The Spectral-Element Method: Introduction

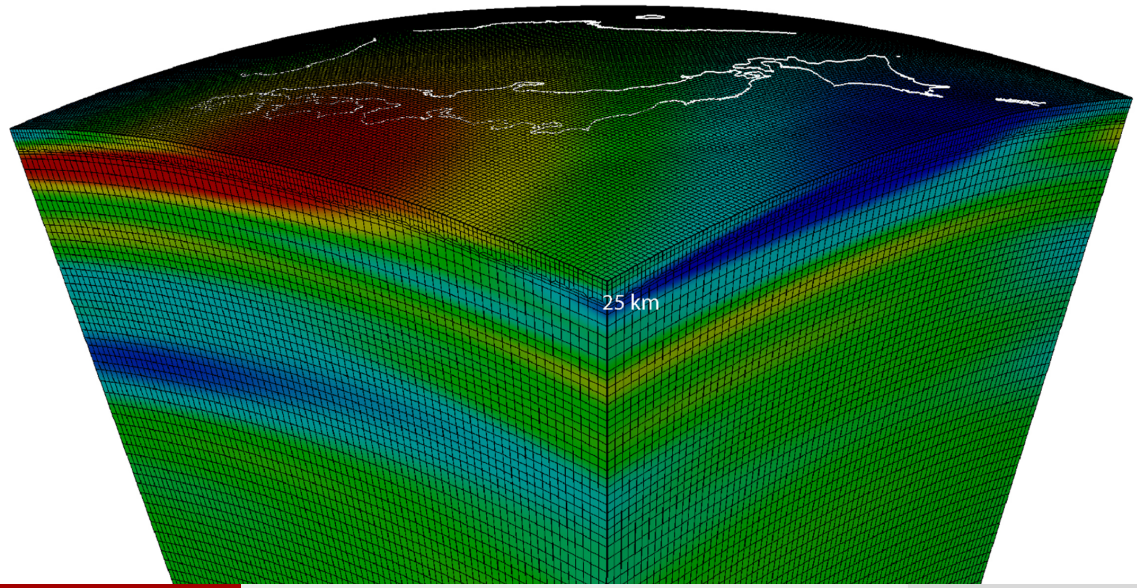
Heiner Igel

Department of Earth and Environmental Sciences
Ludwig-Maximilians-University Munich

Outline

Motivation

- High accuracy for wave propagation problems (exact interpolation)
- Flexibility with Earth model geometries (cubed sphere, curved elements)
- Accurate implementation of boundary conditions (implicit)
- Efficient parallelization possible (explicit time integration)



History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

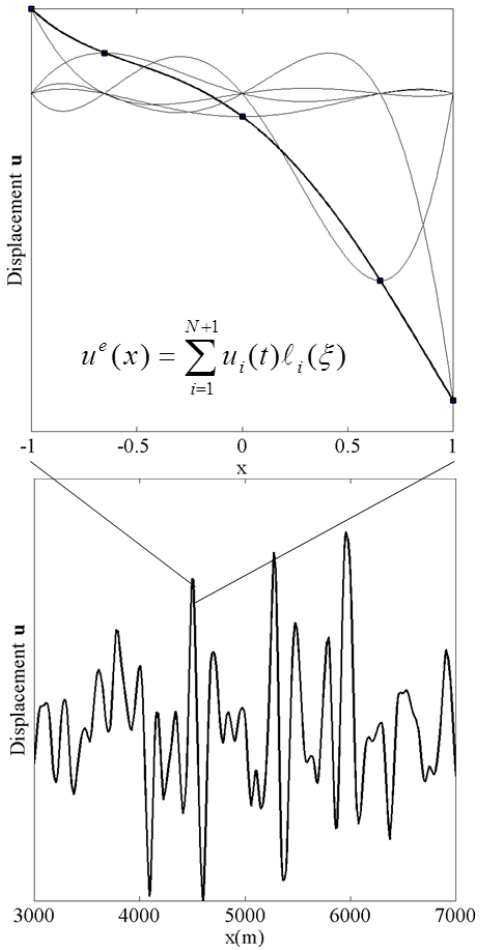
History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

History

- Originated in fluid dynamics (Patera, 1984, Maday and Patera, 1989)
- First applications to seismic wave propagation by Priolo, Carcione and Seriani, 1994)
- Initial concepts around Chebyshev polynomials (Faccioli, Maggio, Quarteroni and Tagliani, 1996)
- Use of Lagrange polynomials (diagonal mass matrix) by Komatitsch and Vilotte (1998)
- Application to spherical geometry using the cubed sphere concept (Chaljub and Vilotte, 2004)
- Global wave simulations using axisymmetry (Nissen-Meyer et al. (2007)
- Spectral elements in spherical coordinates by Fichtner et al. (2009)
- Community code "specfem" widely used for simulaton and inversion (e.g., Peter et al. 2011).
- After 2017 Salvus revolutionizes computational seismology

Spectral Elements in a Nutshell



Ingredients:

- Exact interpolation with Lagrange polynomials
- Numerical Integration (Gauss-Lobatto-Legendre)
- Weak formulation of wave equation
- Time extrapolation using finite-differences

