

Scientific Computing WS 2018/2019

Lecture 15

Jürgen Fuhrmann

juergen.fuhrmann@wias-berlin.de

Problems with “strong formulation”

Writing the PDE with divergence and gradient assumes smoothness of coefficients and at least second derivatives for the solution.

- ▶ δ may not be continuous – what is then $\nabla \cdot (\delta \nabla u)$?
- ▶ Approximation of solution u e.g. by piecewise linear functions what does ∇u mean ?
- ▶ Spaces of twice, and even once continuously differentiable functions is not well suited:
 - ▶ Favorable approximation functions (e.g. piecewise linear ones) are not contained
 - ▶ Though they can be equipped with norms (\Rightarrow Banach spaces) they have no scalar product \Rightarrow no Hilbert spaces
 - ▶ Not complete: Cauchy sequences of functions may not converge to elements in these spaces

Cauchy sequences of functions

- ▶ Let Ω be a Lipschitz domain, let V be a metric space of functions $f : \Omega \rightarrow \mathbb{R}$
- ▶ Regard sequences of functions $f_n = \{f_n\}_{n=1}^{\infty} \subset V$
- ▶ A *Cauchy sequence* is a sequence f_n of functions where the norm of the difference between two elements can be made arbitrarily small by increasing the element numbers:

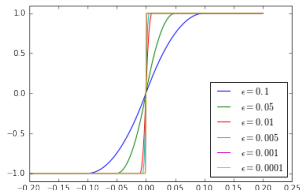
$$\forall \varepsilon > 0 \exists n_0 \in \mathbb{N} : \forall m, n > n_0, \|f_n - f_m\| < \varepsilon$$

- ▶ All convergent sequences of functions are Cauchy sequences
- ▶ A metric space V is *complete* if all Cauchy sequences f_n of its elements have a limit $f = \lim_{n \rightarrow \infty} f_n \in V$ within this space

Completion of a metric space

- ▶ Let V be a metric space. Its completion is the space \bar{V} consisting of all elements of V and all possible limits of Cauchy sequences of elements of V .
- ▶ This procedure allows to carry over definitions which are applicable only to elements of V to more general ones
- ▶ Example: step function

$$f_{\epsilon}(x) = \begin{cases} 1, & x \geq \epsilon \\ -\left(\frac{x-\epsilon}{\epsilon}\right)^2 + 1, & 0 \leq x < \epsilon \\ \left(\frac{x+\epsilon}{\epsilon}\right)^2 - 1, & -\epsilon \leq x < 0 \\ -1, & x < -\epsilon \end{cases} \xrightarrow{\epsilon \rightarrow 0} f(x) = \begin{cases} 1, & x \geq 0 \\ -1, & \text{else} \end{cases}$$



Riemann integral \rightarrow Lebesgue integral

- ▶ Let Ω be a Lipschitz domain, let $C_c(\Omega)$ be the set of continuous functions $f : \Omega \rightarrow \mathbb{R}$ with compact support. (\Rightarrow they vanish on $\partial\Omega$)
- ▶ For these functions, the Riemann integral $\int_{\Omega} f(x) d\mathbf{x}$ is well defined, and $\|f\|_{L^1} := \int_{\Omega} |f(x)| d\mathbf{x}$ provides a norm, and induces a metric.
- ▶ Let $L^1(\Omega)$ be the completion of $C_c(\Omega)$ with respect to the metric defined by the norm $\|\cdot\|_{L^1}$. That means that $L^1(\Omega)$ consists of all elements of $C_c(\Omega)$, and of all limites of Cauchy sequences of elements of $C_c(\Omega)$. Such functions are called *measurable*.
- ▶ For any measurable $f = \lim_{n \rightarrow \infty} f_n \in L^1(\Omega)$ with $f_n \in C_c(\Omega)$, define the *Lebesgue integral*

$$\int_{\Omega} f(x) d\mathbf{x} := \lim_{n \rightarrow \infty} \int_{\Omega} f_n(x) d\mathbf{x}$$

as the limit of a sequence of Riemann integrals of continuous functions

Examples for Lebesgue integrable (measurable) functions

- ▶ Bounded functions which are continuous except in a finite number of points
- ▶ Step functions
- ▶ Equality of L^1 functions is elusive as they are not necessarily continuous: best what we can say is that they are equal “almost everywhere”.
- ▶ In particular, L^1 functions whose values differ in a finite number of points are equal almost everywhere.

