Mathematical modelling in science and engineering

Lecture 2 Introduction to the finite element method

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Model problem

- 1D computational domain $\Omega = (0, 1)$
  - two-point boundary – 0 and 1
- model elliptic problem (second order in one space variable)
  - differential equation [particular model problem]:

$$-\frac{d^2u}{dx^2} = f(x) \qquad [f(x) = -2]$$

  - boundary conditions [particular model problem]:
    - Dirichlet: $u(0) = u_0 \qquad [u_0 = 0]$
    - Neumann: $\frac{du}{dx}(1) = u_1^{'} \qquad [u_1^{'} = 2]$
- two-point boundary value problem with proven existence and uniqueness of results
  - the exact solution for the particular model problem: $u^{\star}(x) = x^2$

Function spaces for the interval (0, 1)

- Assumptions:
  - functions can be added and multiplied by real numbers
  - functions (and their powers) can be integrated
  - functions can be measured using integrals
    - L_1 norm:
      $$\|f\|_{L_1} = \int_0^1 |f(x)| dx$$
    - L_2 norm:
      $$\|f\|_{L_2} = \left(\int_0^1 f(x)^2 dx \right)^{1/2}$$
    - L_p norm:
      $$\|f\|_{L_p} = \left(\int_0^1 |f(x)|^p dx \right)^{1/p}$$
    - L_∞ norm:
      $$\|f\|_{L_\infty} = \lim_{p \to \infty} \left(\int_0^1 |f(x)|^p dx \right)^{1/p} = max|_{x \in [0,1]} |f(x)|$$
  - the difference of two functions can be measured in the same way – giving the distance between the two functions

Function spaces for the interval $(0, 1)$

- the integral of the pointwise product of two functions satisfies the requirements of the inner (scalar) product:

$$(f, g) \equiv \int_0^1 f(x) \cdot g(x) dx$$

  - the L_2 norm of each function can be defined using scalar product:

$$\|f\|_{L_2} = (f, f)^{1/2}$$

- it is possible to define the norms that take into account functions and their derivatives, e.g.:

$$\|f\|_{W^{3,2}} = \left(\int_0^1 \left(f^2 + \left(\frac{df}{dx} \right)^2 + \left(\frac{d^2 f}{dx^2} \right)^2 + \left(\frac{d^3 f}{dx^3} \right)^2 \right) dx \right)^{1/2}$$

  - Sobolev spaces $W^{k,p}$ are the spaces of functions f with finite $\|f\|_{W^{k,p}}$ norms (L_p norms for functions and their k derivatives)
  - especially important are H^k spaces with L_2 norms: $H^k \equiv W^{k,2}$

Function spaces

Sobolev spaces

- the definitions and properties of Sobolev spaces $W^{k,p}$ for the interval $(0,1)$ can be generalized to any interval in 1D and to (almost) arbitrary computational domains (satisfying certain assumptions) in 2D and 3D
- spaces $W^{k,p}$ and especially spaces H^k are important in the mathematical theory of ordinary and partial differential equations
    - further on, we will use the notation $\|f\|$ for the L_2 norm of function f and $\|f\|_k$ (H^k norm) to denote $\|f\|_{W^{k,2}}$ norm
- the space H^1_0 will denote the subspace of H^1 with functions that vanish on the boundary of the computational domain
- we will use several properties of functions in Sobolev spaces (as special cases of vector spaces, normed spaces, Hilbert spaces, Banach spaces etc.)

Weak formulation for the model 1D problem

Derivation (weighted residual approach):

- multiplication of the ODE (or PDE) by a test function $w(x)$

$$\left(-\frac{d^2u}{dx^2} - f(x)\right) \cdot w(x) = 0 \qquad \forall w - \text{at every point } x \in (0,1)$$

- integration over the computational domain (the interval $(0,1)$)

$$\int_0^1 \left(-\frac{d^2u}{dx^2} - f(x)\right) \cdot w(x)dx = 0 \qquad \forall w$$

- application of the generalized integration by parts formulae

$$-\frac{du}{dx}(1)\cdot w(1) + \frac{du}{dx}(0)\cdot w(0) + \int_0^1 \frac{du}{dx}\frac{dw}{dx}dx = \int_0^1 f(x)\cdot w(x)dx \qquad \forall w$$

Weak formulation for the model 1D problem

Derivation (weighted residual approach):

