MU5MES01
Nonlinear structural mechanics by the finite element method.
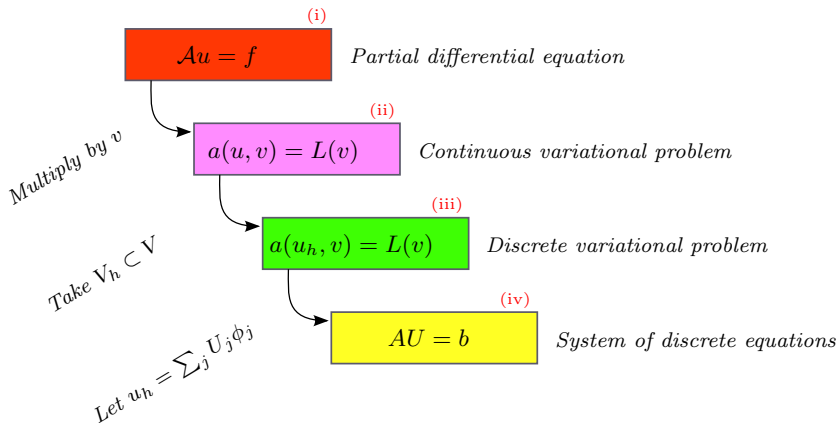
## 1 - Introduction to FEM

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## 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



$\mathcal{A}u = f$ **(i)** — *Partial differential equation*

*Multiply by v*

$a(u, v) = L(v)$ **(ii)** — *Continuous variational problem*

*Take $V_h \subset V$*

$a(u_h, v) = L(v)$ **(iii)** — *Discrete variational problem*

*Let $u_h = \sum_j U_j \phi_j$*

$AU = b$ **(iv)** — *System of discrete equations*

## 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 $\Omega$:

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

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

$$-\int_\Omega (\Delta u)v\,\mathrm{d}x = \int_\Omega \nabla u \cdot \nabla v\,\mathrm{d}x - \underbrace{\int_{\partial\Omega} \frac{\partial u}{\partial n}v\,\mathrm{d}s}_{=0}$$

We find that:

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

## 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:

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

Make an ansatz for the discrete solution:

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

Test against the basis functions:

$$\int_\Omega \nabla(\underbrace{\sum_{j=1}^{N} U_j \phi_j}_{u_h}) \cdot \nabla \phi_i \, \mathrm{d}x = \int_\Omega f \phi_i \, \mathrm{d}x$$

# 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:

$$\mathcal{A}u = f \quad \text{in } \Omega$$

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

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

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

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

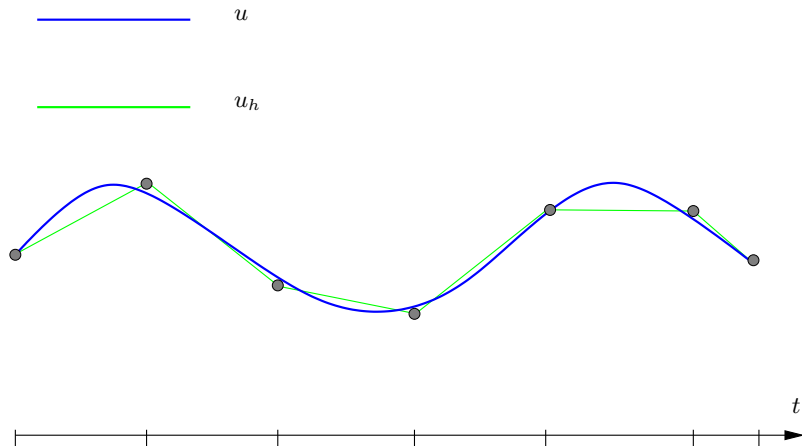(iv) Discrete system of equations for $u_h = \sum_{j=1}^{N} U_j \phi_j$:

$$AU = b$$
$$A_{ij} = a(\phi_j, \phi_i)$$
$$b_i = L(\phi_i)$$

## 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



$u$

$u_h$

$t$

# 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 $\mathcal{R}^d$ (for $d = 1, 2, 3, \dots$) 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)