Spaces of integrable functions

- ▶ For $1 \leq p \leq \infty$, let $L^p(\Omega)$ be the space of measurable functions such that

$$\int_{\Omega} |f(x)|^p dx < \infty$$

equipped with the norm

$$\|f\|_p = \left(\int_{\Omega} |f(x)|^p dx \right)^{\frac{1}{p}}$$

- ▶ These spaces are *Banach spaces*, i.e. complete, normed vector spaces.
- ▶ The space $L^2(\Omega)$ is a *Hilbert space*, i.e. a Banach space equipped with a scalar product (\cdot, \cdot) whose norm is induced by that scalar product, i.e. $\|u\| = \sqrt{(u, u)}$. The scalar product in L^2 is

$$(f, g) = \int_{\Omega} f(x)g(x) dx.$$

Green's theorem for smooth functions

Theorem Let $u, v \in C^1(\bar{\Omega})$ (continuously differentiable). Then for $\mathbf{n} = (n_1 \dots n_d)$ being the outward normal to Ω ,

$$\int_{\Omega} u \partial_i v \, d\mathbf{x} = \int_{\partial\Omega} u v n_i \, ds - \int_{\Omega} v \partial_i u \, d\mathbf{x}$$

Corollaries

- ▶ Let $\mathbf{u} = (u_1 \dots u_d)$. Then

$$\int_{\Omega} \left(\sum_{i=1}^d u_i \partial_i v \right) d\mathbf{x} = \int_{\partial\Omega} v \sum_{i=1}^d (u_i n_i) \, ds - \int_{\Omega} v \sum_{i=1}^d (\partial_i u_i) \, d\mathbf{x}$$
$$\int_{\Omega} \mathbf{u} \cdot \nabla v \, d\mathbf{x} = \int_{\partial\Omega} v \mathbf{u} \cdot \mathbf{n} \, ds - \int_{\Omega} v \nabla \cdot \mathbf{u} \, d\mathbf{x}$$

- ▶ If $v = 0$ on $\partial\Omega$:

$$\int_{\Omega} u \partial_i v \, d\mathbf{x} = - \int_{\Omega} v \partial_i u \, d\mathbf{x}$$
$$\int_{\Omega} \mathbf{u} \cdot \nabla v \, d\mathbf{x} = - \int_{\Omega} v \nabla \cdot \mathbf{u} \, d\mathbf{x}$$

Weak derivative

- ▶ Let $L^1_{loc}(\Omega)$ be the set of functions which are Lebesgue integrable on every compact subset $K \subset \Omega$. Let $C_0^\infty(\Omega)$ be the set of functions infinitely differentiable with zero values on the boundary.
- ▶ For $u \in L^1_{loc}(\Omega)$ we *define* $\partial_i u$ by

$$\int_{\Omega} v \partial_i u d\mathbf{x} = - \int_{\Omega} u \partial_i v d\mathbf{x} \quad \forall v \in C_0^\infty(\Omega)$$

and $\partial^\alpha u$ by

$$\int_{\Omega} v \partial^\alpha u d\mathbf{x} = (-1)^{|\alpha|} \int_{\Omega} u \partial_i v d\mathbf{x} \quad \forall v \in C_0^\infty(\Omega)$$

if these integrals exist.

