt^2 (\boldsymbol{M}^T)^{-1} \left[\boldsymbol{f} - \boldsymbol{K}^T \boldsymbol{u}\right] + 2\boldsymbol{u}(t) - \boldsymbol{u}(t-dt)} \tag{4}$$

Agenda

Finite element formulation

In order to allow for flexibel (variable) space discretization we must introduce elements of variable size and transform the equations to the element level.

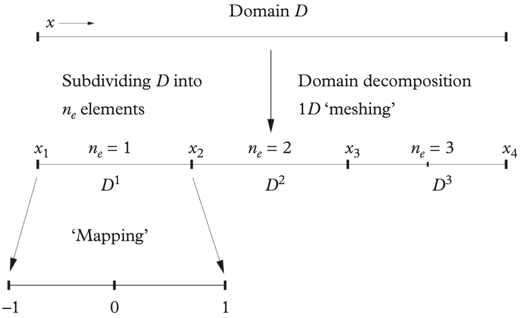


Figure 2: The global domain is subdivided into finite elements which have standard local coordinate system $\xi \in [-1, 1]$.

Finite element formulation

The series expansion is then performed inside of each element

$$\bar{u}(x,t)\big|_{x\in D_e} = \sum_{i=1}^{N_p} u_i^e(t)\varphi_i^e(x) \tag{5}$$

The global integrals (equation 2) are now local to one specific element D_e:

$$\begin{aligned} &\sum_{i=1}^{N_p} \partial_t^2 u_i^e(t) \int_{D_e} \rho(x)\varphi_i^e(x)\varphi_j^e(x)dx \\ + \quad &\sum_{i=1}^{N_p} u_i^e(t) \int_{D_e} \mu(x)\partial_x\varphi_j^e(x)\partial_x\varphi_i^e(x)dx \\ = \quad &\int_{D_e} \varphi_j^e f(x,t)dx \end{aligned} \tag{6}$$

Coordinate transformation

For each element we define a local coordinate system:

$$F_e: \quad [-1, 1] \rightarrow D_e, x = F_e(\xi), \tag{7}$$

$$\xi = \xi(x) = F_e^{-1}(x), e = 1, \ldots n_e \tag{8}$$

where n_e is the number of elements and $\xi \in [-1, 1]$. The global coordinate x can be related to the local coordinate ξ and vice versa via (see Figure 2)

$$x(\xi) = F_e(\xi) = h_e \frac{(\xi + 1)}{2} + x_e, \tag{9}$$

and vice versa

$$\xi(x) = F_e(\xi) = 2\frac{(x - x_e)}{h_e} - 1, \tag{10}$$

Coordinate transformation

A coordinate change $x \to \xi$ leads to

$$\int_{D_e} f(x)dx = \int_{-1}^{1} f(\xi)\frac{dx}{d\xi}d\xi \tag{11}$$

with the Jacobian J

$$J = \frac{dx}{d\xi} = \frac{h_e}{2} \tag{12}$$

The inverse of the Jacobian is required when derivatives of the basis functions are integrated:

$$J^{-1} = \frac{d\xi}{dx} = \frac{2}{h_e} \tag{13}$$

Finite element formulation

This leads finally to the system of linear equations which are solved for each element

$$
\begin{aligned}
& \sum_{i=1}^{N_p} \partial_t^2 u_i^e(t) \int_{-1}^{1} \rho[x(\xi)]\varphi_j^e[x(\xi)]\varphi_i^e[x(\xi)]\frac{dx}{d\xi}d\xi \\
+ \quad & \sum_{i=1}^{N_p} u_i^e(t) \int_{-1}^{1} \mu[x(\xi)]\partial_\xi\varphi_j^e[x(\xi)]\partial_\xi\varphi_i^e[x(\xi)]\left(\frac{d\xi}{dx}\right)^2 \frac{dx}{d\xi}d\xi \\
= \quad & \int_{-1}^{1} \varphi_j^e[x(\xi)]f([x(\xi)],t)\frac{dx}{d\xi}d\xi
\end{aligned}
\tag{14}
$$

Spectral element formulation

We now start to describe the characteristics of the Spectral Element Formulation (SEM) formulation.

