The Spectral-Element Method

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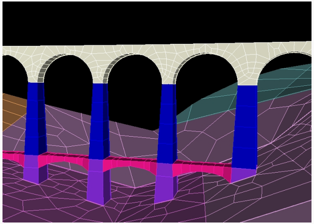
Introduction

Motivation

- High accuracy for wave propagation problems
- Flexibility with Earth model geometries
- Accurate implementation of boundary conditions
- Efficient parallelization possible



1-D elastic wave equation

$$\rho(x)\ddot{u}(x,t) = \partial_x\left[\mu(x)\partial_x u(x,t)\right] \; + \; f(x,t)$$

u displacement

f external force

ρ mass density

μ shear modulus

Boundary condition

No traction perpendicular to the Earth's free surface

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

normal vector n_j, σ_{ij} is the symmetric stress tensor

$$\mu \partial_x u(x, t)|_{x=0,L} = 0$$

where our spatial boundaries are at $x = 0, L$ and the stress-free condition applies at both ends

Spectral Element: Essentials

- Weak formulation of the wave equation
- Transformation to the elemental level (Jacobian)
- Approximation of unknown function u using Lagrange polynomials
- Evaluation of the 1st derivatives of the Lagrange polynomials
- Numerical integration scheme based on GLL quadrature
- Calculation of system matrices at elemental level
- Assembly of global system of equations
- Extrapolation in time using a simple finite-difference scheme

Galerkin Principle

- The underlying principle of the finite-element method
- Developed in context with structural engineering (Boris Galerkin, 1871-1945)
- Also developed by Walther Ritz (1909) - variational principle
- Conversion of a continuous operator problem (such as a differential equation) to a discrete problem
- Constraints on a finite set of basis functions

Weak Formulations

Multiplication of *pde* with test function $w(x)$ on both sides.

G is here the complete computational domain defined with $x \in G = [0, L]$.

$$\int_G w \, \rho \, \ddot{u} \, \mathrm{d}x \; - \int_G w \, \partial_x \left(\mu \, \partial_x u\right) \mathrm{d}x \; = \int_G w \, f \, \mathrm{d}x$$

Integration by parts

$$\int_a^b u v' dx \; = \; [uv]_a^b \; - \; \int_a^b u' v dx$$

Integration by parts

$$\int_G w \, \rho \, \ddot{u} \, \mathrm{d}x \; + \int_G \mu \, \partial_x w \, \partial_x \, u \, \mathrm{d}x = \int_G w \, f \, \mathrm{d}x$$

where we made use of the boundary condition

$$\partial_x u(x,t)|_{x=0} = \partial_x u(x,t)|_{x=L} = 0$$

Wow! **Free surface boundary condition for free**!

The approximate displacement field

$$u(x,t) \approx \overline{u}(x,t) = \sum_{i=1}^{n} u_i(t)\, \psi_i(x).$$

- Discretization of space introduced with this step
- Specific basis function not yet specified
- In principle basis functions defined on entire domain
  (-> PS method)
- Locality of basis functions lead to finite-element type method

Global system after discretization - Galerkin principle

Use approximation of u in weak form and (!) use the same basis function as test function

$$\int\limits_G \psi_i \rho \ddot{\overline{u}} \mathrm{d}x + \int\limits_G \mu \partial_x \psi_i \partial_x \overline{u} \mathrm{d}x = \int\limits_G \psi_i f \mathrm{d}x$$

with the requirement that the medium is at rest a t=0.

Including the function approximation for $u(x, t)$

... leads to an equation for the unknown coefficients $u_i(t)$

$$
\begin{aligned}
&\sum_{i=1}^{n}\left[\ddot{u}_i(t)\int_{G_e}\rho(x)\,\psi_j(x)\,\psi_i(x)\,\mathrm{d}x\right]\\
+&\sum_{i=1}^{n}\left[u_i(t)\int_{G_e}\mu(x)\,\partial_x\psi_j(x)\,\partial_x\psi_i(x)\,\mathrm{d}x\right]\\
=&\int_{G}\psi_i\,f(x,t)\,\mathrm{d}x
\end{aligned}
$$

for all basis functions ψ_j with $j = 1, ..., n$. This is the classical algebro-differential equation for **finite-element** type problems.