- ▶ For smooth functions, weak derivatives coincide with with the usual derivative

Sobolev spaces

- ▶ For $k \geq 0$ and $1 \leq p < \infty$, the Sobolev space $W^{k,p}(\Omega)$ is the space of functions where all up to the k -th derivatives are in L^p :

$$W^{k,p}(\Omega) = \{u \in L^p(\Omega) : \partial^\alpha u \in L^p(\Omega) \forall |\alpha| \leq k\}$$

with the norm

$$\|u\|_{W^{k,p}(\Omega)} = \left(\sum_{|\alpha| \leq k} \|\partial^\alpha u\|_{L^p(\Omega)}^p \right)^{\frac{1}{p}}$$

- ▶ Alternatively, they can be defined as the completion of C^∞ in the norm $\|u\|_{W^{k,p}(\Omega)}$
- ▶ $W_0^{k,p}(\Omega)$ is the completion of C_0^∞ in the norm $\|u\|_{W^{k,p}(\Omega)}$
- ▶ The Sobolev spaces are Banach spaces.

Sobolev spaces of square integrable functions

- ▶ $H^k(\Omega) = W^{k,2}(\Omega)$ with the scalar product

$$(u, v)_{H^k(\Omega)} = \sum_{|\alpha| \leq k} \int_{\Omega} \partial^{\alpha} u \partial^{\alpha} v \, dx$$

is a Hilbert space.

- ▶ $H_0^k(\Omega) = W_0^{k,2}(\Omega)$ with the scalar product

$$(u, v)_{H_0^k(\Omega)} = \sum_{|\alpha|=k} \int_{\Omega} \partial^{\alpha} u \partial^{\alpha} v \, dx$$

is a Hilbert space as well.

- ▶ For this course the most important:

- ▶ $L^2(\Omega)$, scalar product $(u, v)_{L^2(\Omega)} = (u, v)_{0,\Omega} = \int_{\Omega} uv \, dx$

- ▶ $H^1(\Omega)$, scalar product $(u, v)_{H^1(\Omega)} = (u, v)_{1,\Omega} = \int_{\Omega} (uv + \nabla u \cdot \nabla v) \, dx$

- ▶ $H_0^1(\Omega)$, scalar product $(u, v)_{H_0^1(\Omega)} = \int_{\Omega} (\nabla u \cdot \nabla v) \, dx$

- ▶ Inequalities:

$$|(u, v)|^2 \leq (u, u)(v, v) \quad \text{Cauchy-Schwarz}$$

$$\|u + v\| \leq \|u\| + \|v\| \quad \text{Triangle inequality}$$

A trace theorem

The notion of function values on the boundary initially is only well defined for continuous functions. So we need an extension of this notion to functions from Sobolev spaces.

Theorem: Let Ω be a bounded Lipschitz domain. Then there exists a bounded linear mapping

$$\text{tr} : H^1(\Omega) \rightarrow L^2(\partial\Omega)$$

such that

- (i) $\exists c > 0$ such that $\|\text{tr } u\|_{0,\partial\Omega} \leq c \|u\|_{1,\Omega}$
- (ii) $\forall u \in C^1(\bar{\Omega})$, $\text{tr } u = u|_{\partial\Omega}$



Derivation of weak formulation

- ▶ Sobolev space theory provides a convenient framework to formulate existence, uniqueness and approximations of solutions of PDEs.
- ▶ Stationary heat conduction equation with homogeneous Dirichlet boundary conditions:

$$\begin{aligned} -\nabla \cdot \lambda \nabla u(x) &= f(x) \text{ in } \Omega \\ u &= 0 \text{ on } \partial\Omega \end{aligned}$$

Multiply and integrate with an arbitrary *test function* $v \in C_0^\infty(\Omega)$ and apply Green's theorem using $v = 0$ on $\partial\Omega$

$$\begin{aligned} - \int_{\Omega} (\nabla \cdot \lambda \nabla u) v \, d\mathbf{x} &= \int_{\Omega} f v \, d\mathbf{x} \\ \int_{\Omega} \lambda \nabla u \nabla v \, d\mathbf{x} &= \int_{\Omega} f v \, d\mathbf{x} \end{aligned}$$

Weak formulation of homogeneous Dirichlet problem

- ▶ Search $u \in H_0^1(\Omega)$ (here, $\text{tr } u = 0$) such that

$$\int_{\Omega} \lambda \nabla u \nabla v \, d\mathbf{x} = \int_{\Omega} f v \, d\mathbf{x} \quad \forall v \in H_0^1(\Omega)$$

- ▶ Then,

$$a(u, v) := \int_{\Omega} \lambda \nabla u \nabla v \, d\mathbf{x}$$

is a self-adjoint bilinear form defined on the Hilbert space $H_0^1(\Omega)$.

