Part 2 - Finite Elements in 2D and 3D (theoretically)

2.1. Preliminaries

General Notation and Setting

In the following

- d is the space dimension.
- Typically: $d = 1$, $d = 2$ or $d = 3$.
- $\Omega \subset \mathbb{R}^d$ is the computational domain (on which the differential equation is formulated)
- For simplicity, we assume that Ω is <u>convex</u> (i.e. any two points in Ω can be connected by a straight line that does not leave Ω).
- $\partial\Omega$ is the <u>boundary</u> or surface of Ω.

General Notation differential operators

For a function u we denote

- $x = (x_1, \cdots, x_d) \in \Omega$ a point in space;
- the gradient

$$\nabla u(x) = \begin{pmatrix} \partial_{x_1} u(x) \\ \dots \\ \partial_{x_d} u(x) \end{pmatrix};$$

- the Laplacian

$$\Delta u(x) = \sum_{i=1}^{d} \partial_{x_i x_i} u(x).$$

Notation - Two important Lebesgue spaces

- Lebesgue space of square-integrable functions

$$L^2(\Omega) := \{v | \int_\Omega |v|^2 \, \mathrm{d}x < \infty\}$$

L^2-scalar product

$$(u, v)_{L^2(\Omega)} = \int_\Omega u \, v \, \mathrm{d}x$$

and L^2-norm:

$$\|v\|_{L^2(\Omega)} := \left(\int_\Omega |v|^2 \, \mathrm{d}x \right)^{1/2}$$

- Lebesgue space of pointwise bounded functions

$$L^\infty(\Omega) := \{v | \operatorname{ess\,sup}_{x \in \Omega} |v(x)| < \infty\}$$

Notation - H^1-Sobolev spaces

- The Sobolev space of weakly-differentiable is

$$H^1(\Omega) := \{v \in L^2(\Omega) |\ \|\nabla v\|_{L^2(\Omega)} < \infty\}.$$

  Here, ∇v is the weak derivative of v.

- The H^1-space with zero boundary condition is

$$H_0^1(\Omega) := \{v \in H^1(\Omega) |\ v = 0 \text{ on } \partial\Omega\}.$$

- The H^1-scalar product is

$$(u, v)_{H^1(\Omega)} := (u, v)_{L^2(\Omega)} + (\nabla u, \nabla v)_{L^2(\Omega)}.$$

  and the H^1-norm is

$$\|v\|_{H^1(\Omega)} := \sqrt{(v, v)_{H^1(\Omega)}}.$$

Divergence theorem

Recall: the Divergence theorem for (vector functions)

$$\mathbf{F} : \Omega \to \mathbb{R}^d$$

which reads

$$\int_\Omega \nabla \cdot \mathbf{F} = \int_{\partial\Omega} \mathbf{F} \cdot \mathbf{n}.$$

Here $\mathbf{n}$ is the unit outer normal vector on $\partial\Omega$.

Green's formula

Divergence theorem:

$$\int_{\partial\Omega} \mathbf{F} \cdot \mathbf{n} = \int_{\Omega} \nabla \cdot \mathbf{F}.$$

For

- $v, u \in H^1(\Omega)$ and
- a matrix-valued function $\mathbf{k} \in L^\infty(\Omega, \mathbb{R}^{d\times d})$

we set

$$\mathbf{F} := v\, k\, \nabla u : \Omega \to \mathbb{R}^d$$

and conclude the Green's formula

$$\begin{aligned}\int_{\partial\Omega} v\ (k\nabla u \cdot \mathbf{n}) &= \int_{\Omega} \nabla \cdot (k\nabla u\, v) \\ &= \int_{\Omega} (\nabla \cdot k\nabla u)\, v + \int_{\Omega} k\nabla u \cdot \nabla v.\end{aligned}$$

Green's formula

Green's formula:

$$\int_\Omega k\nabla u \cdot \nabla v = -\int_\Omega (\nabla \cdot k\nabla u)\, v + \int_{\partial\Omega} v\, (k\nabla u \cdot \mathbf{n})\,.$$

<u>Example</u>: for $d = 1$ we recover common integration by parts:

$$\begin{aligned}
\int_a^b k u' v' &= -\int_a^b (k u')'\, v + \int_{\partial(a,b)} (k u' \cdot \mathbf{n})\; v \\
&= -\int_a^b (k u')'\, v \\
&\qquad + (k(a) u'(a) \cdot (-1))\; v(a) + (k(b) u'(b) \cdot 1)\; v(b) \\
&= -\int_a^b (k u')'\, v + [k u'\, v]_a^b\,.
\end{aligned}$$

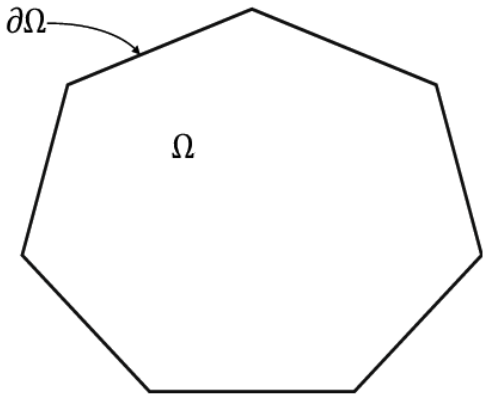
Part 2 - Finite Elements in 2D and 3D

2.2. Elliptic problems with zero Dirichlet boundary condition

General Setting

Let

- $\Omega \subset \mathbb{R}^d$ be a convex and polygonal domain



- source term: $f \in L^2(\Omega)$,
- conductivity/diffusion coefficient: $\mathbf{k} \in L^\infty(\Omega, \mathbb{R}^{d\times d})$ which is elliptic, i.e.,

$$\mathbf{k}(x)\boldsymbol{\xi} \cdot \boldsymbol{\xi} \geq \mathbf{k}_0 |\boldsymbol{\xi}|^2 \qquad \text{for all } \boldsymbol{\xi} \in \mathbb{R}^d$$