Matrix notation

This system of equations with the coefficients of the basis functions (meaning?!) as unknowns can be written in matrix notation

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

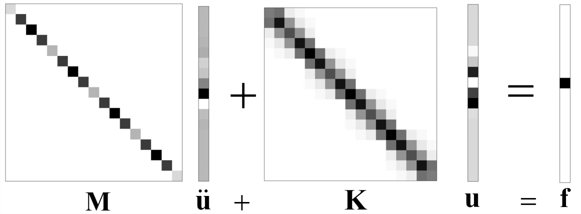
M Mass matrix

K Stiffness matrix

terminology originates from structural engineering problems

Matrix system graphically

The figure gives an actual graphical representation of the matrices for our 1D problem.



The unknown vector of coefficients **u** is found by a simple finite-difference procedure. The solution requires the inversion of mass matrix **M** which is trivial as it is diagonal. That is the key feature of the spectral element method.

Mass and stiffness matrix

Definition of the - at this point - global mass matrix

$$M_{ji} \; = \int\limits_{G} \rho(x) \; \psi_j(x) \; \psi_i(x) \; \mathrm{d}x$$

and the stiffness matrix

$$K_{ji} \; = \int\limits_{G} \mu(x) \; \partial_x \psi_j(x) \; \partial_x \psi_i(x) \; \mathrm{d}x$$

and the vector containing the volumetric forces $f(x, t)$

$$f_j(t) \; = \int\limits_{G} \psi_i \; f(x, t) \; \mathrm{d}x \quad .$$

Time extrapolation of coefficients

A simple centred finite-difference approximation of the 2nd derivative and the following mapping

$$\begin{aligned}
\mathbf{u}^{new} &\rightarrow \mathbf{u}(t + \mathrm{d}t) \\
\mathbf{u} &\rightarrow \mathbf{u}(t) \\
\mathbf{u}^{old} &\rightarrow \mathbf{u}(t - \mathrm{d}t)
\end{aligned}$$

leads us to the solution for the coefficient vector $\mathbf{u}(t + \mathrm{d}t)$ for the next time step as already well known from the other solution schemes in previous schemes.

Solution scheme

$$\mathbf{u}^{new} = \mathrm{d}t^2 \left[\mathbf{M}^{-1} \left(\mathbf{f} - \mathbf{K} \;\; \mathbf{u} \right) \right] + 2\mathbf{u} \; - \mathbf{u}^{old}$$

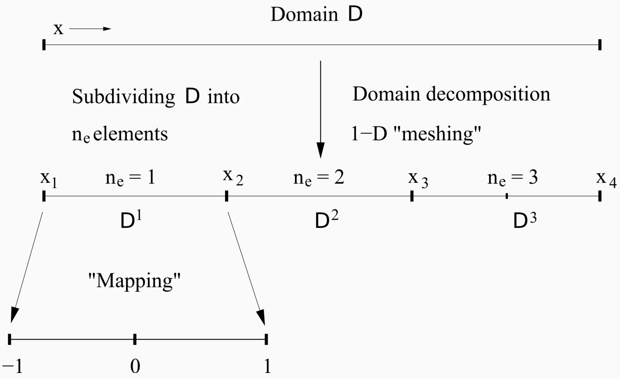
General solution scheme for finite-element method (wave propagation)

Independent of choice of basis functions

Mass matrix needs to be inverted!

To Do: good choice of basis function, integration scheme for calculation of M and K

Element level



In order to facilitate the calculation of the space-dependent integrals we transform each element onto the standard interval [-1,1], illustrated here for $n_e = 3$ elements. The elements share the boundary points.

System at element level

$$\sum_{i=1}^{n}\left[\ddot{u}_i(t)\sum_{e=1}^{n_e}\int_{G_e}\rho(x)\psi_j(x)\psi_i(x)\mathrm{d}x\right]$$
$$+\sum_{i=1}^{n}\left[u_i(t)\sum_{e=1}^{n_e}\int_{G_e}\mu(x)\partial_x\psi_j(x)\partial_x\psi_i(x)\mathrm{d}x\right]$$
$$=\sum_{e=1}^{n_e}\int_{G_e}\psi_j(x)f(x,t)\mathrm{d}x \quad .$$

Because of the sum over n_e there is a global dependence of the coefficients. How can we avoid this?