Elastic wave propagation

1-D elastic wave equation

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

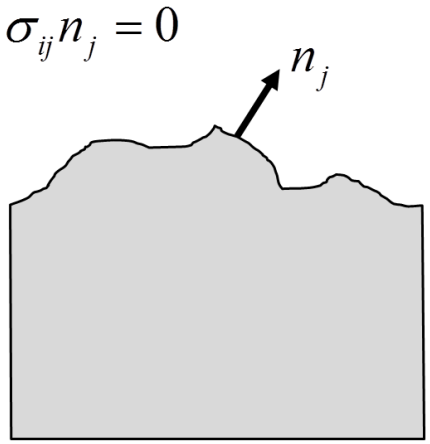
u displacement

f external force

ρ mass density

μ shear modulus

Boundary condition



traction-free surface

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

$\sigma_{ij} \rightarrow$ symmetric stress tensor

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

boundaries are at $x = 0, L$

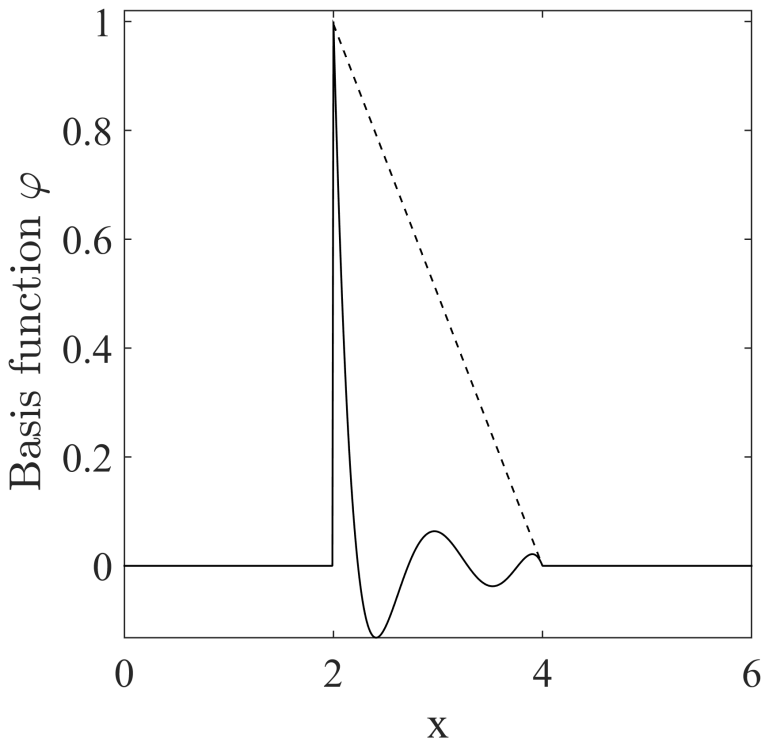
Discretizing the wave field

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

Local basis functions



- 3 elements (length 2)
- Local basis functions defined inside element only
- Linear basis function (dashed)
- Lagrange basis function (solid)

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:

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

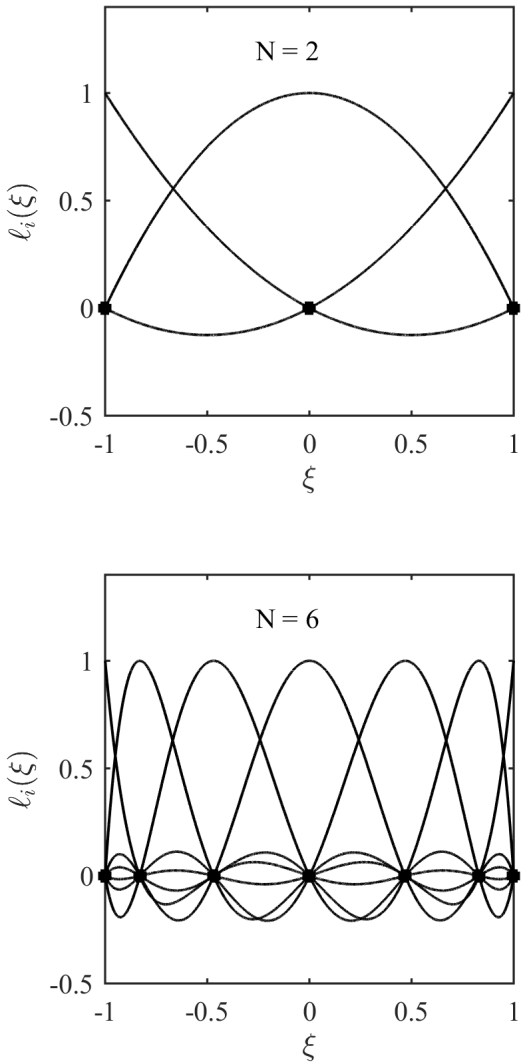
where x_i are fixed points in the interval $[-1, 1]$.

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

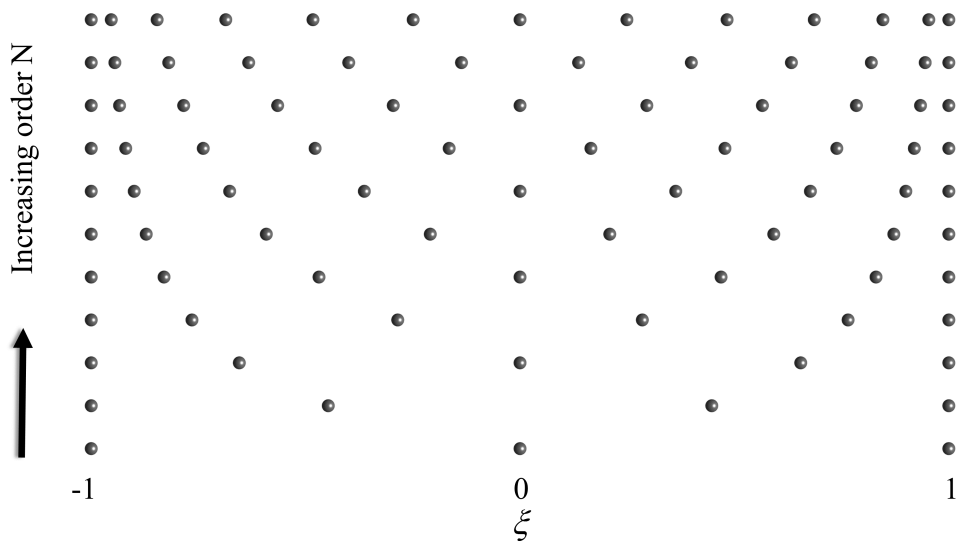


Illustration of the spatial distribution of Gauss-Lobatto-Legendre points in the interval [-1,1] from top to bottom for polynomial order 2 to 12 (from left to right). Note the increasing difference of largest to smallest interval between collocation points! Consequences?

Lagrange polynomials: some properties

Mathematically the collocation property is expressed as

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

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.