- function spaces:
  - V – the subspace of H^1 space for the computational domain (the interval $(0,1)$) with functions satisfying the Dirichlet boundary conditions on the respective parts of the boundary
  - V_0 – the subspace of H^1 space for the computational domain (the interval $(0,1)$) with functions vanishing on the Dirichlet parts of the boundary
- assumption: $u \in V$, i.e. u satisfies (by construction) the Dirichlet boundary conditions, i.e. $u(0) = u_0$
- assumption: $w \in V_0$, i.e. $w(0) = 0$
- application of the assumptions concerning Dirichlet boundary and the formulae for the Neumann (and possibly Robin) boundary conditions (for the model problem $\frac{du}{dx}(1) = u_1^{'}$)

$$\int_0^1 \frac{du}{dx}\frac{dw}{dx}dx = \int_0^1 f(x) \cdot w(x)dx + u_1^{'} \cdot w(1) \qquad \forall w \in V_0$$

Weak formulation for the model 1D problem

Final formulation

Find a function $u(x) \in V$ such that the following holds:

$$\int_0^1 \frac{du}{dx}\frac{dw}{dx}dx = \int_0^1 f(x) \cdot w(x)dx + u_1^{'} \cdot w(1) \qquad \forall w \in V_0$$

It can be proven that:

- If u satisfies the original differential problem then it also satisfies the derived weak formulation
- If u satisfies the derived weak formulation and possess continuous second order derivative then it also satisfies the original differential problem

Equivalence of three problem formulations

Assumption: only zero Dirichlet boundary conditions

Differential formulation

$$-\frac{d^2u}{dx^2} = f(x) \quad \text{in } \Omega \qquad\qquad u(0) = 0 \quad \text{on } \partial\Omega$$

Weak (variational) formulation

Find a function $u \in V$ such that the following holds:

$$(u', w') = (f, w) \qquad \forall w \in V_0$$

Minimization of functional formulation

Find a function $u \in V$ such that the following holds:

$$\frac{1}{2}(u', u') - (f, u) \leq \frac{1}{2}(w', w') - (f, w) \qquad \forall w \in V_0$$

Interpretation in mechanics

The three different formulations have the following origins and interpretations in mechanics
(e.g. for the problem of tensile test, with the displacement u and external force (load) f):

- differential formulation
  - corresponds to Newton's laws of mechanics
- minimization formulation
  - corresponds to the minimization of the total potential energy principle
  - $\frac{1}{2}(u', u')$ - internal elastic energy of the body
  - (f, u) - potential energy of the load
- weak (variational) formulation
  - corresponds to the principle of virtual work

The finite element method

The finite element method is a method for approximating the solutions to boundary value problems

- The two fundamental ingredients of the FEM are:
  - the use of weak variational statements of the problems
  - the discretization of the computational domains into small parts, called elements, within which the solution is approximated using simple polynomials
- The FEM is especially efficient for solving elliptic problems (stationary with no time variable) in complex 3D domains
- The FEM can also be used for solving initial boundary value problems (with time variable), usually in combination with other discretization methods such as the finite difference method or the discontinuous Galerkin method

The finite element method

Discretization of the computational domain:

- The sum of all elements must completely fill the computational domain
- Elements cannot overlap
- Elements should have sufficient quality
  - the ratio of the sizes of edges should be limited
  - the internal angles between the edges should not be too small
- The ratio of the sizes of neighbouring elements should be limited
- Types of meshes:
  - 1D – division into small intervals
  - 2D – popular elements: triangles, quadrilaterals
  - 3D – popular elements: tetrahedra, hexahedra, prisms (less frequent: pyramids)
  - apart from elements with straight edges (and plane faces in 3D) there are elements with curved boundaries

The finite element method

Finite element function spaces:

- elements $\rightarrow$ shape functions, ϕ_i
- computational domain $\rightarrow$ basis functions constructed from shape functions, ψ_j
  - in the standard FEM basis functions are continuous
  - basis functions have as small support (the domain of non-zero values) as possible
- finite element solutions as linear combinations of basis functions

