MU5MES01

Nonlinear structural mechanics by the finite element method.

1 - Introduction to FEM

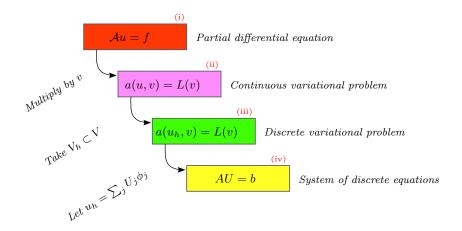
Corrado Maurini, based on slides from Anders Logg

What is FEM?

The finite element method is a framework and a recipe for discretization of differential equations

- Ordinary differential equations
- Partial differential equations
- Integral equations
- A recipe for discretization of PDE
- PDE $\rightarrow Ax = b$
- Different bases, stabilization, error control, adaptivity

The FEM cookbook



The PDE (i)

Consider Poisson's equation, the Hello World of partial differential equations:

$$-\Delta u = f \quad \text{in } \Omega$$
$$u = u_0 \quad \text{on } \partial \Omega$$

Poisson's equation arises in numerous applications:

- heat conduction, electrostatics, diffusion of substances, twisting of elastic rods, inviscid fluid flow, water waves, magnetostatics, ...
- as part of numerical splitting strategies for more complicated systems of PDEs, in particular the Navier-Stokes equations

From PDE (i) to variational problem (ii)

The simple recipe is: multiply the PDE by a test function v and integrate over Ω :

$$-\int_{\Omega} (\Delta u) v \, \mathrm{d}x = \int_{\Omega} f v \, \mathrm{d}x$$

Then integrate by parts and set v = 0 on the Dirichlet boundary:

$$-\int_{\Omega} (\Delta u) v \, dx = \int_{\Omega} \nabla u \cdot \nabla v \, dx - \underbrace{\int_{\partial \Omega} \frac{\partial u}{\partial n} v \, ds}_{=0}$$

We find that:

$$\int_{\Omega} \nabla u \cdot \nabla v \, \mathrm{d}x = \int_{\Omega} f v \, \mathrm{d}x$$

The variational problem (ii)

Find $u \in V$ such that

$$\int_{\Omega} \nabla u \cdot \nabla v \, \mathrm{d}x = \int_{\Omega} f v \, \mathrm{d}x$$

for all $v \in \hat{V}$

The trial space V and the test space \hat{V} are (here) given by

$$V = \{ v \in H^1(\Omega) : v = u_0 \text{ on } \partial \Omega \}$$

$$\hat{V} = \{ v \in H^1(\Omega) : v = 0 \text{ on } \partial \Omega \}$$

From continuous (ii) to discrete (iii) problem

We approximate the continuous variational problem with a discrete variational problem posed on finite dimensional subspaces of V and \hat{V} :

$$V_h \subset V$$
$$\hat{V}_h \subset \hat{V}$$

Find $u_h \in V_h \subset V$ such that

$$\int_{\Omega} \nabla u_h \cdot \nabla v \, \mathrm{d}x = \int_{\Omega} f v \, \mathrm{d}x$$

for all $v \in \hat{V}_h \subset \hat{V}$

From discrete variational problem (iii) to discrete system of equations (iv)

Choose a basis for the discrete function space:

$$V_h = \operatorname{span} \left\{ \phi_j \right\}_{j=1}^N$$

Make an ansatz for the discrete solution:

$$u_h = \sum_{j=1}^{N} U_j \phi_j$$

Test against the basis functions:

$$\int_{\Omega} \nabla \left(\sum_{j=1}^{N} U_{j} \phi_{j} \right) \cdot \nabla \phi_{i} \, \mathrm{d}x = \int_{\Omega} f \phi_{i} \, \mathrm{d}x$$

From discrete variational problem (iii) to discrete system of equations (iv), contd.