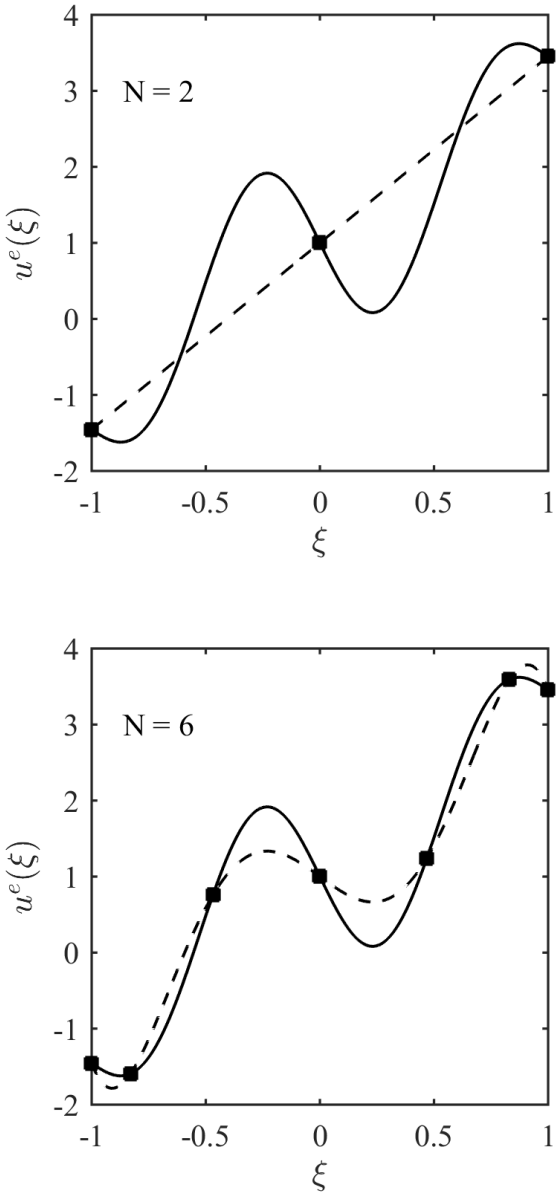
Function approximation

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

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

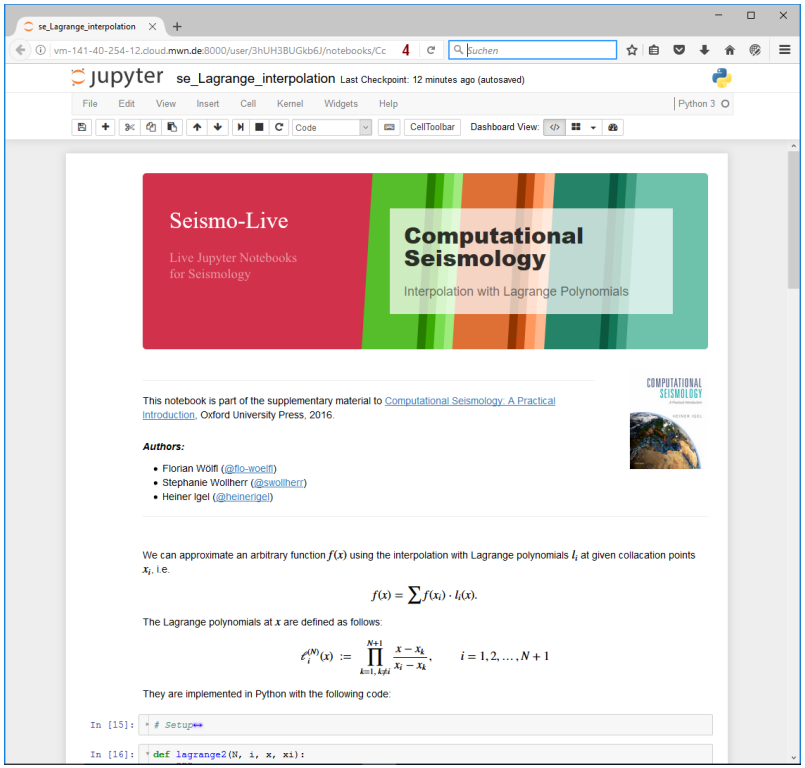
Other options at this point are the Chebyhev polynomials. They have equally good approximation properties (but ...)

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.

Exercise: Lagrange Interpolation



- Visualize Lagrange polynomials
- Interpolate arbitrary function using Lagrange polynomials
- Understand benefit of GLL points (Runge phenomenon)

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

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

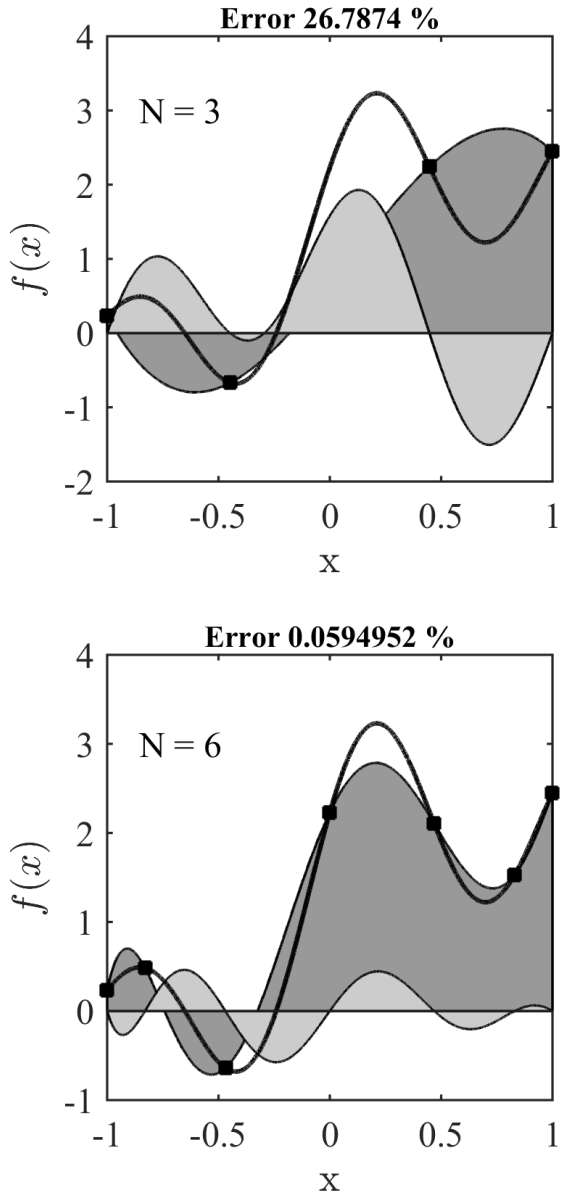
$$w_i = \int_{-1}^{1} \ell_i^{(N)}(x)\mathrm{d}x \quad .$$

Collocation points and integration weights

N	ξ_i	w_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

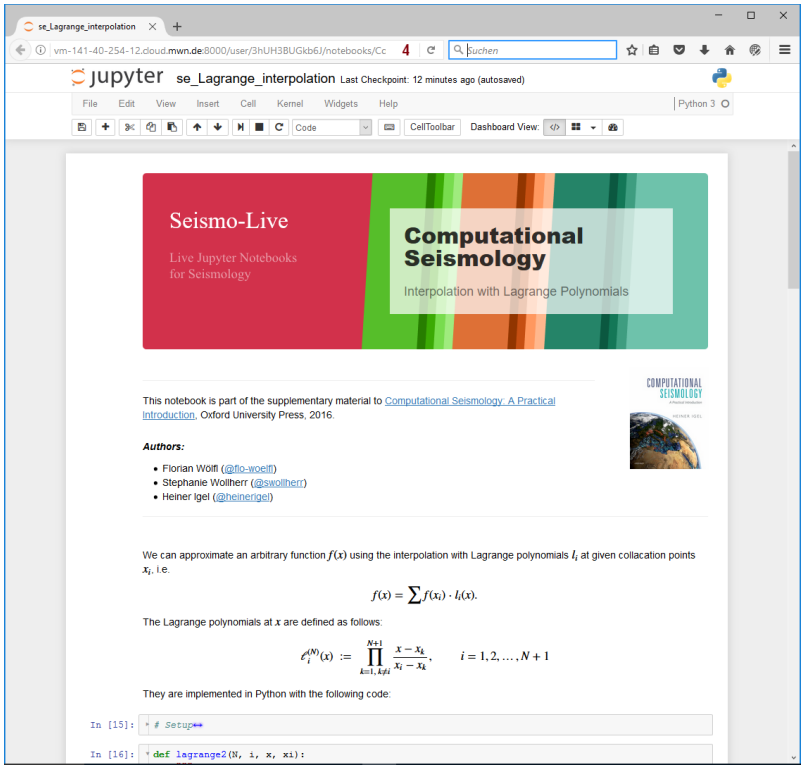
Collocation points and integration weights of the Gauss-Lobatto-Legendre quadrature for order $N = 2, \ldots, 4$.

