The Finite Element Method

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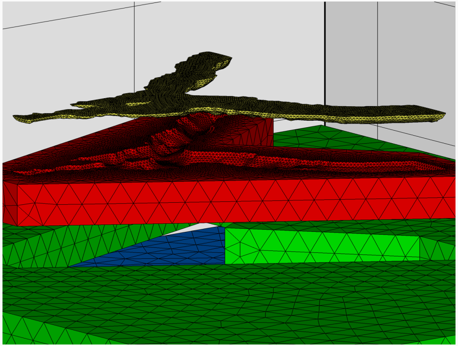
Introduction

Motivation



- Static and time-dependent PDEs
- Arbitrary geometry
- Originated in structrual engineering

History

- As the free-surface boundary condition is implicitly fulfilled study of surface wave propagation (Lysmer 1972, Schlue 1979).
- Seismic scattering problems were simulated with the method in the dissertation by Day (1977).
- In addition to the physical propagation modes, parasitic modes for high-order implementations were found Kelly (1990).
- Li (1994) presented parallel implementations on the legendary CM-2 massively parallel supercomputer.
- Finite-element principles are also the basis for the so-called direct solution method that was introduced by R. Geller and co-workers.
- Problems in seismic shaking hazards and engineering seismology were conducted by the group of J. Bielak and co-workers.
- The methods were later extended to the problem of full waveform inversion (Askan 2008).
- Hybrid methods that make use of advantages of both finite-difference and finite-element methods were presented by Moczo (2010).

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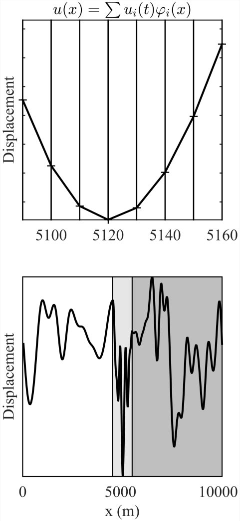
Finite Elements in a Nutshell



1D elastic wave equation with space-dependent density ρ, shear modulus μ, and forcing term $f(x,t)$

$$\rho\partial_t^2 u = \partial_x \, \mu \, \partial_x u + f \ .$$

We seek to find solutions to the displacement field $u(x,t)$, thus, we replace it by a finite sum over (here at first linear) basis functions φ_i. Our unknowns are the coefficients of the basis functions φ_i

$$u(x) \approx \overline{u}(x) = \sum_{i=1}^{N} u_i(t)\varphi_i(x) \ .$$

Finite Elements in a Nutshell

Furthermore, we formulate a so-called *weak* form of the wave equation, multiplying the original strong form by a test function φ_j of the same basis, followed by an integration over the entire physical domain. This leads to a linear system of equations of the form

$$\int_D \rho\, \partial_t^2\, \overline{u}\, \varphi_j\, dx + \int_D \mu\, \partial_x\, \overline{u}\, \partial_x\, \varphi_j\, dx = \int_D f\, \varphi_j\, dx$$

where we seek to find the approximate displacement field $\overline{u}$. Given appropriate initial conditions, the solution at the next time step $\mathbf{u}(t + dt)$ can be found by the following matrix-vector equation

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

where $\mathbf{M}$ and $\mathbf{K}$ are the mass matrix and stiffness matrix, respectively.

Finite Elements in a Nutshell

- Global matrices in the sense that if a physical domain is discretized with N elements, then the matrix sizes is $N \times N$.
- One of the matrices has to be inverted.
- Mass matrix $\mathbf{M}$ consists of elements of the form $\int_D \rho\varphi_i\varphi_j dx$ and the stiffness matrix $\mathbf{K}$ is built up with elements of the form $\int_D \mu\nabla\varphi_i\nabla\varphi_j dx$.
- These integrals can be computed in an elegant way for each element by mapping the physical space to a local reference space.