Rearrange to get:

$$\sum_{j=1}^{N} U_{j} \underbrace{\int_{\Omega} \nabla \phi_{j} \cdot \nabla \phi_{i} \, \mathrm{d}x}_{A_{ij}} = \underbrace{\int_{\Omega} f \phi_{i} \, \mathrm{d}x}_{b_{i}}$$

A linear system of equations:

$$AU = b$$

where

$$A_{ij} = \int_{\Omega} \nabla \phi_j \cdot \nabla \phi_i \, \mathrm{d}x \tag{1}$$

$$b_i = \int_{\Omega} f \phi_i \, \mathrm{d}x \tag{2}$$

The canonical abstract problem

(i) Partial differential equation:

$$Au = f$$
 in Ω

(ii) Continuous variational problem: find $u \in V$ such that

$$a(u, v) = L(v)$$
 for all $v \in \hat{V}$

(iii) Discrete variational problem: find $u_h \in V_h \subset V$ such that

$$a(u_h, v) = L(v)$$
 for all $v \in \hat{V}_h$

(iv) Discrete system of equations for $u_h = \sum_{j=1}^{N} U_j \phi_j$:

$$AU = b$$

$$A_{ij} = a(\phi_j, \phi_i)$$

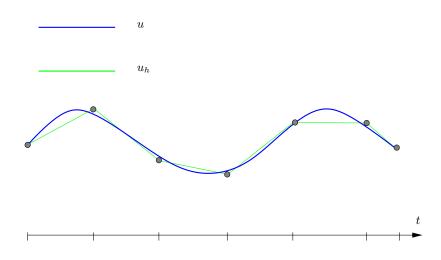
$$b_i = L(\phi_i)$$

Important topics

- How to choose V_h ?
- How to compute A and b
- How to solve AU = b?
- How large is the error $e = u u_h$?
- Extensions to nonlinear problems

How to choose V_h

Finite element function spaces

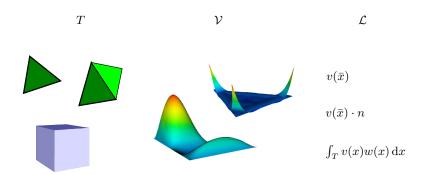


The finite element definition (Ciarlet 1975)

A finite element is a triple $(T, \mathcal{V}, \mathcal{L})$, where

- the domain T is a bounded, closed subset of \mathbb{R}^d (for d = 1, 2, 3, ...) with nonempty interior and piecewise smooth boundary
- the space $\mathcal{V} = \mathcal{V}(T)$ is a finite dimensional function space on T of dimension n
- the set of degrees of freedom (nodes) $\mathcal{L} = \{\ell_1, \ell_2, \dots, \ell_n\}$ is a basis for the dual space \mathcal{V}' ; that is, the space of bounded linear functionals on \mathcal{V}

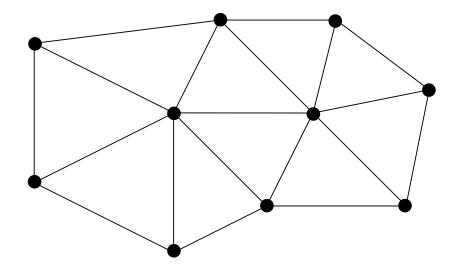
The finite element definition (Ciarlet 1975)



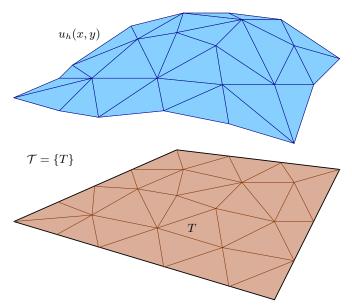
The linear Lagrange element: (T, V, \mathcal{L})

- ullet T is a line, triangle or tetrahedron
- \mathcal{V} is the first-degree polynomials on T
- \mathcal{L} is point evaluation at the vertices