Numerical integration scheme



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

Exercise: Numerical integration



- Appreciate simple GLL quadrature rule
- Numerically integrate arbitrary function
- Understand that this is one source of error in SEM

Weak Form of the Elastic Equation

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

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

where we made use of the boundary condition

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

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

Use approximation of u in weak form and (!) use the same basis function as test function, $w \rightarrow \psi_i$

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

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 $u_i(t)$

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

for all basis functions ψ_j with $j = 1, \ldots, n$. 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

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

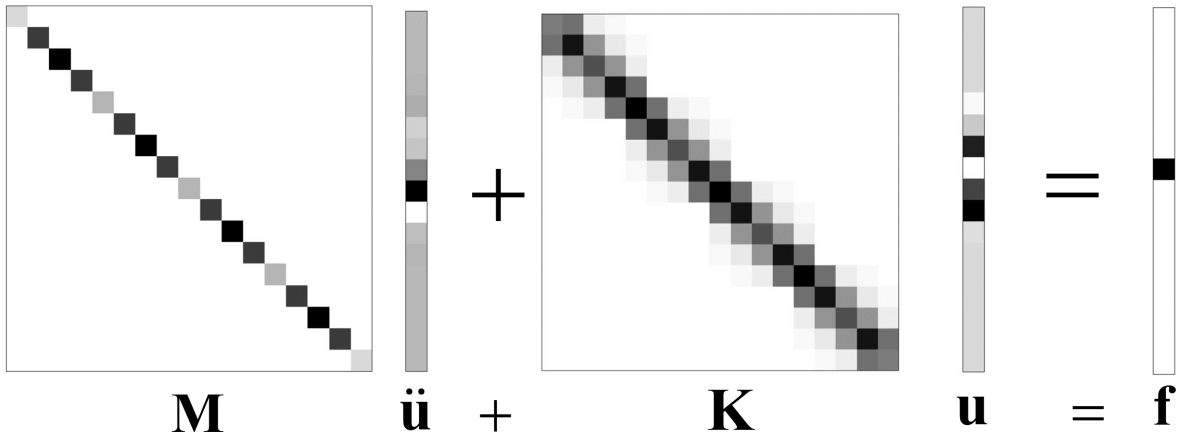
M Mass matrix

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

$$M_{ji} = \int_G \rho(x)\, \psi_j(x)\, \psi_i(x)\, \mathrm{d}x$$

and the stiffness matrix

$$K_{ji} = \int_G \mu(x)\, \partial_x \psi_j(x)\, \partial_x \psi_i(x)\, \mathrm{d}x$$

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

$$f_j(t) = \int_G \psi_i\, f(x, t)\, \mathrm{d}x \quad .$$

Mapping

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)

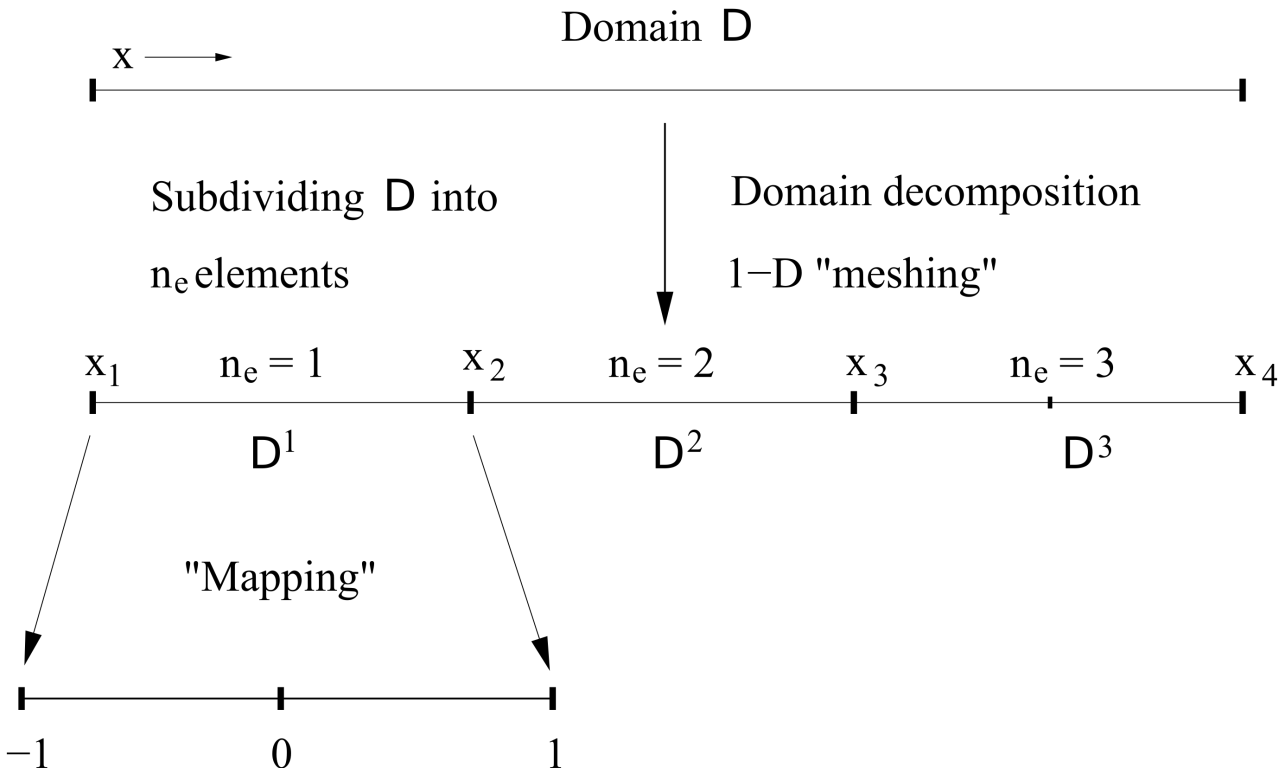
Independent of choice of basis functions

Mass matrix needs to be inverted!