1. We choose Langrange polynomials as basis functions
2. They allow for an exact representation of the wave field at collocation points within each element
3. We make a specific choice for the collocation point: Gauss-Lobatto-Legendre (GLL) points
4. Using the GLL points integration can be performed efficiently using Gauss-Lobatto-Legendre (GLL) quadrature
5. The mass matrix becomes diagonal (and thus easy to invert) because interpolation and integration are formulated for the same GLL points

Agenda

Agenda

Karlsruhe Institute of Technology

Interpolation with Lagrange Polynomials

For a set $n+1$ pair of points $(x_i, f_i)(i = 0, ..., n)$ with $x_i \neq x_j$ when $i \neq j$ it exists only one polynomial P_n of order n with

$$P_n(x_i) = f_i \quad . \tag{15}$$

This polynomial can be constructed by

$$P_n(x) = \sum_{i=0}^{n} f_i L_i(x) \tag{16}$$

with the Lagrange interpolation polynomials

$$L_i(x) := \prod_{k \neq i} \frac{x - x_k}{x_i - x_k}, \quad i = 0, ..., n \tag{17}$$

Interpolation with Lagrange Polynomials

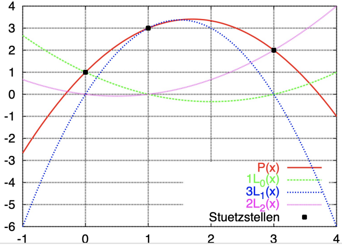
For illustration let us consider the following example for n=2:

i	0	1	2
x_i	0	1	3
f_i	1	3	2

The Langrange interpolation polynomials then are

$$L_0(x) = \frac{(x-1)(x-3)}{(0-1)(0-3)}, L_1(x) = \frac{(x-0)(x-3)}{(1-0)(1-3)}, L_2(x) = \frac{(x-0)(x-1)}{(3-0)(3-1)}$$

$$\begin{aligned} P_2(x) &= 1 \cdot L_0(x) + 3 \cdot L_1(x) + 2 \cdot L_2(x) \\ &= \frac{1}{6}(-5x^2 + 17x + 6) \end{aligned}$$



Lagrange polynomials

In FE/SEM method we seek to approximate $u^e(\xi, t)$ by a sum over space-dependent basis functions φ_i^e weighted by time-dependent coefficients $u_i^e(t)$.

$$u^e(\xi, t) \approx= \sum_{i=1}^{N_p} u_i^e(t)\varphi_i^e(\xi)$$

For these basis functions we choose Lagrange polynomials as defined previously:

$$\varphi_i \;\rightarrow\; \ell_i^{(N)}(\xi) \;:=\; \prod_{j\neq i}^{N+1} \frac{\xi - \xi_j}{\xi_i - \xi_j}, \qquad i, j = 1, 2, \ldots, N+1 \tag{18}$$

where ξ_i are specific points in the interval $[-1, 1]$ (local coordinate system in each element).

Lagrange polynomials

Writing the sum explicitly we obtain

$$\ell_i^{(N)}(\xi) = \frac{\xi - \xi_1}{\xi_i - \xi_1} \frac{\xi - \xi_2}{\xi_i - \xi_2} \cdots \frac{\xi - \xi_N}{\xi_i - \xi_N} \frac{\xi - \xi_{N+1}}{\xi_i - \xi_{N+1}} \tag{19}$$

For specific points we have

$$\ell_{i \neq j}^{(N)}(\xi_j) = \frac{\xi_j - \xi_1}{\xi_i - \xi_1} \cdots \frac{\xi_j - \xi_j}{\xi_i - \xi_j} \cdots \frac{\xi_j - \xi_{N+1}}{\xi_i - \xi_{N+1}} = 0 \tag{20}$$

and

$$\ell_i^{(N)}(\xi_i) = \prod_{j \neq i}^{N+1} \frac{\xi_i - \xi_j}{\xi_i - \xi_j} = 1 \tag{21}$$

which represents the orthogonality of the Lagrange polynomials:

$$\ell_i^{(N)}(\xi_j) = \delta_{ij} \tag{22}$$

Gauss-Lobatto-Legendre (GLL) points

The discretization points ξ_i in the local coordinate system of each element $[-1, 1]$ can be chosen arbitrarily. However, a specific set of points has considerable numerical advantages with respect to the integration and differentiation of the basis functions which are required in the update formula equation 4. These points are called Gauss-Lobatto-Legendre (GLL) points.