(in $1d$, this means $k(x) \geq k_0 > 0$)

General elliptic model problem

Classical solution:

Find $u \in C^2(\Omega)$ such that

$$-\nabla \cdot (k \nabla u) = f \qquad \text{in } \Omega$$

and

$$u = 0 \qquad \text{on } \partial\Omega.$$

Variational (weak) formulation

Find $u \in H_0^1(\Omega)$ such that

$$-\nabla \cdot (k \nabla u) = f \qquad \text{in } \Omega$$

Multiply by $v \in H_0^1(\Omega)$ and integrate over Ω:

$$\begin{aligned}
\int_\Omega f\, v \quad &= \quad -\int_\Omega \nabla \cdot (k \nabla u)\, v \\
&\overset{\text{Green}}{=} \quad \int_\Omega k \nabla u \cdot \nabla v - \int_{\partial\Omega} v\, (k \nabla u \cdot \mathbf{n}) \\
&\overset{v \in H_0^1(\Omega)}{=} \quad \int_\Omega k \nabla u \cdot \nabla v.
\end{aligned}$$

Variational (weak) formulation

Find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega k \nabla u \cdot \nabla v = \int_\Omega f\, v \qquad \text{for all } v \in H_0^1(\Omega).$$

Next step:
replace $H_0^1(\Omega)$ by a finite element space $V_{h,0}$.

How do we construct $V_{h,0}$ for $d > 1$?

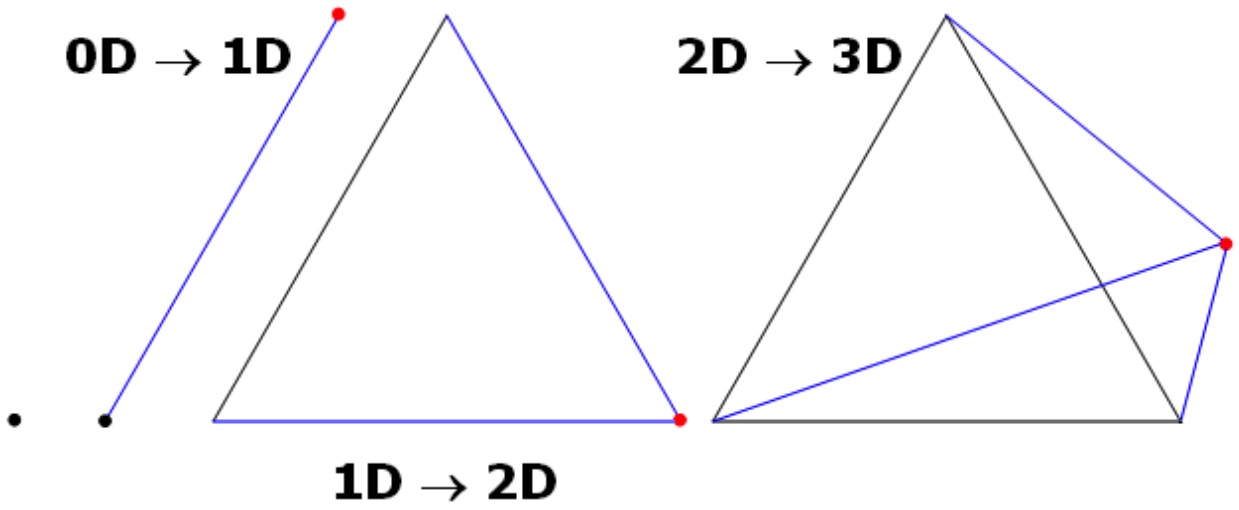
Part 2 - Finite Elements in 2D and 3D

2.3. The finite element space $V_{h,0}$

The mesh - a simplicial partition

What is a simplex? A simplex is an

- interval/line for $d = 1$;
- triangle for $d = 2$;
- tetrahedra for $d = 3$.