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

Getting Down to the Element Level

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

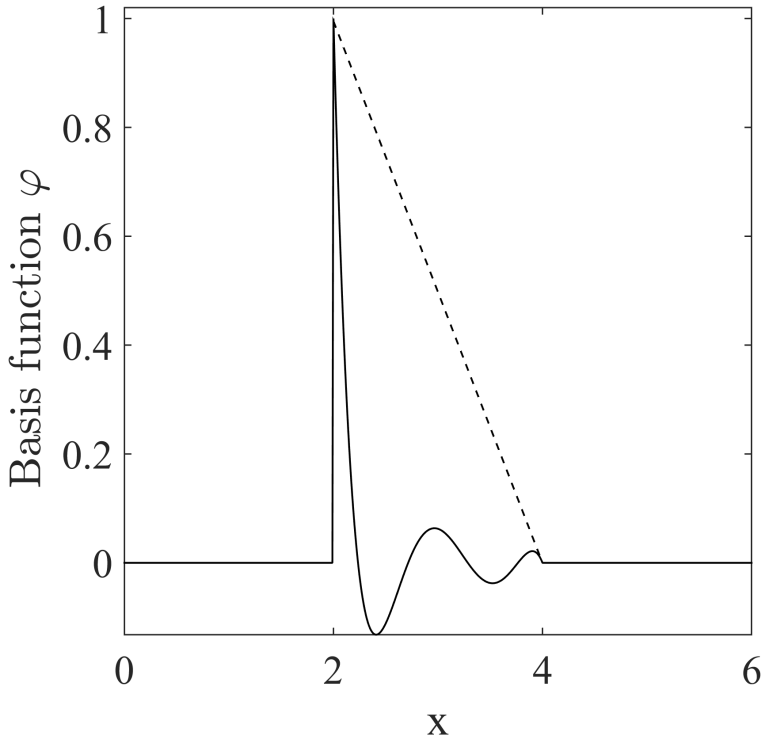


Illustration of local basis functions. By defining basis functions only inside elements the integrals can be evaluated in a local coordinate system. The graph assumes three elements of length two. A finite-element type linear basis function (dashed line) is shown along side a spectral-element type Lagrange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

$$\sum_{i=1}^{n} \ddot{u}_i^e(t) \int_{G_e} \rho(x)\psi_j^e(x)\psi_i^e(x)\mathrm{d}x$$

$$+ \sum_{i=1}^{n} u_i^e(t) \int_{G_e} \mu(x)\partial_x\psi_j^e(x)\partial_x\psi_i^e(x)\mathrm{d}x$$

$$= \int_{G_e} \psi_j^e(x) f(x,t)\mathrm{d}x \quad .$$

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 $\xi \in F_e$

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

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

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

Integration of arbitrary function

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

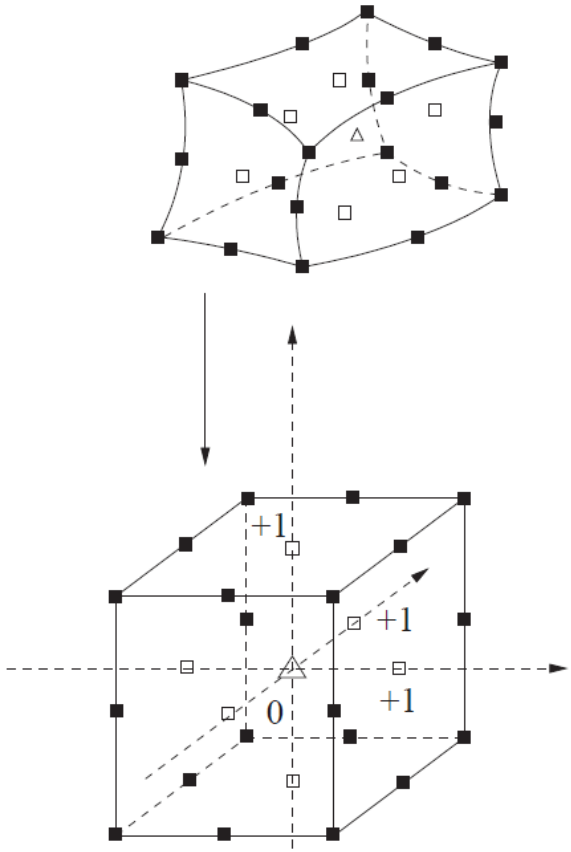
the integrand has to be multiplied by the Jabobian J before integration.

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

we will also need

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

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

$$\sum_{i=1}^{n} \ddot{u}_i^e(t) \int_{-1}^{1} \rho\left[x(\xi)\right] \psi_j^e\left[x(\xi)\right] \psi_i^e\left[x(\xi)\right] \frac{\mathrm{d}x}{\mathrm{d}\xi} \mathrm{d}\xi$$

$$+ \sum_{i=1}^{n} u_i^e(t) \int_{-1}^{1} \mu\left[x(\xi)\right] \frac{\mathrm{d}\psi_j^e\left[x(\xi)\right]}{\mathrm{d}\xi} \frac{\mathrm{d}\psi_i^e\left[x(\xi)\right]}{\mathrm{d}\xi} \left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\right)^2 \frac{\mathrm{d}x}{\mathrm{d}\xi} \mathrm{d}\xi$$

$$= \int_{-1}^{1} \psi_j^e\left[x(\xi)\right] f\left[(x(\xi)), t\right] \frac{\mathrm{d}x}{\mathrm{d}\xi} \mathrm{d}\xi \quad .$$

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.

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.

With the numerical integration scheme we obtain

$$\sum_{i,k=1}^{N+1} \ddot{u}_i^e(t) w_k \rho(\xi) \ell_j(\xi) \ell_i(\xi) \frac{\mathrm{d}x}{\mathrm{d}\xi}\bigg|_{\xi=\xi_k}$$

$$+ \sum_{i,k=1}^{N+1} w_k u_i^e(t) \mu(\xi) \ell_j(\xi) \ell_i(\xi) \left(\frac{\mathrm{d}\xi}{\mathrm{d}x}\right)^2 \frac{\mathrm{d}x}{\mathrm{d}\xi}\bigg|_{\xi=\xi_k}$$

$$\approx \sum_{i,k=1}^{N+1} w_k \ell_j(\xi) f(\xi, t) \frac{\mathrm{d}x}{\mathrm{d}\xi}\bigg|_{\xi=\xi_k}$$

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!