Local basis functions

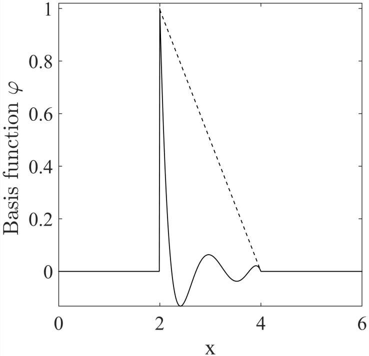


Illustration of local basis functions. By defining basis functions only inside elements the integrals can be evaluated in a local coordinate system. The graph assumes three elements of length two. A finite-element type linear basis function (dashed line) is shown along side a spectral-element type Lagrange polynomial basis function of degree N=5 (solid line).

u inside element

$$\overline{u}(x,t)|_{x\in G_e} = \sum_{i=1}^{n} u_i^e(t)\psi_i^e(x)$$

Now we can proceed with all calculations locally in G_e (inside one element)

Here is the difference to pseudospectral methods

Sum is now over all basis functions inside one element (n turns out to be the order of the polynomial scheme)

Local system of equations

$$
\begin{aligned}
&\sum_{i=1}^{n} \ddot{u}_i^e(t) \int\limits_{G_e} \rho(x)\psi_j^e(x)\psi_i^e(x)\mathrm{d}x \\
+&\sum_{i=1}^{n} u_i^e(t) \int\limits_{G_e} \mu(x)\partial_x\psi_j^e(x)\partial_x\psi_i^e(x)\mathrm{d}x \\
=&\int\limits_{G_e} \psi_j^e(x) f(x,t)\mathrm{d}x \quad .
\end{aligned}
$$

Matrix notation for local system

$$\mathbf{M}^e \cdot \ddot{\mathbf{u}}^e(t) + \mathbf{K}^e \cdot \mathbf{u}^e(t) \;=\; \mathbf{f}^e(t), \qquad e \;=\; 1, \ldots, n_e$$

Here $\mathbf{u}^e$, $\mathbf{K}^e$, $\mathbf{M}^e$, and $\mathbf{f}^e$ are the coefficients of the unknown displacement inside the element, stiffness and mass matrices with information on the density and stiffnesses, and the forces, respectively.

Coordinate transformation

$$F_e : [-1,1] \rightarrow G_e, \qquad x = F_e(\xi),$$
$$\xi = \xi(x) = F_e^{-1}(\xi), \qquad e = 1, \ldots, n_e$$

from our global system $x \in G$ to our local coordinates that we denote $\xi \in F_e$

$$x(\xi) = F_e(\xi) = \Delta e \frac{(\xi + 1)}{2} + x_e$$

where n_e is the number of elements, and $\xi \in [-1,1]$. Thus the physical coordinate x can be related to the local coordinate ξ via

$$\xi(x) = \frac{2(x - x_e)}{\Delta e} - 1$$

Integration of arbitrary function

$$\int_{G_e} f(x)\mathrm{d}x = \int_{-1}^{1} f^e(\xi)\frac{\mathrm{d}x}{\mathrm{d}\xi}\mathrm{d}\xi$$

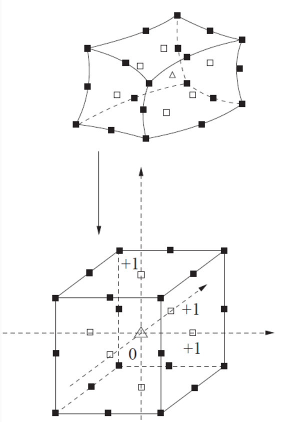
the integrand has to be multiplied by the Jabobian J before integration.

$$J = \frac{\mathrm{d}x}{\mathrm{d}\xi} = \frac{\Delta e}{2} \ .$$

we will also need

$$J^{-1} = \frac{\mathrm{d}\xi}{\mathrm{d}x} = \frac{2}{\Delta e} \ .$$

Skewed 3D elements



In 3D elements might be skewed and have curved boundaries. The calculation of the Jacobian is then carried out analytically by means of shape functions.