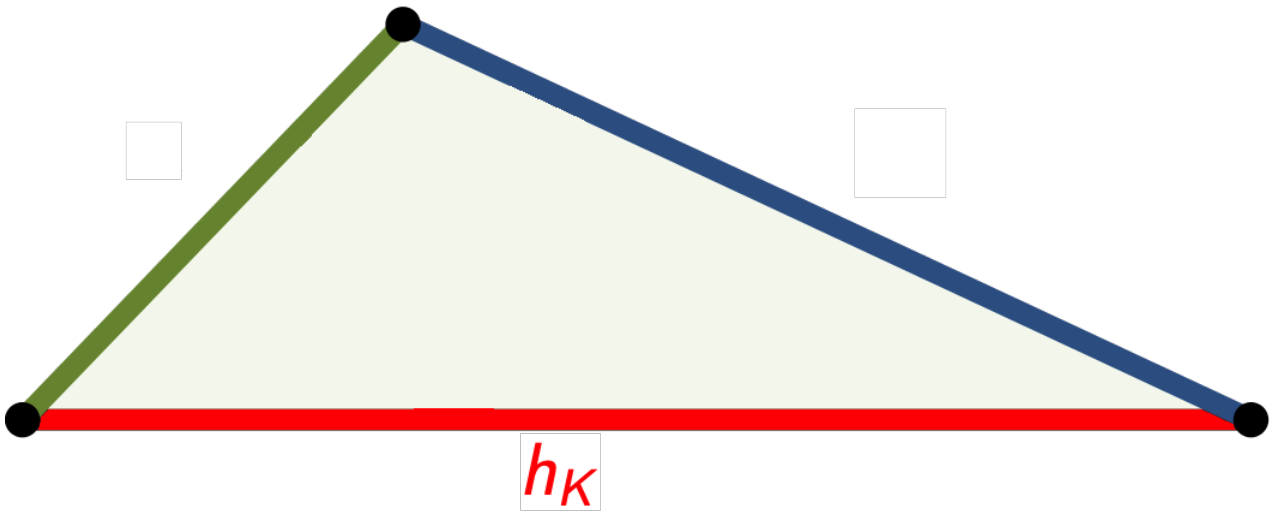
The mesh - a simplicial partition

Every simplex K has two important features, which measure its "quality":

a) The mesh size of a simplex K is

$$h_K := \mathrm{diam}(K);$$

We want it to be <u>small</u>.



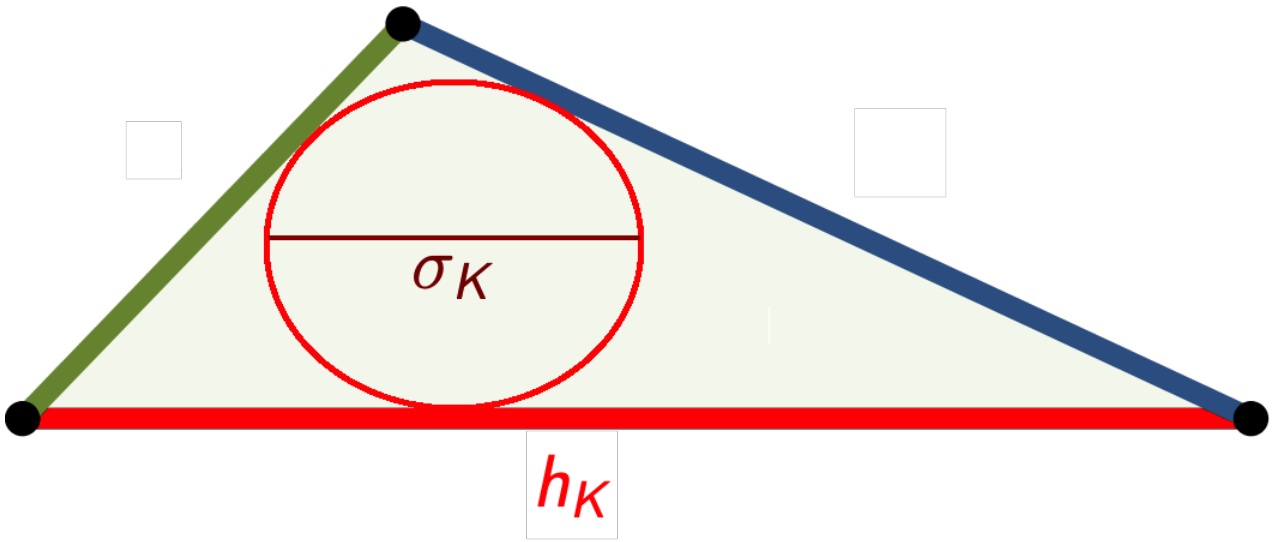
The mesh - a simplicial partition

b) The shape regularity of a simplex K.

For that let σ_K be the incircle diameter.

The shape regularity of K is now

$$\rho_K := \frac{h_K}{\sigma_K} > 1.$$

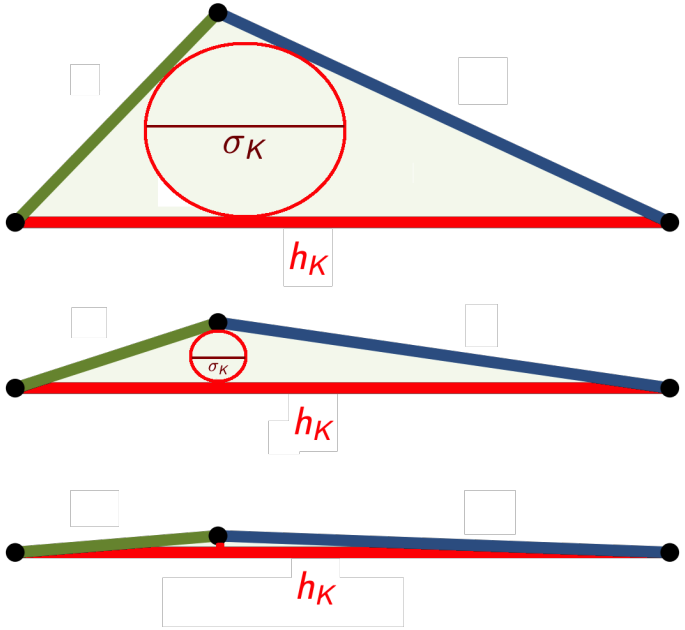


The mesh - a simplicial partition

Why is shape regularity characterized by

$$\rho_K := \frac{h_K}{\sigma_K} > 1?$$

The closer ρ_K is to 1, the more shape regular is K.



We want to avoid small angles!