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

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

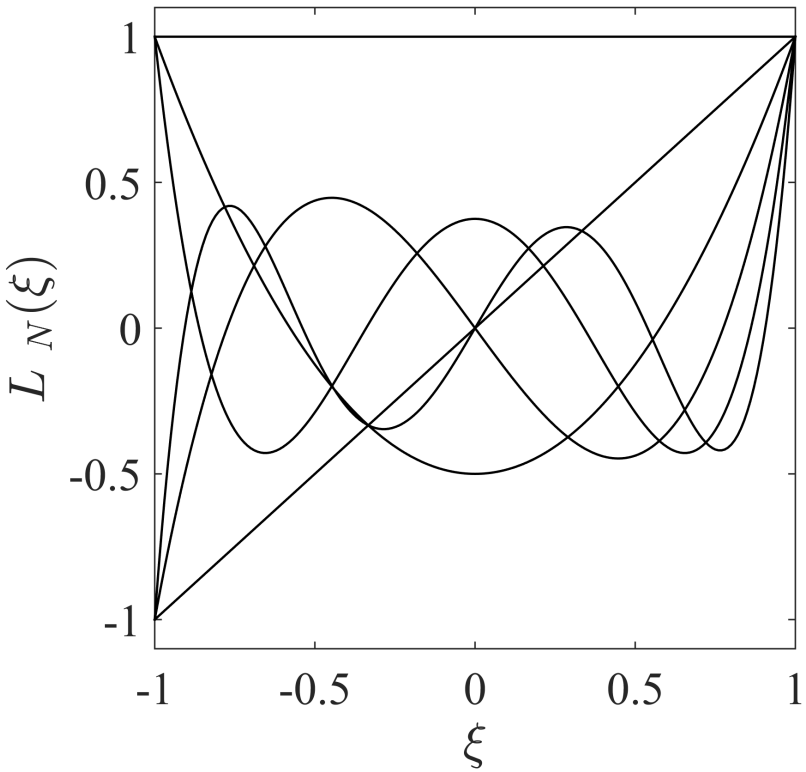
with

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

$$K_{ji}^e = \sum_{k=1}^{N+1} w_k \mu(\xi) \ell_j(\xi) \ell_i(\xi) \left(\frac{\mathrm{d}\xi}{\mathrm{d}x} \right)^2 \frac{\mathrm{d}x}{\mathrm{d}\xi} \Big|_{\xi=\xi_k}$$

$$f_j^e = w_j f(\xi, t) \frac{\mathrm{d}x}{\mathrm{d}\xi} \Big|_{\xi=\xi_j}$$

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

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

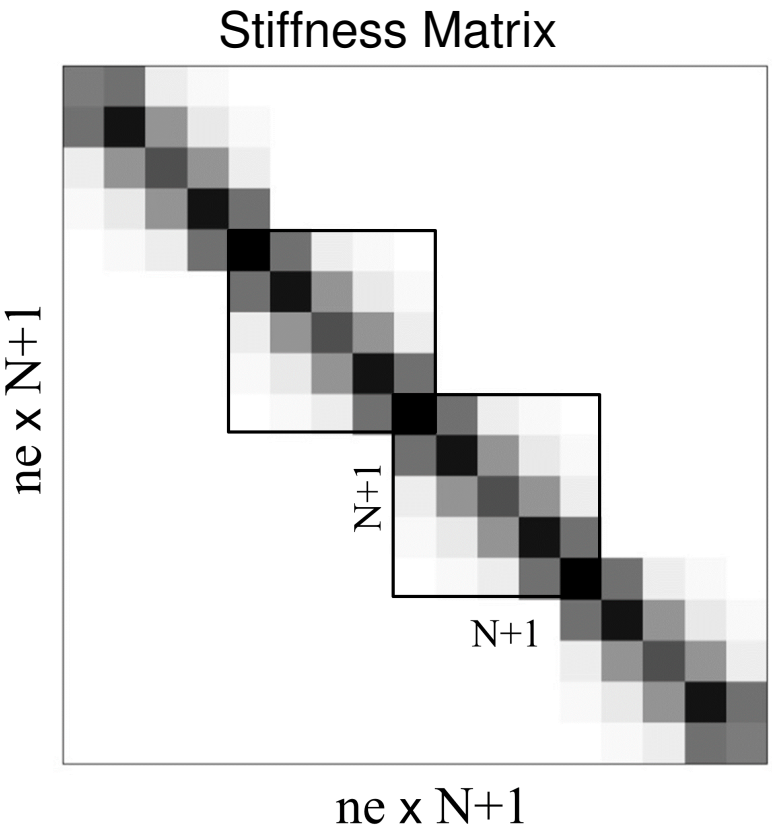
Global Assembly for the diagonal of the stiffness matrix

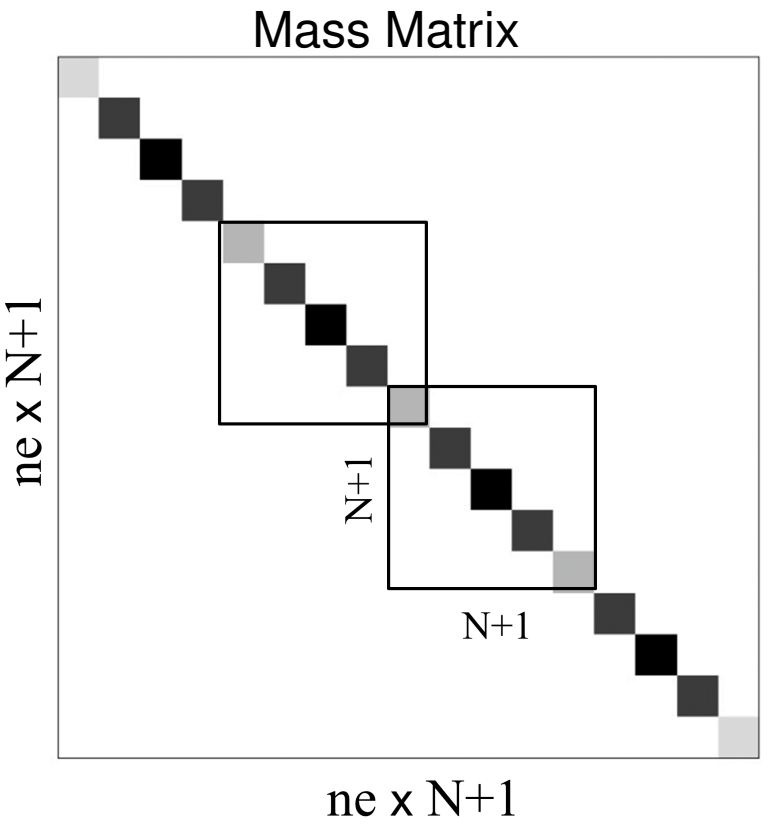
$$\mathbf{K}_g = \begin{pmatrix} K_{1,1}^{(1)} & K_{1,2}^{(1)} & K_{1,3}^{(1)} & & & & \\ K_{2,1}^{(1)} & K_{2,2}^{(1)} & K_{2,3}^{(1)} & & & \mathbf{0} & \\ K_{3,1}^{(1)} & K_{3,2}^{(1)} & K_{3,3}^{(1)} + K_{1,1}^{(2)} & K_{1,2}^{(2)} & K_{1,3}^{(2)} & & \\ & & K_{2,1}^{(2)} & K_{2,2}^{(2)} & K_{2,3}^{(2)}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