Gauss-Lobatto-Legendre (GLL) points

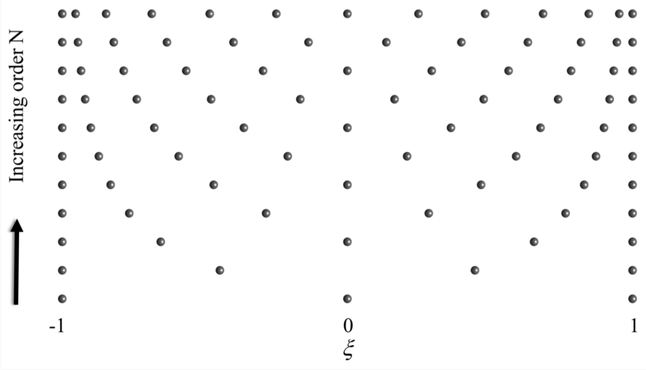


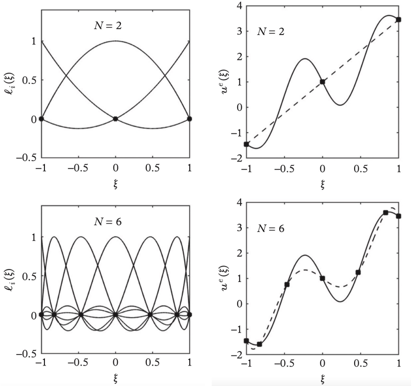
Figure 3: Spatial distribution of Gauss-Lobatto-Legendre (GLL) points in the local coordinate system $\xi \in [-1, 1]$. The point density increases towards the edges with increasing polynomial order N.

N	ξ_i	ω_i
2:	0	4/3
	± 1	1/3
3:	$\pm\sqrt{1/5}$	5/6
	± 1	1/6
4:	0	32/45
	$\pm\sqrt{3/7}$	49/90
	± 1	1/10

Table 1: Collocation points and integration weights of the GLL quadrature for order $N = 2, 3, 4$.

Interpolation with Lagrange polynomials

$$u^e(\xi) = \sum_{i=1}^{N+1} u^e(\xi_i)\ell_i(\xi) \quad \text{with} \quad \ell_i(\xi) = \prod_{j\neq i}^{N+1} \frac{\xi - \xi_j}{\xi_i - \xi_j} \tag{23}$$



Interpolation with Lagrange polynomials for N=2 and N=6. Left: Lagrange Polynomials. Right: Approximation of function (solid) and approximation (dashed). The approximation is exact at the GLL points (squares).

Finite element formulation using Langrange polynomials

We insert equation 23 into our system of linear equations 14 and obtain

$$\sum_{i=1}^{N+1} \partial_t^2 u_i^e(t) \int_{-1}^{1} \rho(\xi)\ell_j^e(\xi)\ell_i^e(\xi)\frac{dx}{d\xi}d\xi \tag{24}$$

$$+ \quad \sum_{i=1}^{N+1} u_i^e(t) \int_{-1}^{1} \mu(\xi)\partial_\xi\ell_j^e(\xi)\partial_\xi\ell_i^e(\xi)\left(\frac{d\xi}{dx}\right)^2 \frac{dx}{d\xi}d\xi$$

$$= \quad \int_{-1}^{1} \ell_j^e(\xi)f(\xi,t)\frac{dx}{d\xi}d\xi$$

where we allow that the material parameters (and forces) vary smoothly within each element.

$$\rho(\xi) := \rho[x(\xi)], \quad \mu(\xi) := \mu[x(\xi)], \quad f(\xi) := f[x(\xi)]. \tag{25}$$