- ▶ It is bounded due to Cauchy-Schwarz:

$$|a(u, v)| = |\lambda| \cdot \left| \int_{\Omega} \nabla u \nabla v \, d\mathbf{x} \right| \leq \|u\|_{H_0^1(\Omega)} \cdot \|v\|_{H_0^1(\Omega)}$$

- ▶ $f(v) = \int_{\Omega} f v \, d\mathbf{x}$ is a linear functional on $H_0^1(\Omega)$. For Hilbert spaces V the dual space V' (the space of linear functionals) can be identified with the space itself.

The Lax-Milgram lemma

Theorem: Let V be a Hilbert space. Let $a : V \times V \rightarrow \mathbb{R}$ be a self-adjoint bilinear form, and f a linear functional on V . Assume a is coercive, i.e.

$$\exists \alpha > 0 : \forall u \in V, a(u, u) \geq \alpha \|u\|_V^2.$$

Then the problem: find $u \in V$ such that

$$a(u, v) = f(v) \quad \forall v \in V$$

admits one and only one solution with an a priori estimate

$$\|u\|_V \leq \frac{1}{\alpha} \|f\|_{V'}$$



Coercivity of weak formulation

Theorem: Assume $\lambda > 0$. Then the weak formulation of the heat conduction problem: search $u \in H_0^1(\Omega)$ such that

$$\int_{\Omega} \lambda \nabla u \nabla v \, d\mathbf{x} = \int_{\Omega} f v \, d\mathbf{x} \quad \forall v \in H_0^1(\Omega)$$

has a unique solution.

Proof: $a(u, v)$ is coercive:

$$a(u, v) = \int_{\Omega} \lambda \nabla u \nabla u \, d\mathbf{x} = \lambda \|u\|_{H_0^1(\Omega)}^2$$



Weak formulation of inhomogeneous Dirichlet problem

$$\begin{aligned} -\nabla \cdot \lambda \nabla u &= f \text{ in } \Omega \\ u &= g \text{ on } \partial\Omega \end{aligned}$$

- ▶ If g is smooth enough, there exists a *lifting* $u_g \in H^1(\Omega)$ such that $u_g|_{\partial\Omega} = g$. Then, we can re-formulate:

$$\begin{aligned} -\nabla \cdot \lambda \nabla (u - u_g) &= f + \nabla \cdot \lambda \nabla u_g \text{ in } \Omega \\ u - u_g &= 0 \text{ on } \partial\Omega \end{aligned}$$

- ▶ Search $u \in H^1(\Omega)$ such that

$$\begin{aligned} u &= u_g + \phi \\ \int_{\Omega} \lambda \nabla \phi \nabla v \, d\mathbf{x} &= \int_{\Omega} f v \, d\mathbf{x} + \int_{\Omega} \lambda \nabla u_g \nabla v \, d\mathbf{x} \quad \forall v \in H_0^1(\Omega) \end{aligned}$$

Here, necessarily, $\phi \in H_0^1(\Omega)$ and we can apply the theory for the homogeneous Dirichlet problem.

Weak formulation of Robin problem

$$\begin{aligned} -\nabla \cdot \lambda \nabla u &= f \text{ in } \Omega \\ \lambda \nabla u \cdot \mathbf{n} + \alpha(u - g) &= 0 \text{ on } \partial\Omega \end{aligned}$$