The mesh - a simplicial partition

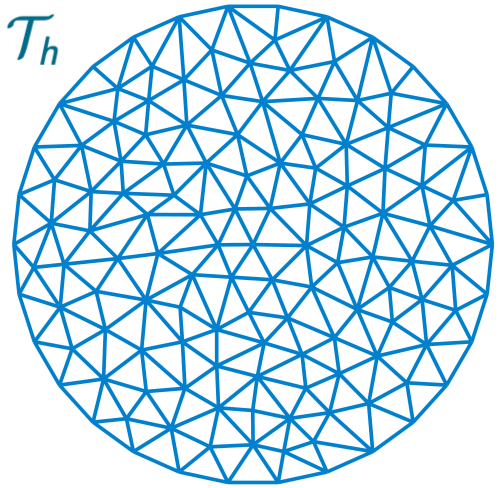
In order to construct $V_{h,0}$, we divide Ω into simplexes in the following way:

- $\mathcal{T}_h$ is a non-overlapping, simplicial partition of Ω,
$$\overline{\Omega} = \bigcup \{K \in \mathcal{T}_h\}$$
- The mesh size is
$$h := \max_{K \in \mathcal{T}_h} h_K;$$
- $\mathcal{T}_h$ is shape regular, i.e.
$$\sigma := \max_{K \in \mathcal{T}_h} \sigma_K$$
is not large (elements of $\mathcal{T}_h$ do not have small angles).

The mesh - a simplicial partition

The domain Ω is divided in simplexes:

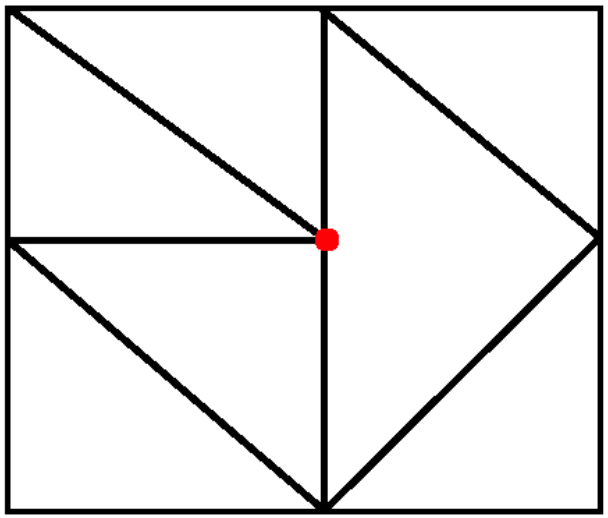
- $\mathcal{T}_h$ is a non-overlapping, simplicial partition of Ω,
- $\mathcal{T}_h$ is shape regular,
- $\mathcal{T}_h$ is quasi-uniform, i.e. all elements have roughly the same diameter h_T.



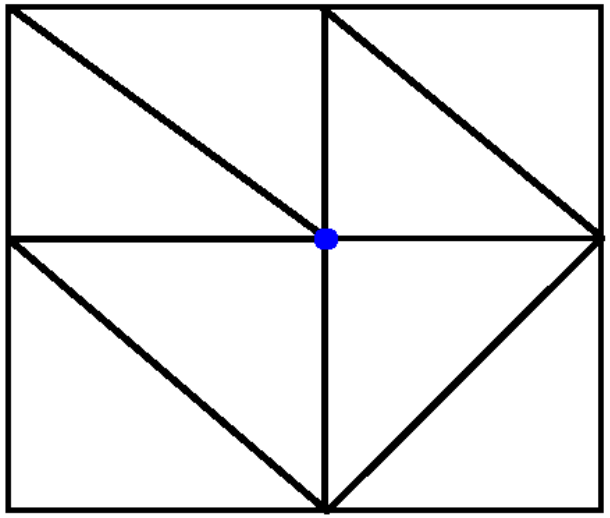
The mesh - a simplicial partition

Finally, the partition $\mathcal{T}_h$ is not allowed to have hanging nodes,

i.e., the corners of a simplex must be always aligned with a corner of all surrounding simplexes.



Hanging node.



Regular node.

The mesh - a simplicial partition

Summary of the properties:

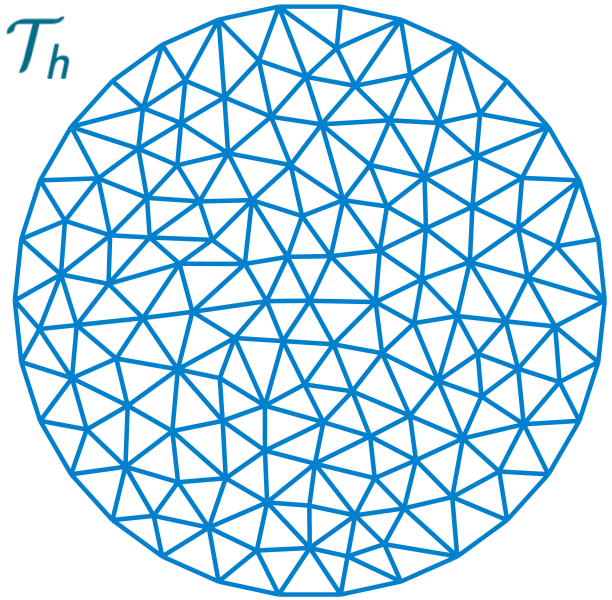
- $\mathcal{T}_h$ is non-overlapping, simplicial partition of Ω,
- $\mathcal{T}_h$ is shape regular,
- $\mathcal{T}_h$ is quasi-uniform,
- $\mathcal{T}_h$ has no hanging nodes.