Agenda

Numerical integration

The integrals appearing in equation 24 can be solved very efficiently by the Gauss-Lobatto-Legendre quadrature. Consider a function $f(x)$ defined in the interval $[-1, 1]$. If we apply a Langrange interpolation the integral can be approximated by a weighted sum of function values at the GLL points:

$$\int_{-1}^{1} f(x)dx \approx \int_{-1}^{1} P_N(x)dx = \sum_{i=1}^{N+1} \omega_i f(x_i) \quad \text{with} \quad P_N(x) = \sum_{i=1}^{N+1} f(x_i)\ell_i^N(x). \tag{26}$$

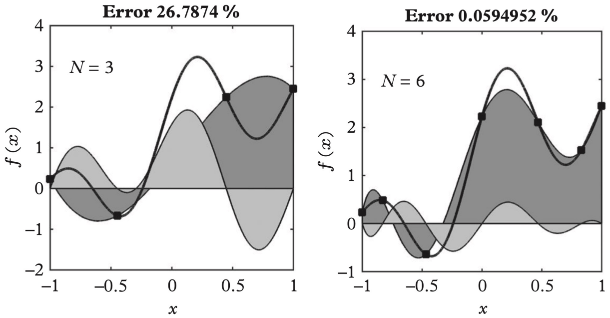
The integration weights can be pre-calculated, examples are given in table 22:

$$\omega_i = \int_{-1}^{1} \ell_i^N(x)dx. \tag{27}$$

Numerical integration

We illustrate the Gauss quadrature with an example:

$$f(\xi) = \sum_{i=1}^{5} \sin\left(\frac{\pi}{a_i}\xi + a_i\right) \quad \text{with} \quad a = [0.5, 1, -3, -2, -5, 4]. \tag{28}$$



Gauss integration with N=3 and N=6. The exact function (thick solid line) is approximated by a Lagrange polynomials (thin solid line) that can be integrated analytically. Thus, the integral of the true function (thick solid) is replaced by an integral over the polynomial function (dark grey). The difference between the true and approximate functions is given in light grey.

Spectral element formulation

We apply the GLL quadrature (equation 26) to our last formulation of the linear system of equation (equation 24) leading to an additional sum over k.

$$
\begin{aligned}
& \sum_{i,k=1}^{N+1} \partial_t^2 u_i^e(t) \omega_k \rho(\xi) \ell_j(\xi) \ell_i(\xi) \frac{dx}{d\xi} \Big|_{\xi=\xi_k} \\
+ \quad & \sum_{i,k=1}^{N+1} \omega_k u_i^e(t) \mu(\xi) \partial_\xi \ell_j(\xi) \partial_\xi \ell_i(\xi) \left(\frac{d\xi}{dx} \right)^2 \frac{dx}{d\xi} \Big|_{\xi=\xi_k} \\
= \quad & \sum_{k=1}^{N+1} \omega_k \ell_j(\xi) f(\xi, t) \frac{dx}{d\xi} \Big|_{\xi=\xi_k}
\end{aligned}
\tag{29}
$$

Spectral element formulation

This can be re-formulated using matrix notation:

$$\sum_{i=1}^{N+1} M_{ji}^e \partial_t^2 u_i^e(t) + \sum_{i=1}^{N+1} K_{ji}^e u_i^e(t) = f_j^e(t), \quad e = 1, \ldots, n_e \tag{30}$$

$$\begin{aligned}
\text{diagonal mass matrix:} \quad M_{ji}^e &= \omega_j \rho(\xi) \frac{dx}{d\xi} \delta_{ij}|_{\xi=\xi_k} \\
\text{stiffness matrix:} \quad K_{ji}^e &= \sum_{k=1}^{N+1} \omega_k \mu(\xi) \partial_\xi \ell_j(\xi) \partial_\xi \ell_i(\xi) \left(\frac{d\xi}{dx}\right)^2 \frac{dx}{d\xi}|_{\xi=\xi_k} \\
\text{force:} \quad f_j^e &= \omega_j f(\xi, t) \frac{dx}{d\xi}|_{\xi=\xi_k}
\end{aligned} \tag{31}$$

The time integration is performed by an explicit (low-order) FD scheme (equation 4).