Vector with information on the source

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

Global assembly graphically





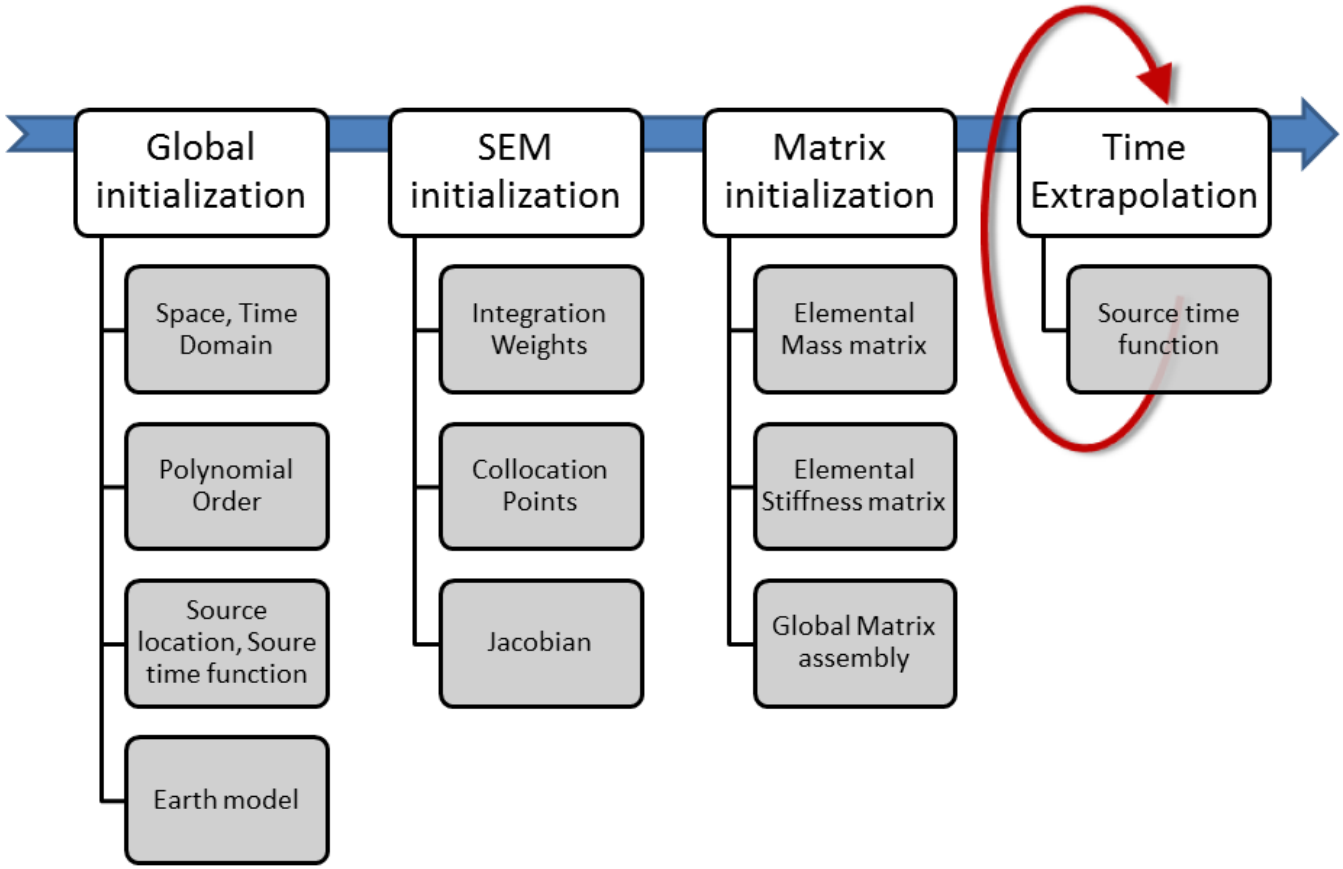
Extrapolation for time-dependent coefficients $\mathbf{u}_g$

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

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

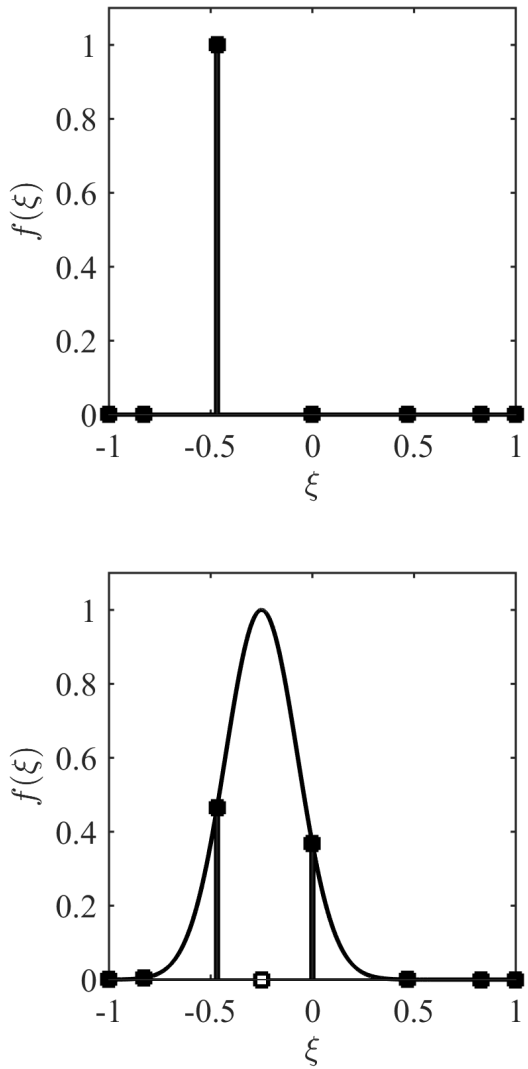
Looks fairly simple, no?