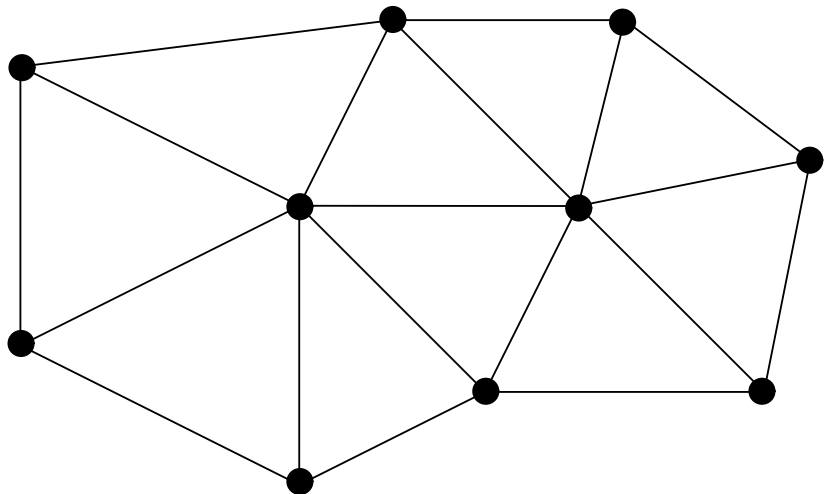$T$
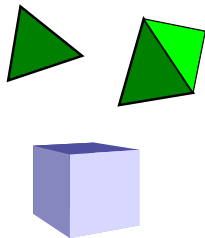
$\mathcal{V}$
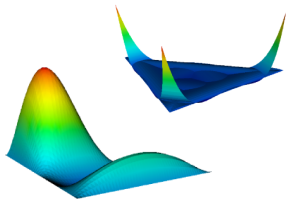
$\mathcal{L}$



$v(\bar{x})$

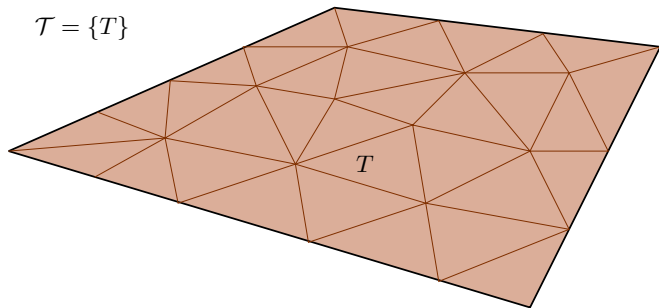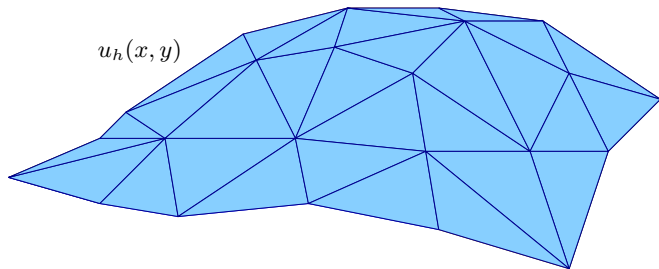$v(\bar{x}) \cdot n$

$\int_T v(x) w(x) \, \mathrm{d}x$

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

- $T$ 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: $V_h$



$u_h(x, y)$

$\mathcal{T} = \{T\}$

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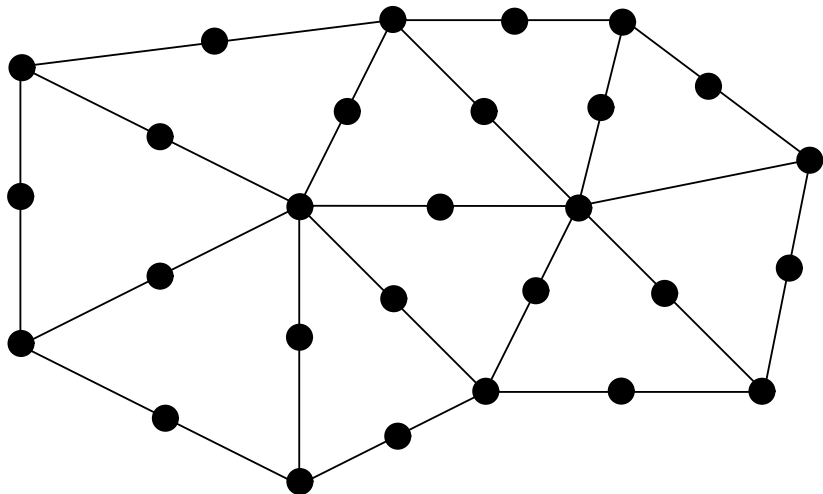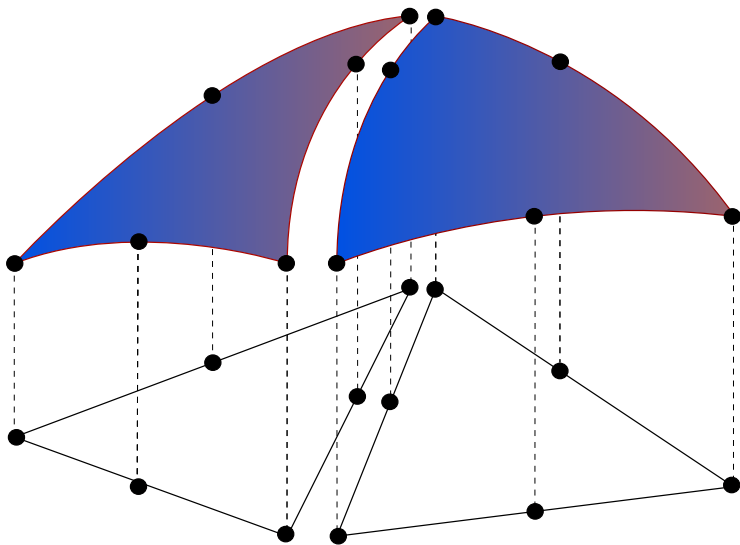
# The quadratic Lagrange element: $(T, \mathcal{V}, \mathcal{L})$