Static Elasticity

Discretization

Departing from the 1D elastic wave equation

$$\rho \partial_t^2 u(x,t) = \partial_x \mu(x) \partial_x u(x,t) + f(x,t)$$

we assume the following:

- Independent in time: $\partial_t^2 u(x,t) = 0$
- Elastic properties of our 1D medium are independent of space: $\mu(x) = \text{const.}$

that leads to the equation

$$-\mu \partial_x^2 u \;= f \;.$$

Illustration

Static elasticity. A string with homogeneous properties (density and shear modulus) is pulled with a certain force. The Poisson equation determines the displacement of the string given appropriate boundary conditions. Don't overdo this experiment, in particular if you have old strings.

Weak form

Transform *strong* form into *weak* form by multiplying the equation with an arbitrary space-dependent test function that we denote as $v \rightarrow v(x)$. Then we integrate the equation on both sides over the entire physical domain D with $x \in D$

$$-\int_D \mu \partial_x^2 \, u \; v \; dx = \int_D f \; v \; dx \; .$$

Performing an integration by parts of the left side:

$$-\int_D \mu \partial_x^2 \, u \; v \; dx = \int_D \mu \; \partial_x \; u \; \partial_x \; v \; dx - [\mu \partial_x u \; v]_{x_{min}}^{x_{max}} \; .$$

where the last term is an anti-derivative.

Free surface

Free-surface condition $\Longrightarrow$ No stress at the boundaries.

As the anti-derivative is evaluated at the domain boundaries this implies that this term vanishes.

$$\mu \int_D \partial_x \, u \, \partial_x \, v \, dx = \int f \, v \, dx$$

which is still a description in the continuous world. To enter the discrete world we replace our exact solution $u(x)$ by a $\overline{u}$, a sum over some basis functions φ_i that we do not yet specify

$$u \approx \overline{u}(x) = \sum_{i=1}^{N} u_i \varphi_i \, .$$

Replacing u by $\overline{u}$, we obtain

$$\mu \int_D \partial_x \, \overline{u} \, \partial_x \, v \, dx = \int f \, v \, dx$$

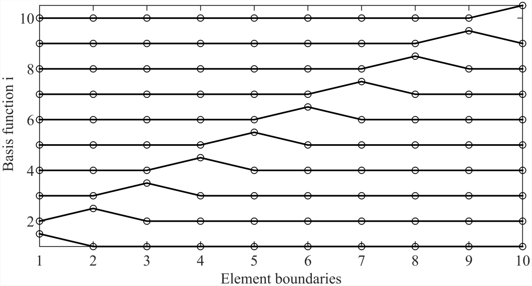
Basis functions

As a choice for our test function $v(x)$ we use the same set of basis functions. Thus $v(x) \rightarrow \varphi_j(x)$.

What is the simplemost choice for our basis functions φ_i? Denoting $x_i, i = 1, 2, ..., N$ as the boundaries of our elements we define our basis functions such that $\varphi_i = 1, x = x_i$ and zero elsewhere. Inside the elements our solution field is described by a linear function:

$$\varphi_i(x) = \begin{cases} \frac{x - x_{i-1}}{x_i - x_{i-1}} & \text{for } x_{i-1} < x \leq x_i \\ \frac{x_{i+1} - x}{x_{i+1} - x_i} & \text{for } x_i < x < x_{i+1} \\ 0 & \text{elsewhere} \end{cases}$$

Basis functions



Linear basis functions for the finite-element method. A 1D domain is discretized with $n - 1$ elements having $n = 10$ element boundaries (open circles). The basis functions $\varphi_i = 1$ at $x = x_i$. With this basis an arbitrary function can be exactly interpolated at the element boundary points x_i.

Galerkin Principle

We are ready to assemble our discretized version of the weak form by replacing the continuous displacement field by its approximation and applying the Galerkin principle. We obtain

$$\mu \int_D \partial_x \left(\sum_{i=1}^{N} u_i \varphi_i \right) \partial_x \, \varphi_j \, dx = \int f \, \varphi_j \, dx$$

$$\sum_{i=1}^{N} u_i \int_D \mu \, \partial_x \, \varphi_i \, \partial_x \, \varphi_j \, dx = \int f \, \varphi_j \, dx$$

which is a system of N equations as we project the solution on the basis functions φ_j with $j = 1, ..., N$. In the second equation we switched the sequence of integration and sum.