Spectral elements: work flow



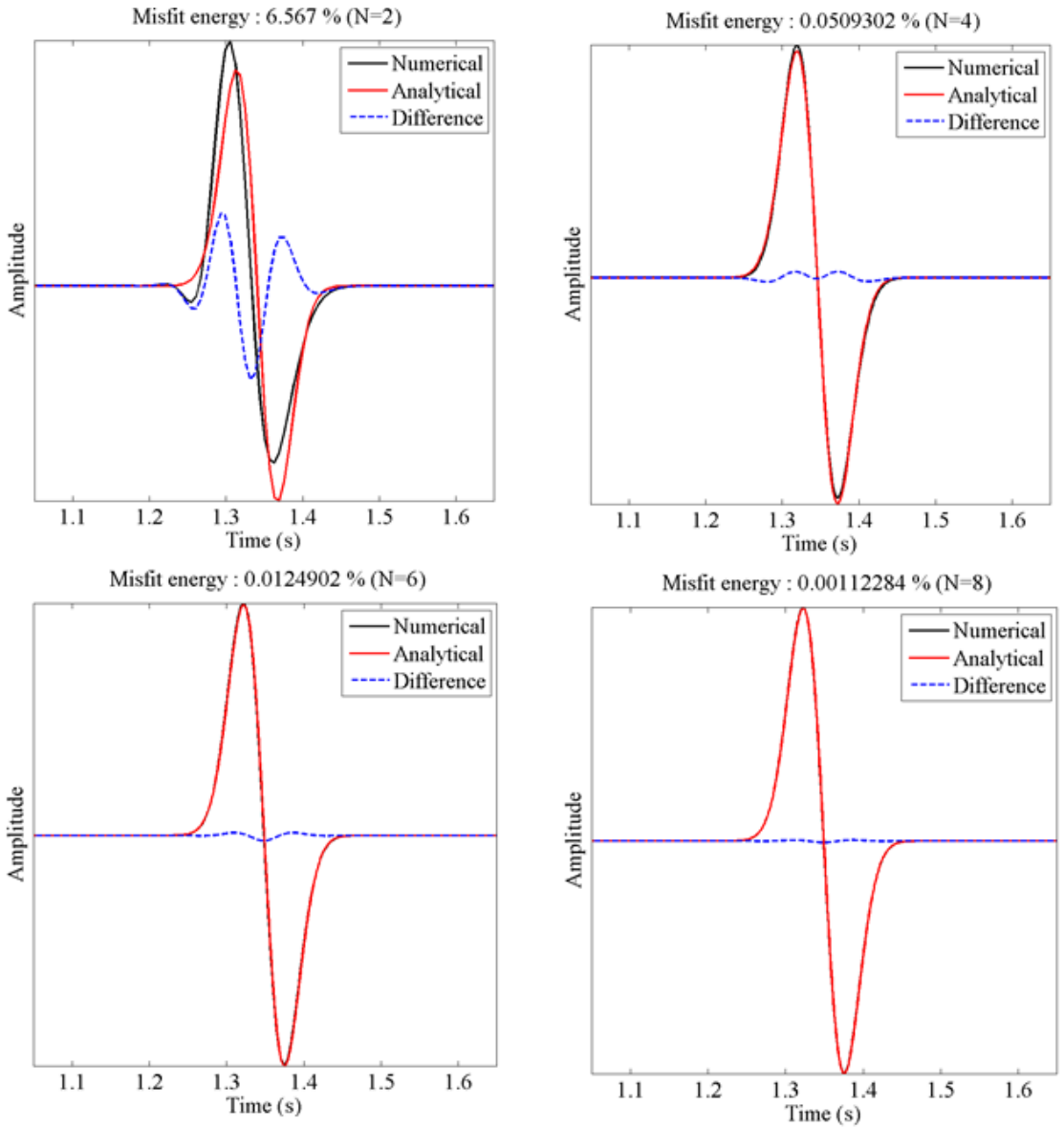
A substantial part consists of preparing the interpolation and integration procedures required to initialize the global mass- and stiffness matrices. The final time-extrapolation is extremely compact and does not require the inversion of a global matrix as is the case in classic finite-element methods.

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).

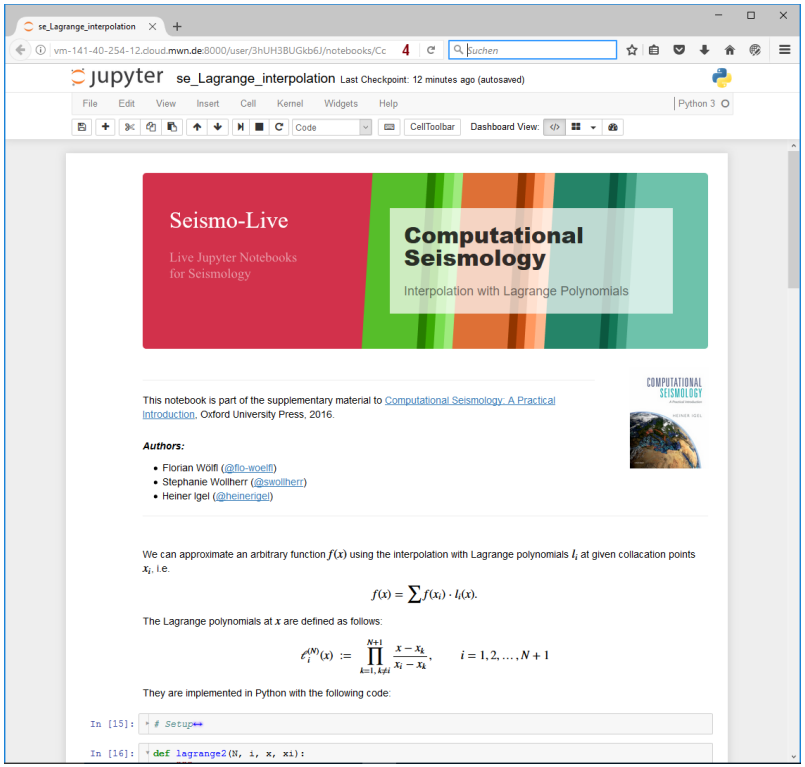
Simulation examples: Varying order N



Summary

- Geometrical flexibility as with finite-element method
- Spectral convergence of Lagrange basis functions (exact interpolation)
- Diagonal structure of the mass matrix (there is a price to pay!)
- No global system matrix inversion necessary
- Errors from numerical integration and time extrapolation
- The spectral-element method is particularly useful where free surface boundaries are important
- Applications in all domains of general and applied elastic wave propagation problems

Exercise: 1D Elastic wave equation with spectral elements



- Calculation of local mass and stiffness matrices
- Global assembly of mass and stiffness matrices
- Time extrapolation scheme
- Influence of polynomial order on accuracy