The linear Lagrange element: \mathcal{L}



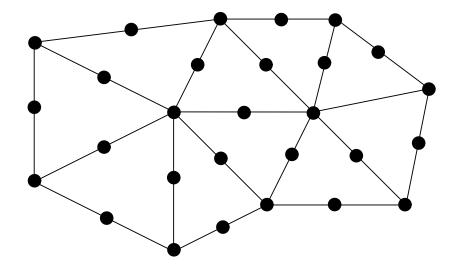
The linear Lagrange element: V_h



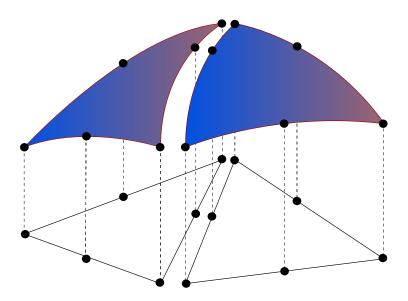
The quadratic Lagrange element: (T, V, \mathcal{L})

- T is a line, triangle or tetrahedron
- \mathcal{V} is the second-degree polynomials on T
- \mathcal{L} is point evaluation at the vertices and edge midpoints

The quadratic Lagrange element: \mathcal{L}

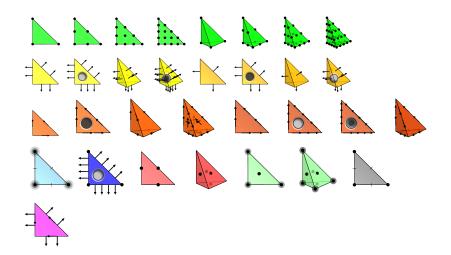


The quadratic Lagrange element: V_h



Nedelec Hermite Brezzi-Douglas-Fortin-Marini Mardal-Tai-Winther **Raviart-Thomas**

Families of elements



Computing the sparse matrix A

Naive assembly algorithm

$$A=0$$
 for $i=1,\dots,N$ for $j=1,\dots,N$ $A_{ij}=a(\phi_j,\phi_i)$ end for

The element matrix

The global matrix A is defined by

$$A_{ij} = a(\phi_j, \phi_i)$$

The element matrix A_T is defined by

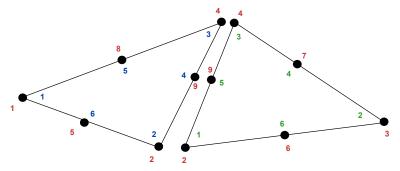
$$A_{T,ij} = a_T(\phi_j^T, \phi_i^T)$$

The local-to-global mapping

The global matrix ι_T is defined by

$$I = \iota_T(i)$$

where I is the global index corresponding to the local index i



The assembly algorithm

$$A = 0$$

for $T \in \mathcal{T}$

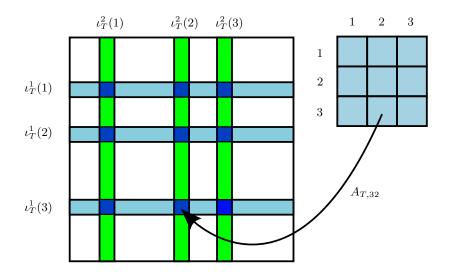
Compute the element matrix A_T

Compute the local-to-global mapping ι_T

Add A_T to A according to ι_T

end for

Adding the element matrix A_T



Solving AU = b

Direct methods

- Gaussian elimination
 - Requires $\sim \frac{2}{3}N^3$ operations
- LU factorization: A = LU
 - Solve requires $\sim \frac{2}{3}N^3$ operations
 - Reuse L and U for repeated solves
- Cholesky factorization: $A = LL^{\top}$
 - Works if A is symmetric and positive definite
 - Solve requires $\sim \frac{1}{3}N^3$ operations
 - Reuse L for repeated solves

Iterative methods

Krylov subspace methods

- GMRES (Generalized Minimal RESidual method)
- CG (Conjugate Gradient method)
 - Works if A is symmetric and positive definite
- BiCGSTAB, MINRES, TFQMR, ...