- $T$ 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

Nedelec Hermite

Mardal-Tai-Winther

Brezzi-Douglas-Fortin-Marini

Brezzi-Douglas-Marini

Lagrange

Argyris

Morley

Raviart-Thomas

DG

Crouzeix-Raviart
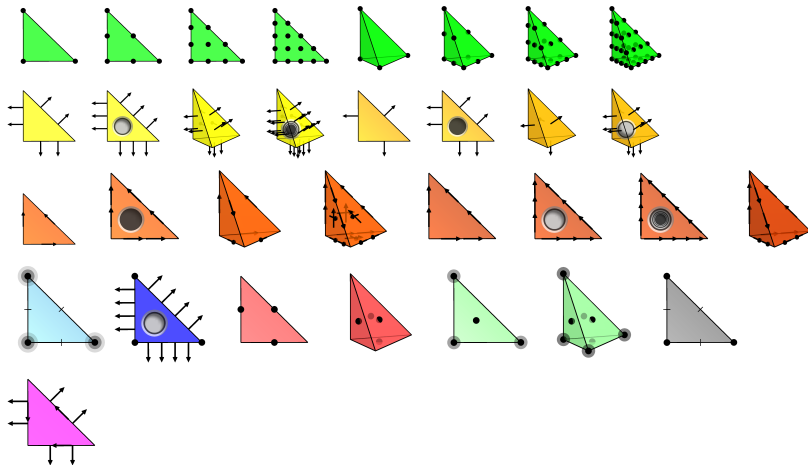
Computing the sparse matrix $A$