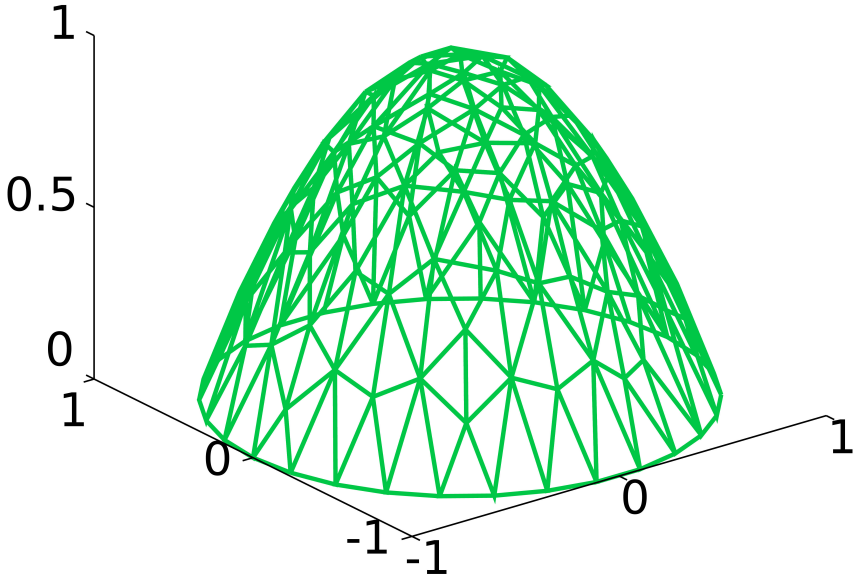
So called Delaunay triangulations have these properties. In Matlab they are part of the PDE-Toolbox and can be generated with `initmesh`.

The $P1$ (Lagrange) finite element space

On the mesh $\mathcal{T}_h$ we define the $P1$ finite element space as

$$V_{h,0} := \{v \in C^0(\Omega) \cap H_0^1(\Omega) | \\ \forall K \in \mathcal{T}_h : \; v_{|K} \text{ is polynomial of degree } 1\}.$$



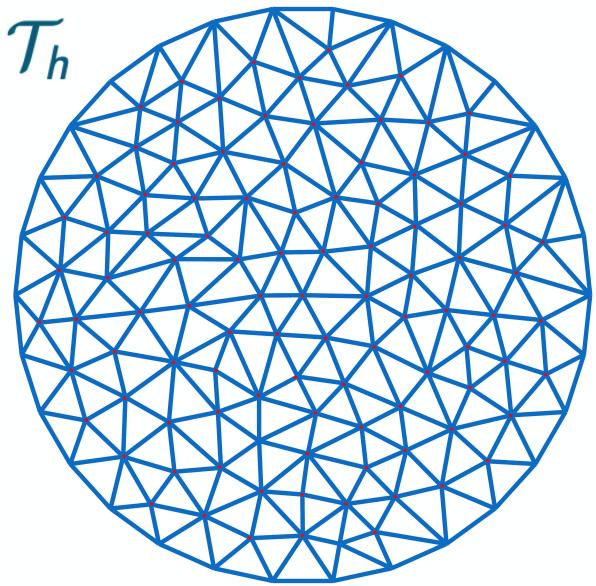


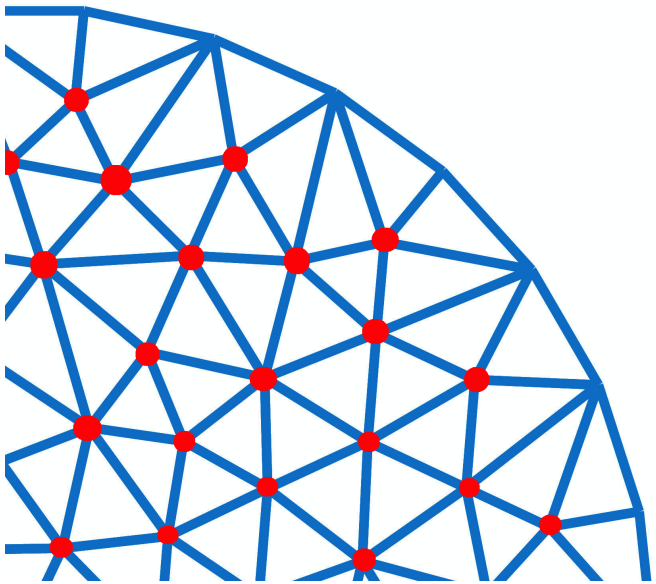
The $P1$ (Lagrange) finite element space

The corners of simplexes (e.g. triangles in $2d$) are called the nodes of $\mathcal{T}_h$.

The set of all nodes is denoted by $\mathcal{N}_h$.

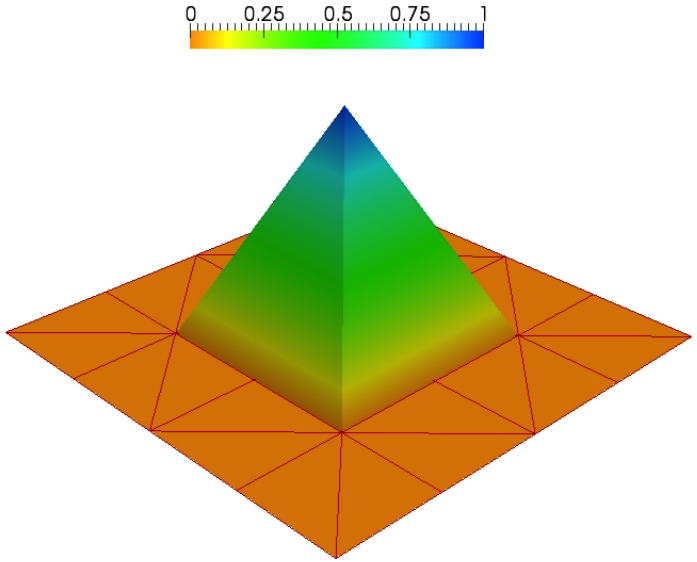
The interior nodes are $\mathcal{N}_{h,0} := \mathcal{N}_h \setminus \partial\Omega$.