Assembly of system of equations

$$
\begin{aligned}
&\sum_{i=1}^{n} \ddot{u}_i^e(t) \int_{-1}^{1} \rho\left[x(\xi)\right] \psi_j^e\left[x(\xi)\right] \psi_i^e\left[x(\xi)\right] \frac{\mathrm{d}x}{\mathrm{d}\xi} \mathrm{d}\xi \\
&+ \sum_{i=1}^{n} u_i^e(t) \int_{-1}^{1} \mu\left[x(\xi)\right] \frac{\mathrm{d}\psi_j^e\left[x(\xi)\right]}{\mathrm{d}\xi} \frac{\mathrm{d}\psi_i^e\left[x(\xi)\right]}{\mathrm{d}\xi} \left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\right)^2 \frac{\mathrm{d}x}{\mathrm{d}\xi} \mathrm{d}\xi \\
&= \int_{-1}^{1} \psi_j^e\left[x(\xi)\right] f\left[(x(\xi)), t\right] \frac{\mathrm{d}x}{\mathrm{d}\xi} \mathrm{d}\xi \quad .
\end{aligned}
$$

System of n equations for each index j corresponding to one particular basis function. We need to find basis functions that allows efficient and accurate calculation of the required integrals.

Lagrange polynomials

Remember we seek to approximate $u(x,t)$ by a sum over space-dependent basis functions ψ_i weighted by time-dependent coefficients $u_i(t)$.

$$u(x,t) \;\approx\; \overline{u}(x,t) \;=\; \sum_{i=1}^{n} u_i(t)\,\psi_i(x)$$

Our final choice: Lagrange polynomials:

$$\psi_i \;\to\; \ell_i^{(N)} \;:=\; \prod_{k=1,\;k\neq i}^{N+1} \frac{\xi-\xi_k}{\xi_i-\xi_k}, \qquad i = 1,2,\ldots,N+1$$

where x_i are fixed points in the interval $[-1,1]$.

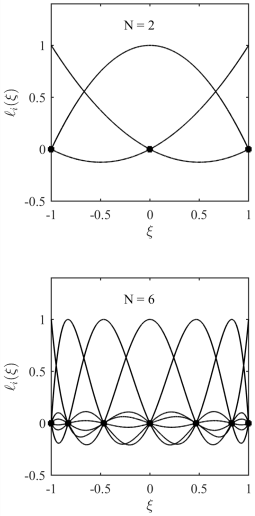
Orthogonality of Lagrange polynomials

$$\ell_{\mathbf{i}}^{(\mathbf{N})}(\xi_{\mathbf{j}}) = \delta_{\mathbf{ij}}$$

They fulfill the condition that they *exactly* interpolate (or approximate) the function

at N+1 collocation points. Compare with discrete Fourier series on regular grids or Chebyshev polynomials on appropriate grid points (-> pseudospectral method).

Lagrange polynomials graphically



Top: Family of $N + 1$ Lagrange polynomials for $N = 2$ defined in the interval $\xi \in [-1, 1]$. Note their maximum value in the whole interval does not exceed unity.

Bottom: Same for $N = 6$. The domain is divided into N intervals of uneven length. When using Lagrange polynomials for function interpolation the values are exactly recovered at the collocation points (squares).

Gauss-Lobatto-Legendre points

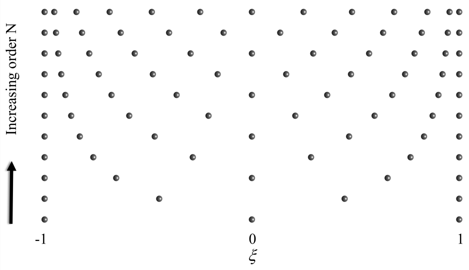


Illustration of the spatial distribution of Gauss-Lobatto-Legendre points in the interval [-1,1] from top to bottom for polynomial order 2 to 12 (from left to right). Note the increasing difference of largest to smallest interval between collocation points! Consequences?

Lagrange polynomials: some properties

Mathematically the collocation property is expressed as

$$\ell_i^{(N)}(\xi_i) = 1 \;\text{ and }\; \dot{\ell}_i^{(N)}(\xi_i) \;=\; 0$$

where the dot denotes a spatial derivative. The fact that

$$|\ell_i^{(N)}(\xi)| \leq 1, \qquad \xi \in [-1, 1]$$

minimizes the interpolation error in between the collocation points due to numerical inaccuracies.

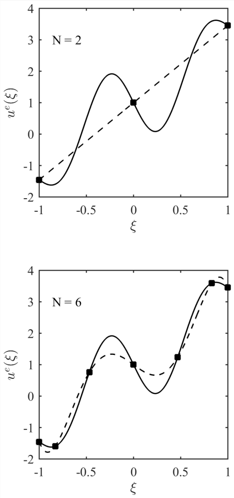
Function approximation

This is the final mathematical description of the unknown field $u(x, t)$ for the spectral-element method based on Lagrange polynomials.

$$u^e(\xi) = \sum_{i=1}^{N+1} u^e(\xi_i)\ell_i(\xi)$$

Other options at this point are the Chebyhev polynomials. They have equally good approximation properties (but ...)