Matrix-Vector Notation

The discrete system thus obtained can be written using matrix-vector notation. Defining the solution vector **u** as

$$\mathbf{u} = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{pmatrix}$$

the source vector **f** as

$$\mathbf{f} = \begin{pmatrix} \int_D f \, \varphi_1 \, dx \\ \int_D f \, \varphi_2 \, dx \\ \vdots \\ \int_D f \, \varphi_N \, dx \end{pmatrix}$$

Matrix-Vector Notation

and the matrix containing the integral over the basis function derivatives as **K**

$$\mathbf{K} \rightarrow K_{ij} = \mu \int_D \partial_x \, \varphi_i \, \partial_x \, \varphi_j$$

Solution

System of equations can be written in component form as

$$u_i \, K_{ij} = f_j$$

where we use the Einstein summation convention and in matrix-vector notation

$$\mathbf{K}^T \, \mathbf{u} = \mathbf{f}$$

Note: Matrix **K** is called the it stiffness matrix.
This system of equations has as many unknowns as equations. Provided that the matrix is positive definite we can determine its inverse:

$$\mathbf{u} = (\mathbf{K}^T)^{-1}\mathbf{f}$$

Boundary Conditions

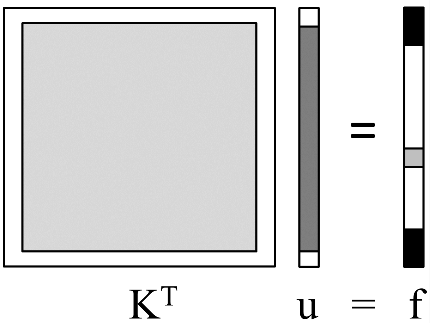
In case you would like to invoke specific values at the boundaries the approximate solution becomes

$$\bar{u} \;=\; u_1\varphi_1 + \sum_{i=2}^{N-1} u_i\varphi_i \;+\; u_N\varphi_N$$

where u_1 and u_N are the boundary values. The weak form becomes

$$\begin{aligned}\sum_{i=2}^{N-1} \mu \int_D \partial_x\, \varphi_i\, \partial_x\, \varphi_j\, dx = \int_D f\, \varphi_j\, dx \\ + u(x_{min}) \int_D \partial_x\, \varphi_1\, \partial_x\, \varphi_j\, dx \\ + u(x_{max}) \int_D \partial_x\, \varphi_N\, \partial_x\, \varphi_j\, dx\end{aligned}$$

Boundary Conditions



Graphical representation of the matrix-vector system with boundary conditions. The global system matrix has $N-2 \times N-2$ elements. The system *feels* the boundary conditions through a modified source terms. The red spot indicates the source location inside the medium.

Reference Element, Mapping

Mapping the physical domain to a reference element. In our case we center the local coordinate system denoted as ξ at point x_i and obtain

$$\xi = x - x_i$$

$$h_i = x_i - x_{i-1}$$

where h_i denotes the size of element i defined in the interval $x \in [x_i, x_{i+1}]$. The local basis functions becomes

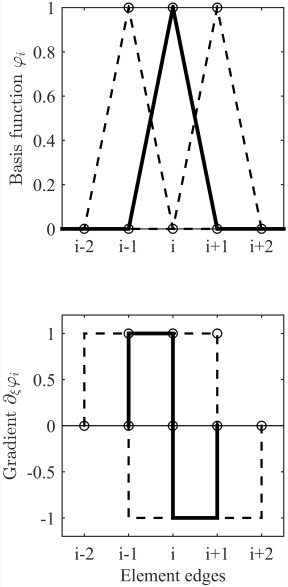
$$\varphi_i(\xi) = \begin{cases} \frac{\xi}{h} + 1 & \text{for } -h < \xi \leq 0 \\ 1 - \frac{\xi}{h} & \text{for } 0 < \xi < h \\ 0 & \text{elsewhere} \end{cases}$$

Reference Element, Mapping

and their derivatives

$$\partial_\xi \, \varphi_i(\xi) = \begin{cases} \frac{1}{h} & \text{for } -h < \xi \leq 0 \\ -\frac{1}{h} & \text{for } 0 < \xi < h \\ 0 & \text{elsewhere} \end{cases}$$

Reference Element, Mapping



Basis functions and their derivatives. **Top:** The basis function φ_i (thick solid line) is shown along with the neighboring functions $\varphi_{i\pm1}$ (thin dotted lines). **Bottom:** The same for their derivatives with respect to the space coordinate ξ.