The $P1$ (Lagrange) finite element space

The FE space $V_{h,0}$ is spanned by the nodal basis ("hat functions"), i.e., $V_{h,0} = \text{span}\{\phi_z \mid z \in \mathcal{N}_{h,0}\}$



Here we have $\phi_z \in V_{h,0}$, which is uniquely determined by the conditions

$$\phi_z(z) = 1 \qquad \text{and} \qquad \phi_z(\tilde{z}) = 0 \quad \text{for } \tilde{z} \in \mathcal{N}_h \setminus \{z\}.$$

The $P1$ (Lagrange) finite element space

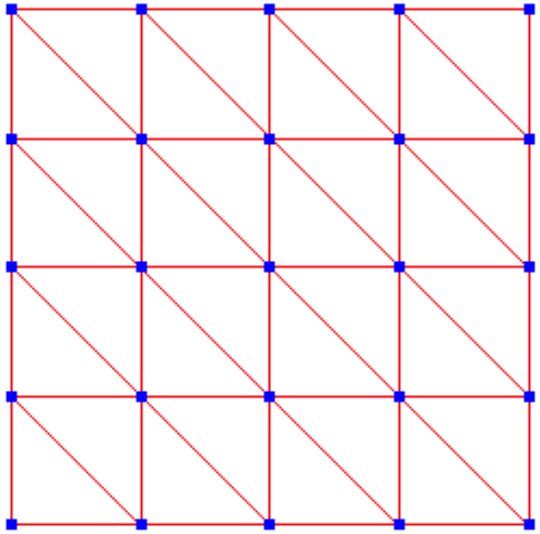
Note:

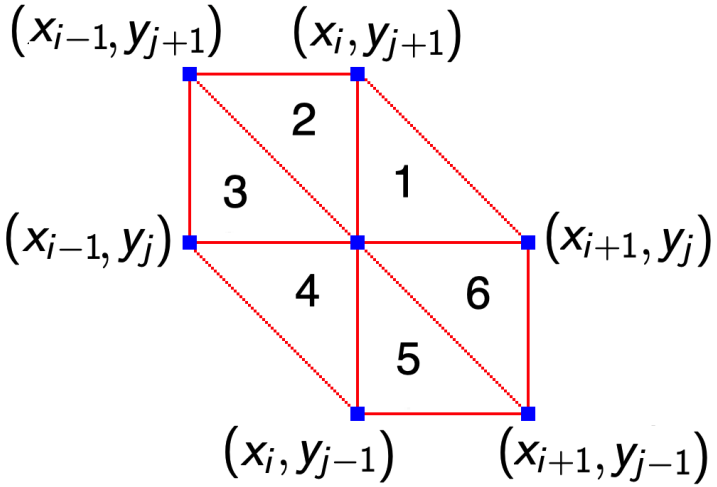
any $v_h \in V_{h,0}$ is uniquely determined by its nodal values $v_h(z)$, i.e.,

$$v_h(x) = \sum_{z \in \mathcal{N}_{h,0}} v_h(z)\, \phi_z(x).$$

Example: $P1$ basis function in 2D

We consider the mesh below and the node $z = (x_i, y_j)$.





The corresponding nodal basis function $\phi_z(x, y) = \phi_{ij}(x, y)$ is:

$$\phi_{ij}(x, y) = \begin{cases} 1 - \frac{1}{h}(x - x_i) - \frac{1}{h}(y - y_j) & \text{for } (x, y) \in 1 \\ 1 - \frac{1}{h}(y - y_j) & \text{for } (x, y) \in 2 \\ 1 + \frac{1}{h}(x - x_i) & \text{for } (x, y) \in 3 \\ 1 + \frac{1}{h}(x - x_i) + \frac{1}{h}(y - y_j) & \text{for } (x, y) \in 4 \\ 1 + \frac{1}{h}(y - y_j) & \text{for } (x, y) \in 5 \\ 1 - \frac{1}{h}(x - x_i) & \text{for } (x, y) \in 6 \\ 0 & \text{else.} \end{cases}$$

Part 2 - Finite Elements in 2D and 3D

2.4. The finite element method

Finite element approximation

We seek $u \in H_0^1(\Omega)$ such that

$$(k\nabla u, \nabla v)_{L^2(\Omega)} = (f, v)_{L^2(\Omega)} \quad \text{for all } v \in H_0^1(\Omega).$$

To find a P1 finite element approximation u_h, we replace $H_0^1(\Omega)$ by $V_{h,0}$. This yields:

Find $u_h \in V_{h,0}$ such that

$$(k\nabla u_h, \nabla v_h)_{L^2(\Omega)} = (f, v_h)_{L^2(\Omega)} \quad \text{for all } v_h \in V_{h,0}.$$