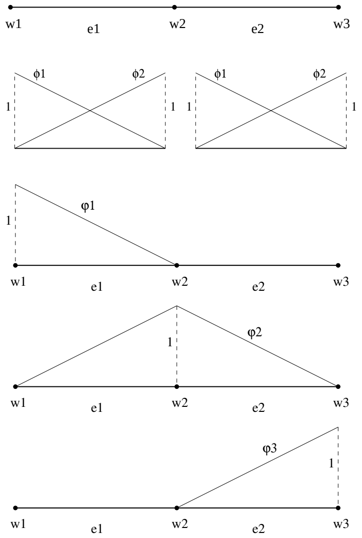
$$u^h(x) = \mathrm{U}^h_1\psi_1 + \mathrm{U}^h_2\psi_2 + \mathrm{U}^h_3\psi_3 + \ldots + \mathrm{U}^h_N\psi_N = \sum_j^N \mathrm{U}^h_j\psi_j$$

$$u^h(x) \in V^h(x) = \mathrm{span}\,\{\psi_1, \psi_2, \psi_3, \ldots, \psi_N\}$$

  - coefficients U^h_j of linear combination (degrees of freedom) form a discrete FEM solution to the approximation problem
  - N – the size of vector $\mathbf{U}^h$, i.e. the number of degrees of freedom, is the size of a particular FEM problem

Finite element formulation for the model 1D problem

- The division of computational domain into elements
- Shape functions ϕ_i inside elements
- Basis functions ψ_j for the whole computational domain

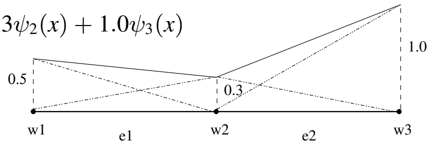


Example:

- domain: $(0,1)$
- elements: $e_1 - (0,0.5)$ and $e_2 - (0.5,0)$
- element vertices (finite element nodes): $\{w_1, w_2, w_3\} - \{0, 0.5, 1.0\}$

Finite element interpolation

- Using finite element spaces it is possible to construct not only approximate solutions but also interpolants (functions that agree with a set of discrete values)
- Finite element interpolation is especially easy for the spaces where finite element degrees of freedom correspond to the values at specific points (warning: there are spaces where it is not true!)
    - for typical finite element spaces with linear basis (shape) functions the values of degrees of freedom are the values of finite element solutions at element vertices
    - Example:
        - interpolation for the set of points: $\{(w_1, 0.5), (w_2, 0.3), (w_3, 1.0)\}$
        - $\mathbf{U}^h = \{0.5, 0.3, 1.0\}$
        - $u^h(x) = 0.5\psi_1(x) + 0.3\psi_2(x) + 1.0\psi_3(x)$



Finite element formulation for the model 1D problem

- Weak formulation:
  Find a function $u^h \in V^h \subset V$ such that the following holds:
  $$\left(\frac{du^h}{dx}, \frac{dw^h}{dx}\right) = (f, w) + u_1^{'} \cdot w^h(1) \qquad \forall w^h \in V_0^h \subset V_0$$
- Domain discretization:
  Partition of $(0, 1)$ into subintervals (x_{j-1}, x_j) of length $h_j = x_j - x_{j-1}$ with $h = \max h_j$
- Finite element discretization (approximation):
  $$u^h = \sum_j^N \mathrm{U}_j^h \psi_j \qquad w^h = \sum_i^N \mathrm{W}_i^h \psi_i$$

Hence:

$$\left(\frac{d\sum_j^N \mathrm{U}_j^h \psi_j}{dx}, \frac{d\sum_i^N \mathrm{W}_i^h \psi_i}{dx}\right) = \sum_i^N \mathrm{W}_i^h \sum_j^N \mathrm{U}_j^h \left(\frac{d\psi_j}{dx}, \frac{d\psi_i}{dx}\right)$$

Finite element approximation for the model 1D problem

- General finite element solution procedure consists of two steps:
  - creation of the system of linear equations:

$$\sum_{i}^{N} \mathrm{W}_i^h \left(\sum_{j}^{N} \mathrm{U}_j^h \left(\frac{d\psi_j}{dx}, \frac{d\psi_i}{dx} \right) - (f, \psi_i) - u_1' \cdot \psi_i(1) \right) = 0 \qquad \forall \mathbf{W}^h = \{\mathrm{W}_1^h, \mathrm{W}_2^h, ..., \mathrm{W}_N^h\}$$

Hence:

$$\sum_{j}^{N} \mathrm{U}_j^h \left(\frac{d\psi_j}{dx}, \frac{d\psi_i}{dx} \right) = (f, \psi_i) + u_1' \cdot \psi_i(1) \qquad i = 1, 2, ..., N$$

i.e.