Stiffness Matrix

We can now proceed with calculating the elements of the stiffness matrix K defined as

$$K_{ij} = \mu \int_D \partial_x \varphi_i \, \partial_x \, \varphi_j \, dx$$

with the corresponding expression in local coordinates ξ

$$K_{ij} = \mu \int_{D_\xi} \partial_\xi \varphi_i \, \partial_\xi \varphi_j \, d\xi \ .$$

Stiffness Matrix

Let us calculate some of the elements of matrix K_{ij} starting with the diagonal elements. For example, for K_{11} we obtain

$$
\begin{aligned}
K_{11} &= \mu \int_D \partial_x \, \varphi_1 \, \partial_x \, \varphi_1 \; dx \\
&= \mu \int_0^h \frac{-1}{h} \frac{-1}{h} d\xi \; = \frac{\mu}{h^2} \int_0^h d\xi = \frac{\mu}{h}
\end{aligned}
$$

Stiffness Matrix

For diagonal element A_{22} the derivatives overlap in element 1 and 2 implying the integration has to be performed for the interval $\xi \in [-h, h]$.

$$
\begin{aligned}
K_{22} &= \mu \int_D \partial_x \, \varphi_2 \, \partial_x \, \varphi_2 \, dx \\
&= \ \mu \int_{-h}^{0} \partial_\xi \, \varphi_2 \, \partial_\xi \, \varphi_2 \, d\xi + \mu \int_{0}^{h} \partial_\xi \, \varphi_2 \, \partial_\xi \, \varphi_2 \, d\xi \\
&= \frac{\mu}{h^2} \int_{-h}^{0} d\xi + \frac{\mu}{h^2} \int_{0}^{h} = \frac{2\mu}{h}
\end{aligned}
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Stiffness Matrix

Equivalently, the off-diagonal terms overlap only in one element, for example

$$
\begin{aligned}
K_{12} &= \mu \int_D \partial_x \varphi_1 \, \partial_x \varphi_2 \, dx \\
&= \mu \int_0^h \partial_\xi \varphi_1 \, \partial_\xi \varphi_2 \, d\xi = \mu \int_0^h \frac{-1}{h} \frac{1}{h} d\xi \\
&= \frac{-\mu}{h^2} \int_0^h d\xi = \frac{-\mu}{h} \\
K_{21} &= K_{12}
\end{aligned}
$$

Stiffness Matrix

Finally, the stiffness matrix for an elastic physical system with constant shear modulus μ and element size h reads

$$K_{ij} = \frac{\mu}{h} \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}$$

Note: Space-dependent terms in our linear system are proportional to the 3-point operator matrix for a 2nd finite-difference derivative

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Simulation Example

Parameter	Value
x_{max}	1
nx	20
μ	1
h	0.0526
u(0)	0.15
u(1)	0.05

The physical domain is defined in the interval $x \in [0, 1]$ and we apply a unit forcing at $x = 0.75$ at one of the boundary element points.