Agenda

Numerical differentiation

For the calculation of the stiffness matrix K_{ji}^{e} in equation 31 we need the space derivatives $\partial_\xi \ell_i$ of the Langrange polynomials. These can be precalculated using Legendre polynomials:

$$L_N(\xi) = \frac{1}{2^N N!} \frac{d^N}{\xi^N} \left(\xi^2 - 1\right)^N \tag{32}$$

The Legendre Polynomials can be calculated using the following recursive formula

$$\begin{aligned} L_0(\xi) &= 1 \\ L_1(\xi) &= \xi \\ L_{n\geq 2}(\xi) &= \frac{1}{n}\left[(2n-1)\xi L_{n-1}(\xi) - (n-1)L_{n-2}(\xi)\right]. \end{aligned}$$

Numerical differentiation

The derivatives of the Lagrange polynomials can be calculated using:

$$\partial_\xi \ell_i = \sum_{j=0}^{N} d_{ji} \ell_k, \quad k = 0, \dots, N, \tag{33}$$

with

$$d_{ji} = \begin{cases} -\frac{1}{4}N(N+1) & \text{if } i = j = 0 \\ \frac{L_N(\xi_i)}{L_N(\xi_j)} \frac{1}{\xi_i - \xi_j} & \text{if } 0 \le i \le N, 0 \le j \le N, i \ne j \\ 0 & \text{if } 1 \le i = j \le N-1 \\ \frac{1}{4}N(N+1) & \text{if } i = j = N \end{cases} \tag{34}$$

For a spectral-element simulation of a specific order N, a matrix with the derivatives $\partial_\xi \ell_k(\xi_i)$ for each polynomial k at all $N+1$ collocation points ξ is precalculated and used to evaluate the integrals.

Agenda

Spectral Element Method: Conclusions

- The SEM combines the flexibility of FE methods with respect to computational meshes with the spectral convergence of Lagrange basis functions used inside the elements.
- The enormous success of the SEM is based upon the diagonal structure of the mass matrix that needs to be inverted to extrapolate the system in time combined with the spectral convergence of the basis functions.
- The diagonal mass matrix is made possible by superimposing the collocation points of both interpolation and integration schemes (Gauss-Lobatto-Legendre integration).
- Due to the diagonality, no matrix inversion techniques need to be employed, allowing straightforward parallelization of the algorithm.

Spectral Element Method: Conclusions

- Spectral element solutions are usually formulated for hexahedral computational grids. For complex models (surface topography, internal curved boundaries) this might involve cumbersome mesh generation. Formulations for triangles or tetrahedra are in principle possible but the advantage of a diagonal mass matrix is lost.
- The spectral element method is particularly useful for simulation problems where an uneven free surface plays an important role, and/or in which surface waves need to be accurately modelled. The reason is that the free-surface boundary is implicitly solved.
- Several well-engineered community codes are available for Cartesian and spherical geometries including basin scale, continental scale, and global Earth (or planetary scale) calculation.
- For further studies the book of Heiner Igel (LMU) (see References) is recommended.

Agenda

Example of SEM

- In this example we present an application of SEM to a model on scale relevant for seismic exploration. The model has significant topography of the free surface.
- The code SPECFEM 2D by CNRS (France) and Princeton University (USA) has been applied (Komatitsch & Vilotte 1998).
- The resulting seismograms have been compared with the FD method (SOFI2D, KIT)
- The results/figures are taken from the master thesis of Daniel Krieger (Krieger 2019).
- The goal of the thesis was to compare FD and SEM based FWI in the presence of free surface topography

FD and SEM in the presence of free surface topography

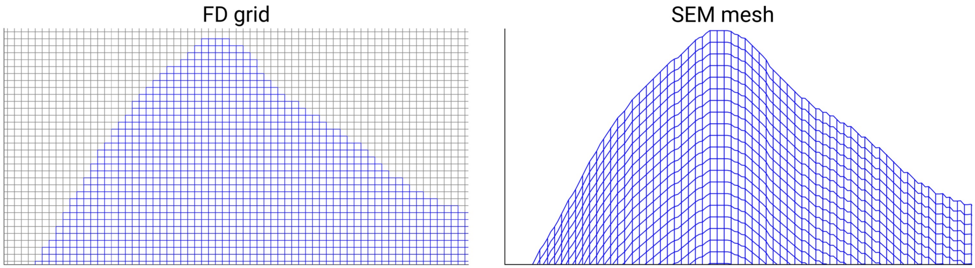


Figure 4: Qualitative comparison of the free surface in the FD model which is defined on a regular grid (left) and the SEM model which is defined on an irregular mesh (right). In the FD model grey represents vacuum grid-points.