Multigrid methods

- GMG (Geometric MultiGrid)
- AMG (Algebraic MultiGrid)

Preconditioners

• ILU, ICC, SOR, AMG, Jacobi, block-Jacobi, additive Schwarz, ...

See also PETSc manual for their practical use:

https://www.mcs.anl.gov/petsc/petsc-current/docs/manual.pdf

Which method should I use?

Rules of thumb

- Direct methods for small systems
- Iterative methods for large systems
- Break-even at ca 100–1000 degrees of freedom
- Use a symmetric method for a symmetric system
 - Cholesky factorization (direct)
 - CG (iterative)
- Use a multigrid preconditioner for Poisson-like systems
- GMRES with ILU preconditioning is a good default choice

Norms and apriori error estimations

Measuring functions: norms

Commonly used (semi-)norms

Let $u: x \in \Omega \subset \mathbb{R}^n \to u(x)\mathbb{R}^m$ be a generic function:

• sup-norm:

$$||u||_{\infty,\Omega} = \sup_{\Omega} |u(x)|$$

• L^2 -norm:

$$||u||_{0,\Omega} = \sqrt{\int_{\Omega} u(x) \cdot u(x) dx}$$

 \bullet H¹-norm:

$$||u||_{1,\Omega} = \sqrt{\int_{\Omega} u(x) \cdot u(x) + \int_{\Omega} \nabla u(x) \cdot \nabla u(x)} \equiv \sqrt{\int_{\Omega} \nabla u(x) \cdot \nabla u(x) dx}$$

• Energy norm for the variational problem $\min_u \frac{1}{2}a(u,u) - l(u)$:

$$||u||_E = \sqrt{\frac{a(u,u)}{2}}$$

Measuring functions

Exemple in FEniCS

Let $u: x \in \Omega \subset \mathbb{R}^n \to u(x)\mathbb{R}^m$ be a generic function:

• L^2 -norm:

$$||u||_{0,\Omega} = \sqrt{\int_{\Omega} u(x) \cdot u(x) dx}$$

```
integral = assemble(inner(u,u)*dx)
norm_L2 = sqrt(integral)
```

Theory can help you to validate your implementation!

A priori estimates for the Poisson problem (or Linear elasticity)

If

•
$$u \in H_0^1(\Omega) \cap H^{k+1}(\Omega)$$

•
$$V_h = \{v_h \in C(\Omega) : v_h \in P^k(T) \ \forall \ T \in \mathcal{T}\}$$

then

$$E_1(h) := \|u - u_h\|_{1,\Omega} \le Ch^k \|u\|_{k+1,\Omega}$$

$$E_0(h) := \|u - u_h\|_{0,\Omega} \le Ch^{k+1} \|u\|_{k+1,\Omega}$$

where
$$\|\cdot\|_{l,\Omega} = \|\cdot\|_{H^{l}(\Omega)}$$
 for $l = 0, 1, k + 1$.

Taking log on each side

$$\log(E_1(h)) \le \log(Ch^k ||u||_{k+1,\Omega}) = k \log(h) + \log(C||u||_{k+1,\Omega})$$

Method of manufactured solutions

Recipe

- \bullet Take a suitable function u
- 2 Compute $-\Delta u$ to obtain f
- Sompute boundary values (trivial if only Dirichlet boundary conditions are used)
- Solve the corresponding variational problem

$$a(u_h, v) = L(v)$$

for a sequence of meshes Ω_h and compute the error $E_i(h) = ||u - u_h||_{i,\Omega_i}$ for i = 0, 1

6 Plot $\log(E_i(h))$ against $\log(h)$ and determine k

Exercice

See TP 1.2

Types of error estimators

• A priori estimates

(from mathematical analysis before calculating the solution):

$$||u - u_h|| \leqslant Ch^k ||u||_{\Omega, k+1}$$

This requires that the data are "regular". See Chap 6 in the Szabo-Babuska book for understanding the issues with "singularities":

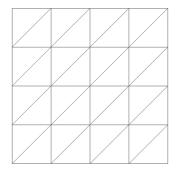
https://classes.engineering.wustl.edu/2009/fall/mase5510/Chapter_6.pdf.