## Naive assembly algorithm

$A = 0$

**for** $i = 1, \ldots, N$

    **for** $j = 1, \ldots, N$

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

    **end for**

**end for**

# The element matrix

The global matrix $A$ is defined by

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

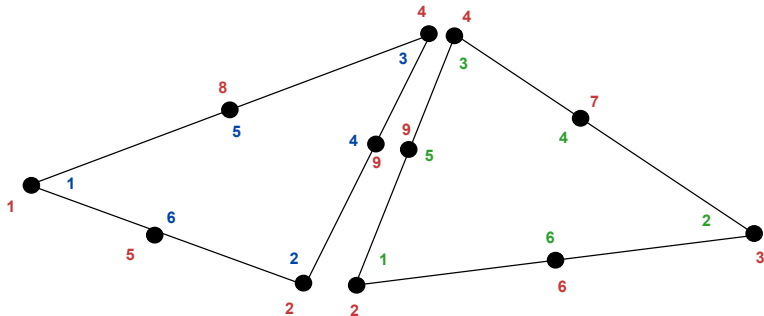The *element matrix* $A_T$ is defined by

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

# The local-to-global mapping

The global matrix $\iota_T$ is defined by

$$I = \iota_T(i)$$

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

## The assembly algorithm
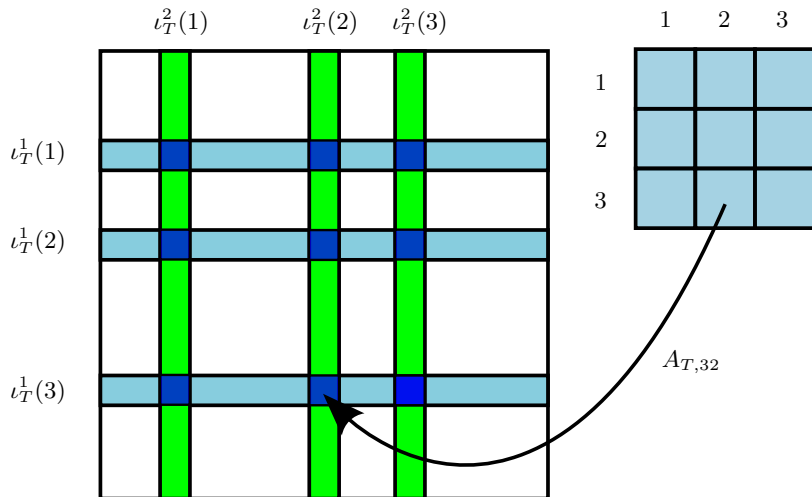
$A = 0$

**for** $T \in \mathcal{T}$

    Compute the element matrix $A_T$

    Compute the local-to-global mapping $\iota_T$

    Add $A_T$ to $A$ according to $\iota_T$

**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

# Types of error estimators

- *A priori* estimates

  (from mathematical analysis before calculating the solution):

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

  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

# Measuring functions: norms

## Commonly used (semi-)norms

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

- sup-norm:

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

- $L^2$-norm:

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

- $H^1$-norm:

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

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

- $L^2$-norm:

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

```
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

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

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

   for a sequence of meshes $\Omega_h$ and compute the error $E_i(h) = \|u - u_h\|_{i,\Omega_i}$ for $i = 0, 1$
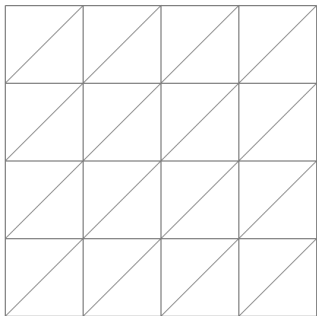5. Plot $\log(E_i(h))$ against $\log(h)$ and determine $k$

### Exercice

See TP 1.2

## A priori estimates

If $u \in H^{k+1}(\Omega)$ and $V_h = P^k(\mathcal{T}_h)$ then

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

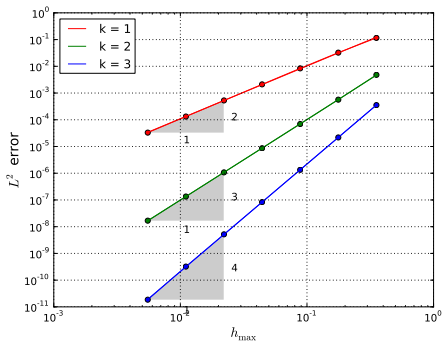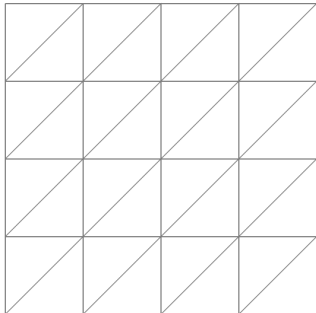$$\|u - u_h\|_{L^2(\Omega)} \leqslant Ch^{k+1} \|u\|_{\Omega, k+1}$$



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

## *A priori* estimates

If $u \in H^{k+1}(\Omega)$ and $V_h = P^k(\mathcal{T}_h)$ then

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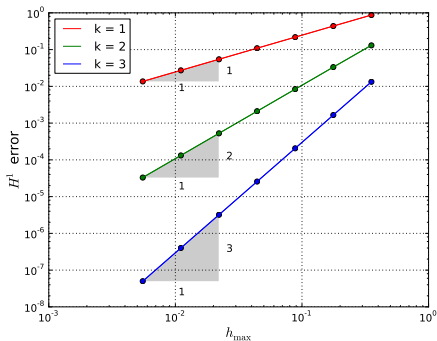$$\|u - u_h\|_{L^2(\Omega)} \leqslant Ch^{k+1} \|u\|_{\Omega,k+1}$$
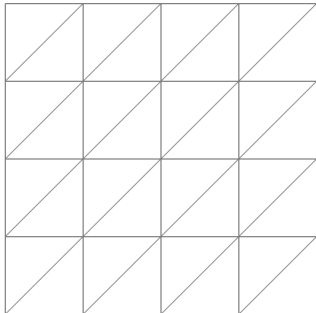


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These estimates are based on the regularity of the solution: it can be wrost than this in the presence of singularities!!

# Linear elasticity

## Linear elasticity

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

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

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

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

.

**Homework:**

1. Consider the energy functional

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

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 $\underline{b}$, $\underline{T}$, $\bar{\underline{u}}$?

3. 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?