Interpolation with Lagrange Polynomials



The function to be approximated is given by the solid lines. The approximation is given by the dashed line exactly interpolating the function at the GLL points (squares). **Top:** Order $N = 2$ with three grid points. **Bottom:** Order $N = 6$ with seven grid points.

Spectral-element system with basis functions

Including the Legendre polynomials in our local (element-based) system leads to

$$\sum_{i=1}^{N+1} \ddot{u}_i^e(t) \int_{-1}^{1} \rho(\xi)\ell_j(\xi)\ell_i(\xi)\frac{\mathrm{d}x}{\mathrm{d}\xi}\mathrm{d}\xi$$

$$+ \sum_{i,k=1}^{N+1} u_i^e(t) \int_{-1}^{1} \mu(\xi)\dot{\ell}_j(\xi)\dot{\ell}_i(\xi)\left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\right)^2 \frac{\mathrm{d}x}{\mathrm{d}\xi}\mathrm{d}\xi$$

$$= \int_{-1}^{1} \ell_j(\xi) f(\xi, t)\frac{\mathrm{d}x}{\mathrm{d}\xi}\mathrm{d}\xi$$

Because we want that ρ, μ, and f vary inside one element there is no way out carrying out the integration numerically.

Integration scheme for an arbitrary function $f(x)$

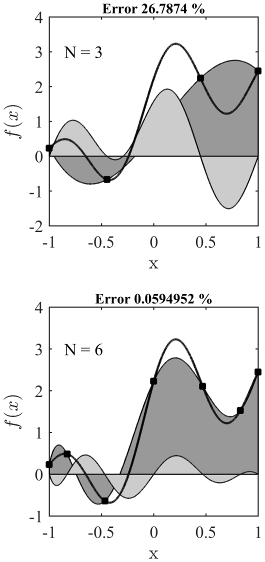
$$\int_{-1}^{1} f(x)\mathrm{d}x \approx \int_{-1}^{1} P_N(x)\mathrm{d}x = \sum_{i=1}^{N+1} w_i f(x_i)$$

defined in the interval $x \in [-1, 1]$ with

$$P_N(x) = \sum_{i=1}^{N+1} f(x_i)\ell_i^{(N)}(x)$$

$$w_i = \int_{-1}^{1} \ell_i^{(N)}(x)\mathrm{d}x \quad .$$

Numerical integration scheme



- Exact function (thick solid line)
- Approximation by Lagrange polynomials (thin solid line)
- Difference between true and approximate function (light gray)

Collocation points and integration weights

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	$1/10$

Collocation points and integration weights of the Gauss-Lobatto-Legendre quadrature for order $N = 2, \dots, 4$.

After integration

With the numerical integration scheme we obtain

$$
\begin{aligned}
&\sum_{i,k=1}^{N+1} \ddot{u}_i^e(t) w_k \rho(\xi) \ell_j(\xi) \ell_i(\xi) \frac{\mathrm{d}x}{\mathrm{d}\xi}\bigg|_{\xi=\xi_k} \\
&+ \sum_{i,k=1}^{N+1} w_k u_i^e(t) \mu(\xi) \ell_j(\xi) \ell_i(\xi) \left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\right)^2 \frac{\mathrm{d}x}{\mathrm{d}\xi}\bigg|_{\xi=\xi_k} \\
&\approx \sum_{i,k=1}^{N+1} w_k \ell_j(\xi) f(\xi, t) \frac{\mathrm{d}x}{\mathrm{d}\xi}\bigg|_{\xi=\xi_k}
\end{aligned}
$$

What is still missing is a formulation for the derivative of the Lagrange polynomials at the collocation points. But: Major progress! We have replaced the integrals by sums!

cont'd...