Simulation Example

```python
# -----------------------------------------------------
# Initialization of setup
# -----------------------------------------------------
nx = 20              # Number of boundary points
u  = np.zeros(nx)    # Solution vector
f  = np.zeros(nx)    # Source vector
mu = 1               # Constant shear modulus

# Element boundary points
x = np.linspace(0, 1, nx)   # x in [0,1]
h = x[2] - x[1]             # Constant element size

# -----------------------------------------------------
# Assemble stiffness matrix K_ij (Eq 6.30)
# -----------------------------------------------------
K = np.zeros((nx, nx))
for i in range(1, nx-1):
    for j in range(1, nx-1):
        if i == j:
            K[i, j] = 2*mu/h
        elif i == j + 1:
            K[i, j] = -mu/h
        elif i + 1 == j:
            K[i, j] = -mu/h
        else:
            K[i, j] = 0
```

```python
# ---------------------------------------------------------------
# Souce term is a spike at i = 3*nx/4
f[int(3*nx/4)] = 1

# Boundary condition at x = 0
u[0] = 0.15 ; f[1] = u[0]/h

# Boundary condition at x = 1
u[nx-1] = 0.05 ; f[nx-2] = u[nx-1]/h

# ---------------------------------------------------------------
# Finite element solution. (Eq 6.19)
# ---------------------------------------------------------------
u[1:nx-1] = np.linalg.inv(K[1:nx-1, 1:nx-1]) @ np.transpose(f[1:nx-1])
```

Relaxation method

Starting with the Poisson equation $-\mu\partial_x^2 u = f$, omitting space dependencies, we replace the l.h.s. with a finite-difference approximation and obtain

$$-\mu\frac{u(x-h) - 2u(x) + u(x+h)}{h^2} = f$$

and after rearranging

$$u(x) = \frac{u(x-h) + u(x+h)}{2} - \frac{h^2}{2\mu}f\ .$$

This equation can be used as an iterative procedure with an initial guess for the the unknown field u.

Simulation Example

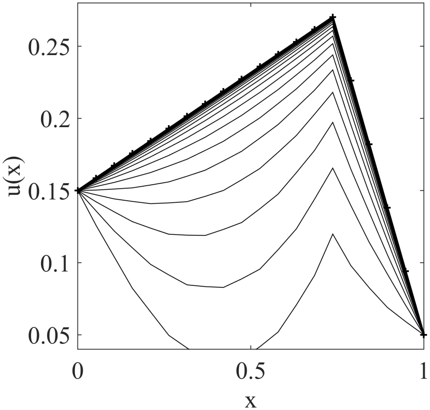
With discretization $u_i = u(x_i)$ and iteration step k this can be written as

$$u_i^{k+1} = \frac{u_{i+1}^k - u_{i-1}^k}{2} - \frac{h^2}{2\mu} f_i$$

with initial guess $u_i^{k=1} = 0$ - also called a *relaxation method*.

```
# ------------------------------------------------------------
for it in range(nt):
    # Calculate the average of u (omit boundaries)
    for i in range(1, nx-1):
        du[i] =u [i+1] + u[i-1]
    u = 0.5*( f*h**2/mu + du )
    u[0] = 0.15     # Boundary condition at x=0
    u[nx-1] = 0.05 # Boundary condition at x=1
    fd = u
```

Simulation Example



Simulation example comparing the finite-element solution (thick solid line) with a finite-difference based relaxation method (thin lines) that iteratively converges to the correct solution (see text for details). 500 iterations were employed for the relaxation method and the solution is shown after any 25 iterations.

Summary

- The finite-element method was originally developed mostly for static structural engineering problems.
- The *element* concept relates to describing the solution field in an analogous way inside each element, thereby facilitating the required calculations of the system matrices.
- The finite-element approach can in principle be applied to elements of arbitrary shape. Most used shapes are triangles (tetrahedra) or quadrilateral (hexahedral) structures.
- The finite-element method is a series expansion method. The continuous solution field is replaced by a finite sum over (not necessarily orthogonal) basis functions.
- For static elastic problems or the elastic wave propagation problem finite-element analysis leads to a (large) system of linear equations. In general, the matrices are of size $N \times N$ where N is the number of degrees of freedom.
- Because of the specific interpolation properties of the basis functions, their coefficients take the meaning of the values of the solution field at specific node points.

Summary

- In an initialization step the global stiffness and mass matrices have to be calculated. They depend on integrals over products of basis functions and their derivatives.
- If equation parameters (e.g., elastic parameters, density) vary inside elements, then numerical integration has to be performed.
- The stress-free surface condition can be implicitly solved. This is a major advantage for example for the simulation of surface waves.
- The classic finite-element method plays a minor role in seismology as its high-order sister, the spectral-element method, is more efficient.