Finite element approximation

The FE approximation $u_h \in V_{h,0}$ solves

$$(k\nabla u_h, \nabla v_h)_{L^2(\Omega)} = (f, v_h)_{L^2(\Omega)} \quad \text{for all } v_h \in V_{h,0}.$$

Since $\{\phi_{z_i}\}_{z_i \in \mathcal{N}_{h,0}}$ is a basis of $V_{h,0}$ this is the same as

$$(k\nabla u_h, \nabla \phi_{z_i})_{L^2(\Omega)} = (f, \phi_{z_i})_{L^2(\Omega)} \quad \text{for all } z_i \in \mathcal{N}_{h,0}.$$

We write

$$u_h = \sum_{z_j \in \mathcal{N}_{h,0}} \xi_j \, \phi_{z_j} \qquad \text{where } \xi_j = u_h(z_j),$$

and obtain

$$\sum_{z_j \in \mathcal{N}_{h,0}} \xi_j \, (k\nabla \phi_{z_j}, \nabla \phi_{z_i})_{L^2(\Omega)} = (f, \phi_{z_i})_{L^2(\Omega)}.$$

Finite element approximation

Finite Element Approximation

$$u_h = \sum_{z_j \in \mathcal{N}_{h,0}} \xi_j \, \phi_{z_j} \qquad \text{where } \xi_j = u_h(z_j) \text{ \underline{is unknown}},$$

solves

$$\sum_{z_j \in \mathcal{N}_{h,0}} \xi_j \underbrace{(k \nabla \phi_{z_j}, \nabla \phi_{z_i})_{L^2(\Omega)}}_{=\mathbf{A}_{ij}} = \underbrace{(f, \phi_{z_i})_{L^2(\Omega)}}_{\mathbf{b}_i}.$$

which can be written as system of equations

$$\begin{pmatrix} \mathbf{A}_{11} & \cdots & \mathbf{A}_{1,N} \\ \vdots & \ddots & \vdots \\ \mathbf{A}_{N,1} & \cdots & \mathbf{A}_{N,N} \end{pmatrix} \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_N \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \vdots \\ \mathbf{b}_N \end{pmatrix},$$

where N is the number of basis functions.

Notes on the FE-matrix properties

The entries of the matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$ are given by

$$\mathbf{A}_{ij} = (k \nabla \phi_{z_j}, \nabla \phi_{z_i})_{L^2(\Omega)}.$$

We observe:

- $\mathbf{A}$ is sparse, i.e. most entries are zero.
- If k is symmetric, then $\mathbf{A}$ is symmetric too, i.e., $\mathbf{A}_{ij} = \mathbf{A}_{ji}$.
- $\mathbf{A}$ is positive definite$^{(*)}$, i.e.,

$$\mathbf{A}\boldsymbol{\xi} \cdot \boldsymbol{\xi} > 0 \qquad \text{for all } \boldsymbol{\xi} \in \mathbb{R}^N \setminus \{0\}.$$

Hence: the system $\mathbf{A}\boldsymbol{\xi} = \boldsymbol{b}$ is uniquely solvable.

How do we see the positive definiteness?

Concerning $(*)$:

The entries are $\mathbf{A}_{ij} = (k\nabla\phi_{z_j}, \nabla\phi_{z_i})_{L^2(\Omega)}$.

For any $\xi \in \mathbb{R}^N \setminus \{0\}$ we define

$$v := \sum_j \xi_j \, \phi_{z_j}$$

and observe (with the assumed ellipticity of k)

$$\mathbf{A}\xi \cdot \xi = \sum_{ij} \mathbf{A}_{ij}\xi_i\xi_j = (k\nabla \sum_i \xi_i\phi_{z_j}, \nabla \sum_i \xi_j\phi_{z_i})_{L^2(\Omega)}$$

$$= (k\nabla v, \nabla v)_{L^2(\Omega)} \geq k_0 \|\nabla v\|^2_{L^2(\Omega)} > 0.$$

Condition number of the FE-matrix

$\mathbf{A} \in \mathbb{R}^{N \times N}$ is FE matrix; solve $\mathbf{A}\boldsymbol{\xi} = \mathbf{b}$.

If $\mathbf{A}$ is positive definite and symmetric, it makes sense to use an iterative solver (like the CG method).

The convergence speed of iterative solvers depends on the condition number $\kappa(\mathbf{A})$ of the matrix. The larger $\kappa(\mathbf{A})$ the slower the convergence.

The condition number of the stiffness matrix is (without proof)

$$\kappa(A) = \|A\| \, \|A^{-1}\| = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} \leq C h^{-2}.$$

This means, the smaller the mesh size, the longer the iterative method needs to converge.

Note on the FE-matrix

We come back to how to generate the matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$ in Matlab and how to compute the entries

$$\mathbf{A}_{ij} = (k \nabla \phi_{z_j}, \nabla \phi_{z_i})_{L^2(\Omega)}.$$

Before that, we quickly discuss different boundary conditions.