Model

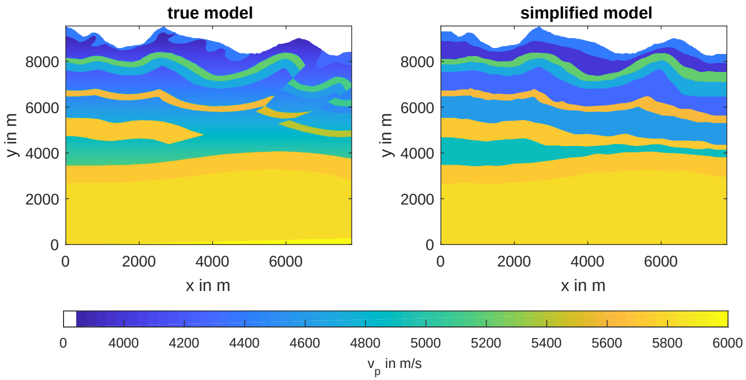


Figure 5: P-wave velocity structure of the simplified model (right) which is used. Models of S-wave velocity and mass density were derived by linear relations.

Full Mesh

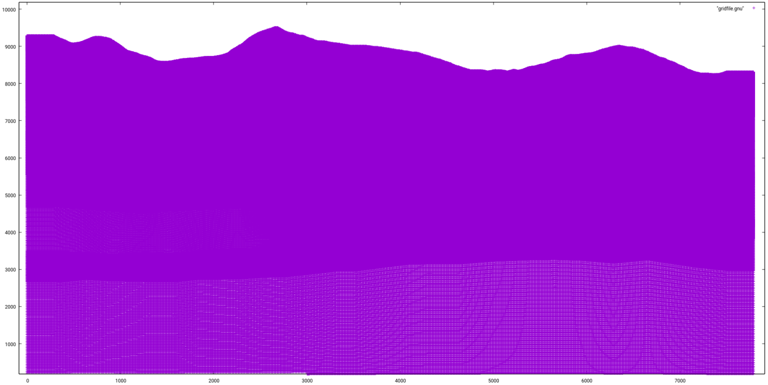


Figure 6: Full SEM mesh.

Mesh Zoom 1

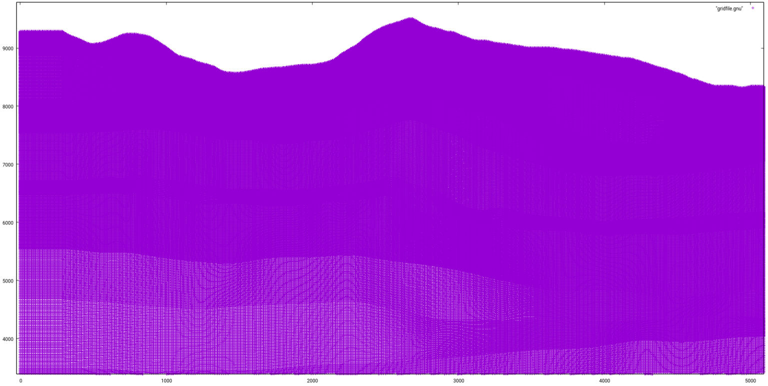


Figure 7: Zoomed SEM mesh.

Mesh Zoom 2

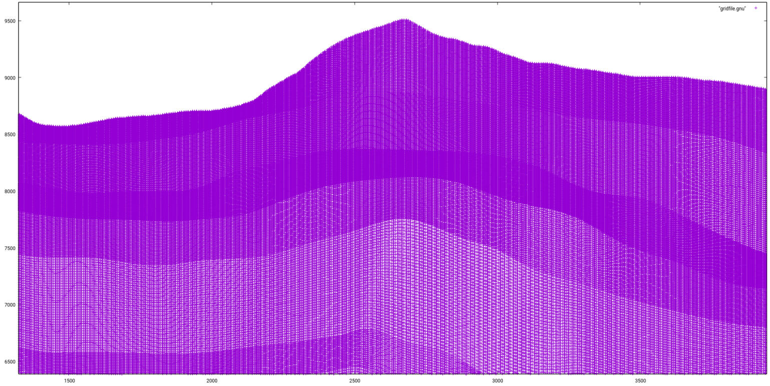


Figure 8: Zoomed SEM mesh.