- A posteriori estimates (based on the postprocessing of the solution):
 - Explicit residual-based error estimators
 - Implicit error estimator based on local problems
 - Gradient recovery estimators
 - Hierarchic error estimators
 - Goal-oriented error estimators

A priori estimates

If
$$u \in H^{k+1}(\Omega)$$
 and $V_h = P^k(\mathcal{T}_h)$ then
$$\|u - u_h\| \leqslant Ch^k \|u\|_{\Omega, k+1}$$

$$\|u - u_h\|_{L^2(\Omega)} \leqslant Ch^{k+1} \|u\|_{\Omega, k+1}$$

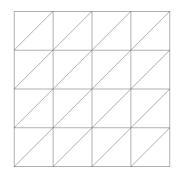


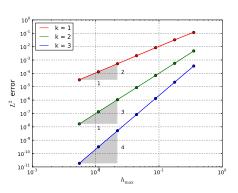
These estimates are based on the regularity of the solution: it can be wrost than this in the presence of singularities!!

A priori estimates

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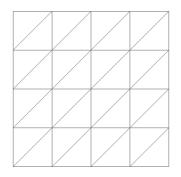


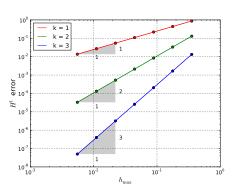
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Linear elasticity

Linear elasticity

The variational problem for linear isotropic elasticity is the following: Find $u \in \mathcal{C} \equiv \{u : H^1(\Omega), \underline{u} = \underline{\overline{u}} \text{ on } \partial_u \Omega\}$ such that

$$\int_{\Omega} \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}(\underline{u})) : \underline{\underline{\varepsilon}}(\underline{v}) \, d\underline{x} = \int_{\partial \Omega_f} \underline{T} \cdot \underline{v} \, ds + \int_{\partial \Omega} \underline{b} \cdot \underline{v} \, d\underline{x}$$
 (3)

 $\forall v \in \mathcal{C}_0 \equiv \{u : H^1(\Omega), \ \underline{u} = \underline{0} \text{ on } \partial_u \Omega\}$ where

$$\underline{\underline{\underline{\sigma}}}(\underline{\underline{\varepsilon}}) = \lambda \operatorname{tr}(\underline{\underline{\varepsilon}})\underline{\underline{I}} + 2\mu\underline{\underline{\varepsilon}}, \qquad \varepsilon(u) = \operatorname{sym}(\nabla u)$$

.

Homework:

Consider the energy functional

$$\mathcal{E}(\underline{u}) = \int_{\Omega} \frac{1}{2} \underline{\underline{\sigma}}(\underline{\underline{\varepsilon}}(\underline{u})) : \underline{\underline{\varepsilon}}(\underline{u}) \, d\underline{x} - \int_{\partial \Omega_f} \underline{T} \cdot \underline{u} \, ds - \int_{\partial \Omega} \underline{b} \cdot \underline{u} \, d\underline{x}.$$

Show that the variational formulation for linear elasticity is equivalent to the stationarity condition

$$\mathcal{E}'(\underline{u})(\underline{v}) = 0, \quad \forall \underline{u} \in \mathcal{C}_0, \quad \text{with } \mathcal{E}'(\underline{u})(\underline{v}) = \left. \frac{d\mathcal{E}(\underline{u} + h\underline{v})}{dh} \right|_{h=0}.$$

- ② What is the physical interpretation of \underline{b} , \underline{T} , $\underline{\bar{u}}$?
- 8 After a Galerkin approximation, the associated discrete problem will be in the form

$$AU = b$$

Following the procedure illustrated in class for the scalar Poisson equation, give the expression of A_{ij} , b_j , U_i in the case of linear elasticity. How to account for Dirichlet BC's?