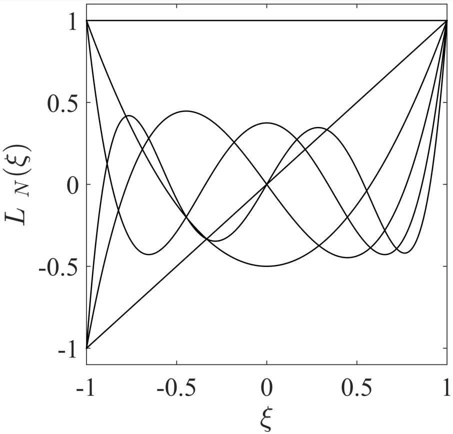
Solution equation for our spectral-element system at the element level

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

with

$$\begin{aligned}
M_{ji}^{e} &= w_j \rho(\xi) \frac{\mathrm{d}x}{\mathrm{d}\xi} \delta_{ij} \Big|_{\xi=\xi_j} \\
K_{ji}^{e} &= \sum_{k=1}^{N+1} w_k \mu(\xi) \ell_j(\xi) \ell_i(\xi) \left(\frac{\mathrm{d}\xi}{\mathrm{d}x} \right)^2 \frac{\mathrm{d}x}{\mathrm{d}\xi} \Big|_{\xi=\xi_k} \\
f_j^{e} &= w_j f(\xi, t) \frac{\mathrm{d}x}{\mathrm{d}\xi} \Big|_{\xi=\xi_j}
\end{aligned}$$

Illustration of Legendre Polynomials



The Legendre polynomials are used to calculate the first derivatives of the Legendre polynomials. They can also be used to calculate the integration weights of the GLL quadrature.

$$\dot{\ell}(\xi_i) = \sum_{j=1}^{N} \tilde{d}_{ij}^{(1)} \ell(\xi_j)$$

$$\partial_x u^e(\xi) = \sum_{i=1}^{N+1} u^e(\xi_i) \dot{\ell}_i(\xi)$$

Global Assembly and Solution

Global Assembly for the diagonal of the mass matrix

$$\mathbf{M}_g = \begin{pmatrix} M_{1,1}^{(1)} \\ M_{2,2}^{(1)} \\ M_{3,3}^{(1)} \\ \\ \\ \\ \\ \end{pmatrix} + \begin{pmatrix} \\ \\ M_{1,1}^{(2)} \\ M_{2,2}^{(2)} \\ M_{3,3}^{(2)} \\ \\ \\ \end{pmatrix} + \begin{pmatrix} \\ \\ \\ \\ M_{1,1}^{(3)} \\ M_{2,2}^{(3)} \\ M_{3,3}^{(3)} \end{pmatrix} = \begin{pmatrix} M_{1,1}^{(1)} \\ M_{2,2}^{(1)} \\ M_{3,3}^{(1)} + M_{1,1}^{(2)} \\ M_{2,2}^{(2)} \\ M_{3,3}^{(2)} + M_{1,1}^{(3)} \\ M_{2,2}^{(3)} \\ M_{3,3}^{(3)} \end{pmatrix}$$

Global Assembly for the diagonal of the stiffness matrix

$$
\mathbf{K}_g = \begin{pmatrix}
K^{(1)}_{1,1} & K^{(1)}_{1,2} & K^{(1)}_{1,3} & & & & \\
K^{(1)}_{2,1} & K^{(1)}_{2,2} & K^{(1)}_{2,3} & & & \mathbf{0} & \\
K^{(1)}_{3,1} & K^{(1)}_{3,2} & K^{(1)}_{3,3} + K^{(2)}_{1,1} & K^{(2)}_{1,2} & K^{(2)}_{1,3} & & \\
 & & K^{(2)}_{2,1} & K^{(2)}_{2,2} & K^{(2)}_{2,3} & & \\
 & & K^{(2)}_{3,1} & K^{(2)}_{3,2} & K^{(2)}_{3,3} + K^{(3)}_{1,1} & K^{(3)}_{1,2} & K^{(3)}_{1,3} \\
 & \mathbf{0} & & & K^{(3)}_{2,1} & K^{(3)}_{2,2} & K^{(3)}_{2,3} \\
 & & & & K^{(2)}_{3,1} & K^{(2)}_{3,2} & K^{(2)}_{3,3}
\end{pmatrix}
$$

Vector with information on the source

$$\mathbf{f}_g = \begin{pmatrix} f_1^{(1)} \\ f_2^{(1)} \\ f_3^{(1)} + f_1^{(2)} \\ f_2^{(2)} \\ f_3^{(2)} + f_1^{(3)} \\ f_2^{(3)} \\ f_3^{(3)} \end{pmatrix}$$