Seismograms

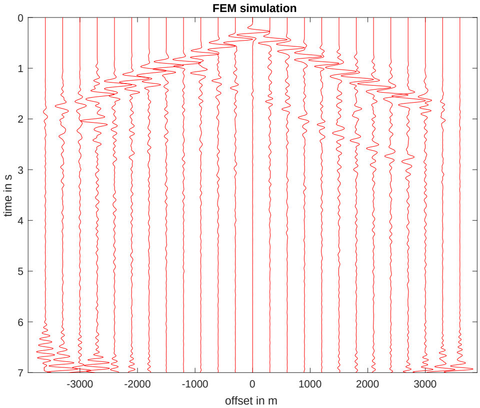
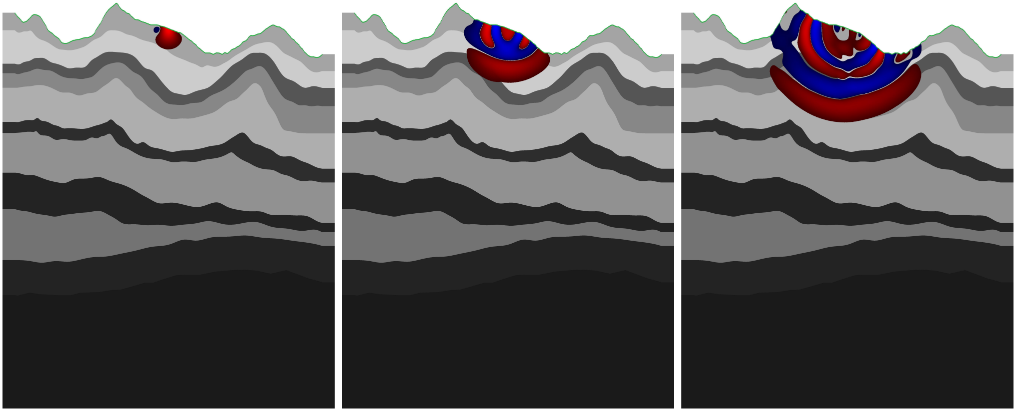
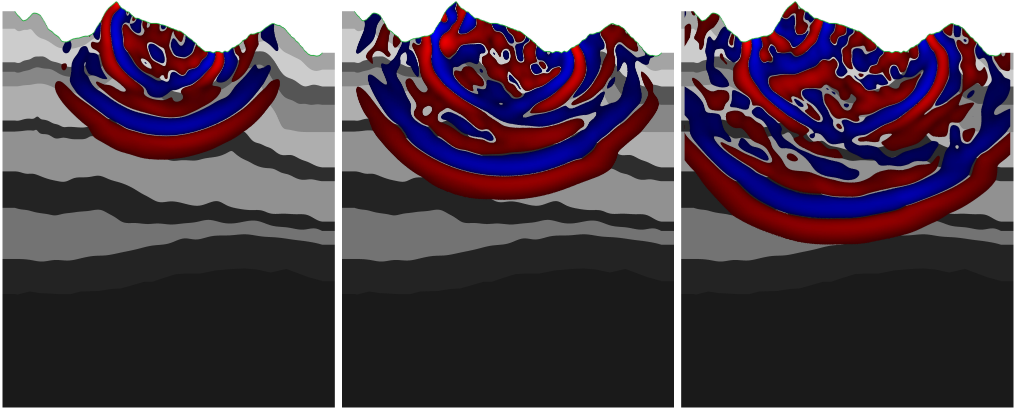


Figure 9: Seismograms obtained from SEM.