$$\sum_{j}^{N} \mathrm{A}_{i,j} \mathrm{U}_j^h = \mathrm{b}_i \qquad i = 1, 2, ..., N$$

with: $\mathrm{A}_{i,j} = \left(\frac{d\psi_j}{dx}, \frac{d\psi_i}{dx} \right)$ and $\mathrm{b}_i = (f, \psi_i) + u_1' \cdot \psi_i(1)$

  - solution of the system of linear equations

Finite element approximation for the model 1D problem

- For the particular problem
  ($f(x) = -2, \quad u(0) = u_0 = 0, \quad \frac{du}{dx}(1) = u'_1 = 2$)
  the solution procedure leads to the system of linear equations:

$$\begin{pmatrix} -2 & 2 & 0 \\ 2 & -4 & 2 \\ 0 & 2 & -2 \end{pmatrix} = \begin{pmatrix} 0.5 \\ 1.0 \\ -1.5 \end{pmatrix}$$

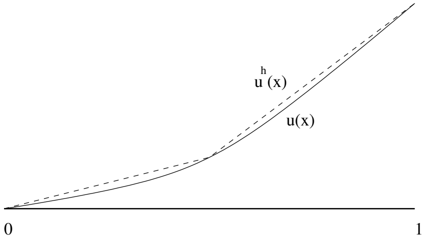
- The application of the Dirichlet boundary condition can be accomplished by the assumption $\mathrm{U}^h_1 = 0$, that, after substituting to the system of equations, lead to the final system:

$$\begin{array}{rcrcr} -4\mathrm{U}^h_2 & + & 2\mathrm{U}^h_3 & = & 1 \\ 2\mathrm{U}^h_2 & - & 2\mathrm{U}^h_3 & = & -1.5 \end{array}$$

- The final solution is the vector $\mathbf{U}^h = [0.0, 0.25, 1.0]$

Finite element approximation for the model 1D problem

The exact and approximate solutions for the particular case of the model problem:



The error:

$$e^h = u^h - u$$

Finite element approximation

Finite element approximations to elliptic problems have several important properties:

- For many problems it is relatively easy to prove the existence and uniqueness of exact and approximate finite element solutions using the corresponding weak formulations
  - this concerns in particular the model 1D problem considered
- FEM approximate solutions satisfy the best approximation property:
  - for the model 1D problem:

$$\|(u^h - u)'\| < \|(w^h - u)'\| \qquad \forall w^h \in V_0^h$$

- Using the interpolant of the exact solution as the function w^h in the formula above and the interpolation error estimate it is possible to estimate the error of the finite element solution as:
  - for the model 1D problem:

$$\|e^h\| = \|u^h - u\| < Ch^2 \cdot \max |u''|$$

Finite element approximation

The properties of FEM approximations have important consequences:

- one can control the error of finite element solutions by a suitable choice of element sizes
- with the maximal element size going to zero finite element solutions converge to the exact solution

Additional observations:

- the error depends on the second order derivative of the exact solution, not the gradient (as is often incorrectly stated)
- with the element size going to zero, the number of elements in the computational domain and the number of degrees of freedom in the system of linear equations associated with the problem go to infinity
    - however: the computational cost does not grow quadratically with the number of degrees of freedom, since the matrices of linear systems are very sparse
        - for really large problems the number of zeros in the system matrices can easily exceed 99,99%

Finite element approximation

The geometric interpretation of the finite element method:

- the integral on the left hand side of the weak finite element statement for many problems (especially for elliptic PDEs) can be interpreted as a special form of scalar product, for example:

$$(u, v)_E = \int_0^1 \frac{du}{dx}\frac{dv}{dx}dx$$

- the definition of the scalar product leads to the definition of a norm (so called energy norm – due to some interpretations in mechanics):

$$\|u\|_E^2 = (u, u)_E$$

Finite element approximation

The geometric interpretation of the finite element method:

- the finite element formulation can then be interpreted as the condition of orthogonalization of the error with respect to the space V^h using the scalar product $(.,.)_E$:

$$(u_h - u, v_h)_E = 0 \qquad \forall v_h \in V_h$$

- hence, the finite element solution u_h can be interpreted as the projection of the exact solution u onto the space V_h
- with the finite element solution u_h being the closest function in V_h to the exact solution u with the distance measured by the energy norm