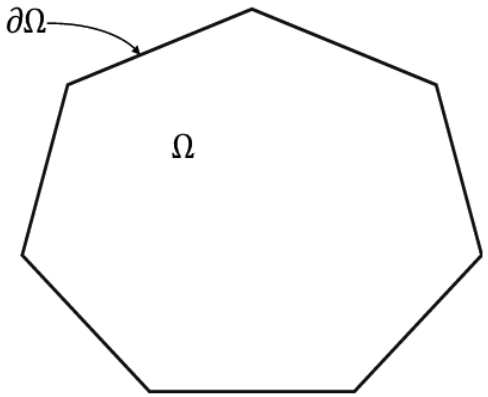
Part 2 - Finite Elements in 2D and 3D

2.5. Elliptic problems with general Dirichlet or Neumann boundary conditions

Reminder: assumptions

Let

- $\Omega \subset \mathbb{R}^d$ be a convex and polygonal domain



- source term: $f \in L^2(\Omega)$,
- conductivity/diffusion coefficient: $\mathbf{k} \in L^\infty(\Omega, \mathbb{R}^{d\times d})$ which is elliptic, i.e.,

$$\mathbf{k}(x)\boldsymbol{\xi} \cdot \boldsymbol{\xi} \geq \mathbf{k}_0 |\boldsymbol{\xi}|^2 \qquad \text{for all } \boldsymbol{\xi} \in \mathbb{R}^d$$

(in $1d$, this means $k(x) \geq k_0 > 0$)

General Dirichlet boundary condition

Find $u \in H^1(\Omega)$ such that

$$-\nabla \cdot (k \nabla u) = f \qquad \text{in } \Omega$$

and

$$u = g \qquad \text{on } \partial\Omega.$$

$g \in H^1(\Omega)$ is given Dirichlet boundary funct.
(that we only need to know on $\partial\Omega$)

General Dirichlet boundary condition

Variational formulation (using Green's formula):

Find $u \in H^1(\Omega)$ with $u - g \in H_0^1(\Omega)$ and

$$(k\nabla u, \nabla v)_{L^2(\Omega)} = (f, v)_{L^2(\Omega)}$$

for all $v \in H_0^1(\Omega)$.

Finite element approximation:

Find $u_h \in V_h$ with $u_h(z) = g(z)$ for all boundary nodes $z \in \mathcal{N}_h \cap \partial\Omega$ and

$$(k\nabla u_h, \nabla v_h)_{L^2(\Omega)} = (f, v_h)_{L^2(\Omega)}$$

for all $v_h \in V_{h,0}$.

General Dirichlet boundary condition

Finite element approximation:

Find $u_h \in V_h$ with $u_h(z) = g(z)$ for $z \in \mathcal{N}_h \cap \partial\Omega$:

$$(k\nabla u_h, \nabla v_h)_{L^2(\Omega)} = (f, v_h)_{L^2(\Omega)}$$

for all $v_h \in V_{h,0}$.

We write

$$u_h = \sum_{z_i \in \mathcal{N}_h} u_h(z_i)\,\phi_i = \sum_{z_i \in \mathcal{N}_{h,0}} \xi_i\,\phi_i + \sum_{z_i \in \mathcal{N}_h \cap \partial\Omega} g(z_i)\,\phi_i,$$

where ξ_i is unknown.

General Dirichlet boundary condition

Finite element approximation:

$$u_h = \sum_{z_i \in \mathcal{N}_{h,0}} \xi_i \, \phi_i + \sum_{z_i \in \mathcal{N}_h \cap \partial\Omega} g(z_i) \, \phi_i,$$

where the unknown ξ_i solve

$$\sum_{z_i \in \mathcal{N}_{h,0}} \xi_i (k \nabla \phi_i, \nabla \phi_j)_{L^2(\Omega)}$$

$$= (f, \phi_j)_{L^2(\Omega)} - \sum_{z_i \in \mathcal{N}_h \cap \partial\Omega} g(z_i) (k \nabla \phi_i, \nabla \phi_j)_{L^2(\Omega)}$$

for all ϕ_j with $z_j \in \mathcal{N}_{h,0}$.

Again, problem can be written as algebraic system of equations that we can solve.

General Neumann boundary condition

Find $u \in H^1(\Omega)$ such that

$$-\nabla \cdot (k \nabla u) + u = f \qquad \text{in } \Omega$$

and

$$k \nabla u \cdot \mathbf{n} = g_N \qquad \text{on } \partial\Omega.$$

$g_N \in L^2(\partial\Omega)$ is a given Neumann boundary function and $\mathbf{n}$ the unit outer normal on $\partial\Omega$.

General Neumann boundary condition

Find $u \in H^1(\Omega)$ such that

$$-\nabla \cdot (k \nabla u) + u = f \qquad \text{in } \Omega$$

and

$$k \nabla u \cdot \mathbf{n} = g_N \qquad \text{on } \partial\Omega.$$

Recall the Green's formula:

$$\begin{aligned} -\int_\Omega (\nabla \cdot k \nabla u)\, v &= \int_\Omega k \nabla u \cdot \nabla v - \int_{\partial\Omega} (k \nabla u \cdot \mathbf{n})\, v \\ &= \int_\Omega k \nabla u \cdot \nabla v - \int_{\partial\Omega} g_N\, v \end{aligned}$$

General Neumann boundary condition

Variational formulation (using Green's formula):

Find $u \in H^1(\Omega)$ with

$$\begin{aligned}(k\nabla u, \nabla v)_{L^2(\Omega)} + (u, v)_{L^2(\Omega)} \\ = \ (f, v)_{L^2(\Omega)} + (g_N, v)_{L^2(\partial\Omega)}\end{aligned}$$

for all $v \in H^1(\Omega)$.

Finite element approximation:

Find $u_h \in V_h$ with

$$\begin{aligned}(k\nabla u_h, \nabla v_h)_{L^2(\Omega)} + (u_h, v_h)_{L^2(\Omega)} \\ = \ (f, v_h)_{L^2(\Omega)} + (g_N, v_h)_{L^2(\partial\Omega)}\end{aligned}$$

for all $v_h \in V_h$. (can be solved as usual)