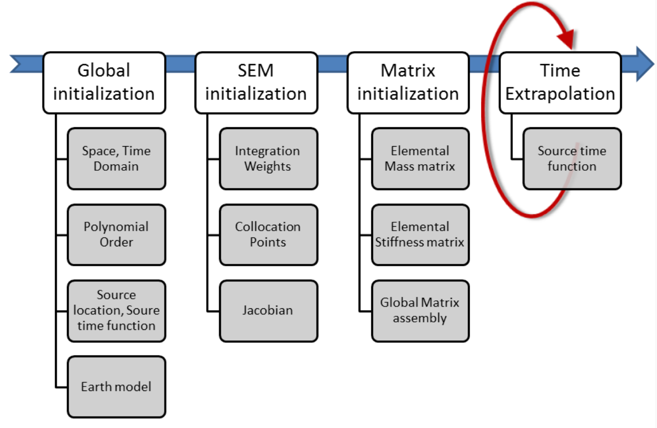
Extrapolation for time-dependent coefficients $\mathbf{u}_g$

This is our final algorithm as it is implemented using Matlab or Python

$$\mathbf{u}_g(t+\mathrm{d}t) \; = \mathrm{d}t^2 \left[\mathbf{M}_g{}^{-1} \left(\mathbf{f}_g(t) - \mathbf{K}_g \;\; \mathbf{u}_g(t)\right) \right] \\ + 2\mathbf{u}_g\mathbf{(t)} \; - \mathbf{u}_g(t-\mathrm{d}t)$$

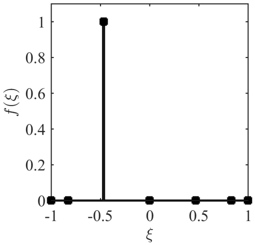
Looks fairly simple, no?

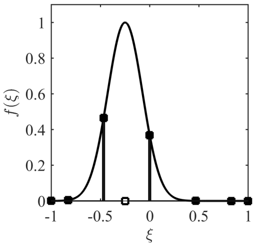
Spectral elements: work flow



A substantial part consists of preparing the interpolation and integration procedures required to initialize the global mass- and stiffness matrices. The final time-extrapolation is extremely compact and does not require the inversion of a global matrix as is the case in classic finite-element methods.

Point source initialization

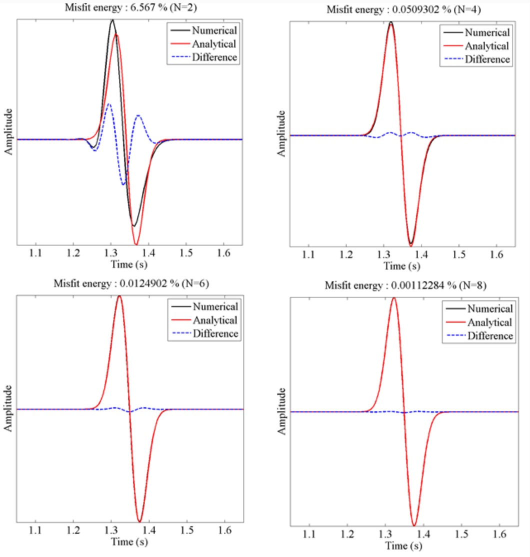




Top: A point-source polynomial representation (solid line) of a δ-function (red bar).

Bottom: A finite-source polynomial representation (solid line) as a superposition of point sources injected at some collocation points. For comparison with analytical solutions it is important to note that the spatial source function actually simulated is the polynomial representation of the (sum over) δ-function(s).

sem1d: simulation examples



Summary

- The spectral element method combines the flexibility of finite-element methods concerning computational meshes with the spectral convergence of Lagrange basis functions used inside the elements.
- The enormous success of the spectral element method is based upon the diagonal structure of the mass matrix that needs to be inverted to extrapolate the system in time. Due to this diagonality no matrix inversion techniques need to be employed allowing straight forward parallelisation of the algorithm. The diagonal mass matrix is possible through the coincidence of the collocation points of both interpolation and integration schemes (Gauss-Lobatto-Legendre).

Summary

- The errors of the spectral-element scheme accumulate from the (usually low-order finite-difference) time extrapolation scheme and the numerical integration using Gauss-Lobatto-Legendre quadrature.
- The spectral-element method is particularly useful for simulation problems where the free-surface plays an important role, and/or in which surface waves need to be accurately modelled. Technically the reason is that the free-surface boundary is implicitly solved.
- A well engineered community code (SPECFEM3D, www.geodynamics.org) is available for Cartesian and spherical geometries including global Earth (or planetary scale) calculations.