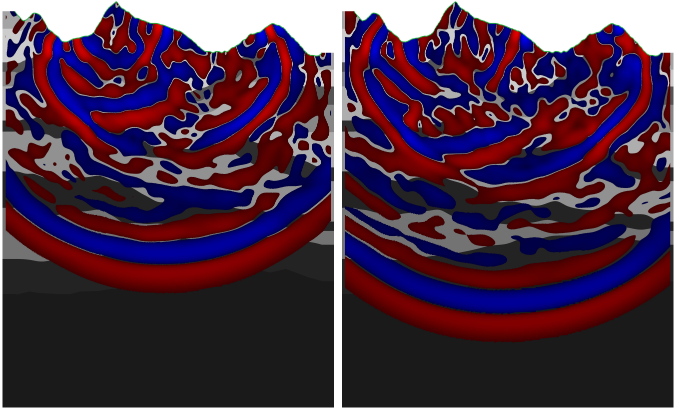
Wavefield at t = 0.2 s, 0.4 s, 0.6 s



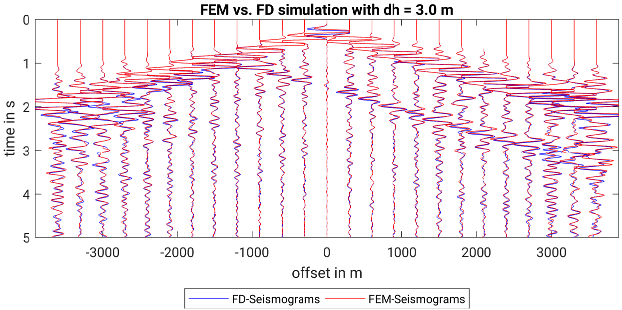
Wavefield at t = 0.8 s, 1.0 s, 1.2 s

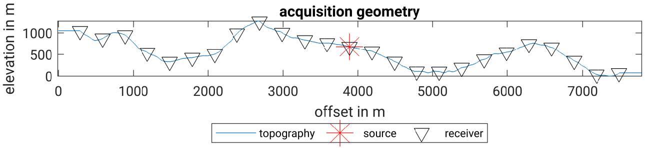


Wavefield at t = 1.4 s, 1.6 s



Seismogram comparisons





Agenda

1. Review of Finite Elements
2. Getting down to the element level
3. Spectral element method
   3.1 Lagrange polynomials
   3.2 Numerical integration
   3.3 Numerical differentiation
   3.4 Conclusions
4. Example
5. References

References

Igel, H. (2016), *Computational Seismology: A Practical Introduction*, 1. edn, Oxford University Press.
URL: *https://global.oup.com/academic/product/computational-seismology-9780198717409?cc=de&lang=en&*

Komatitsch, D. & Vilotte, J. P. (1998), 'The spectral-element method: an efficient tool to simulate the seismic response of 2D and 3D geological structures', *bssa* **88**(2), 368–392.

Krieger, D. (2019), 2D elastic full-waveform inversion of land seismic data with topographic variations, Master's thesis, Karlsruhe Institute of Technology.
URL: *https://publikationen.bibliothek.kit.edu/1000094788*

Questions

1. What are the main improvements of the SEM compared to the FE method ?
2. What are the main advantages/disadvantages of SEM compared with the FD method ?
3. How can we increase the accuracy of the SEM ? How does this compare with the FD method ?
4. Let us discuss the important properties of the different ingredients of the SEM. a) Lagrange Polynomials, b) GLL points and integration. c) Numerical differentiation. How do these properties "work together" ?
5. Why does the mass matrix finally becomes diagonal and why is this important ?
6. Do we need to consider a CFL stability condition in the SEM ?

Questions

7 Do we also have numerical dispersion in the SEM ?

8 Boundary conditions: How can we implement the free surface with topography in SEM (and FD) ? Do we need to consider specific boundary conditions between neighboring elements in the SEM ?

9 Which of the three methods a) FD, b) Reflectivity method, c) SEM should/can be applied in the following scenarios: 1) Layered medium, 2) Alps, 3) Global Earth, 4) Earthquakes, 5) Shallow seismic, 6) Non-destructive testing of concrete, 7) Medical imaging.

10 Does it make sense to combine the two methods FD and SEM ? In which scenarios could this be beneficial ? How would you implement this ?