- ▶ Multiply and integrate with an arbitrary *test function* from $C_c^\infty(\Omega)$:

$$\begin{aligned} - \int_{\Omega} (\nabla \cdot \lambda \nabla u) v \, d\mathbf{x} &= \int_{\Omega} f v \, d\mathbf{x} \\ \int_{\Omega} \lambda \nabla u \nabla v \, d\mathbf{x} + \int_{\partial\Omega} (\lambda \nabla u \cdot \mathbf{n}) v \, ds &= \int_{\Omega} f v \, d\mathbf{x} \\ \int_{\Omega} \lambda \nabla u \nabla v \, d\mathbf{x} + \int_{\partial\Omega} \alpha u v \, ds &= \int_{\Omega} f v \, d\mathbf{x} + \int_{\partial\Omega} \alpha g v \, ds \end{aligned}$$

Weak formulation of Robin problem II

- ▶ Let

$$a^R(u, v) := \int_{\Omega} \lambda \nabla u \nabla v \, d\mathbf{x} + \int_{\partial\Omega} \alpha uv \, ds$$

$$f^R(v) := \int_{\Omega} fv \, d\mathbf{x} + \int_{\partial\Omega} \alpha gv \, ds$$

- ▶ Search $u \in H^1(\Omega)$ such that

$$a^R(u, v) = f^R(v) \quad \forall v \in H^1(\Omega)$$

- ▶ If $\lambda > 0$ and $\alpha > 0$ then $a^R(u, v)$ is coercive.

Neumann boundary conditions

- ▶ Homogeneous Neumann:

$$\lambda \nabla u \cdot \mathbf{n} = 0 \text{ on } \partial\Omega$$

- ▶ Inhomogeneous Neumann:

$$\lambda \nabla u \cdot \mathbf{n} = g \text{ on } \partial\Omega$$

- ▶ Weak formulation: Search $u \in H^1(\Omega)$ such that

$$\int_{\Omega} \nabla u \nabla v \, d\mathbf{x} = \int_{\partial\Omega} g v \, ds \quad \forall v \in H^1(\Omega)$$

Not coercive due to the fact that we can add an arbitrary constant to u and $a(u, u)$ stays the same!

Further discussion on boundary conditions

- ▶ Mixed boundary conditions:
One can have different boundary conditions on different parts of the boundary. In particular, if Dirichlet or Robin boundary conditions are applied on at least a part of the boundary of measure larger than zero, the bilinear form becomes coercive.
- ▶ Natural boundary conditions: Robin, Neumann
These are imposed in a “natural” way in the weak formulation
- ▶ Essential boundary conditions: Dirichlet
Explicitly imposed on the function space
- ▶ Coefficients $\lambda, \alpha \dots$ can be functions from Sobolev spaces as long as they do not change integrability of terms in the bilinear forms

The Galerkin method I

- ▶ Weak formulations “live” in Hilbert spaces which essentially are infinite dimensional
- ▶ For computer representations we need finite dimensional approximations
- ▶ The Galerkin method and its modifications provide a general scheme for the derivation of finite dimensional approximations
- ▶ Finite dimensional subspaces of Hilbert spaces are the spans of a set of basis functions, and are Hilbert spaces as well \Rightarrow e.g. the Lax-Milgram lemma is valid there as well

The Galerkin method II

- ▶ Let V be a Hilbert space. Let $a : V \times V \rightarrow \mathbb{R}$ be a self-adjoint bilinear form, and f a linear functional on V . Assume a is coercive with coercivity constant α , and continuity constant γ .
- ▶ Continuous problem: search $u \in V$ such that

$$a(u, v) = f(v) \quad \forall v \in V$$

- ▶ Let $V_h \subset V$ be a finite dimensional subspace of V
- ▶ “Discrete” problem \equiv Galerkin approximation:
Search $u_h \in V_h$ such that

$$a(u_h, v_h) = f(v_h) \quad \forall v_h \in V_h$$

By Lax-Milgram, this problem has a unique solution as well.

Céa's lemma

- ▶ What is the connection between u and u_h ?
- ▶ Let $v_h \in V_h$ be arbitrary. Then

$$\begin{aligned}\alpha \|u - u_h\|^2 &\leq a(u - u_h, u - u_h) \quad (\text{Coercivity}) \\ &= a(u - u_h, u - v_h) + a(u - u_h, v_h - u_h) \\ &= a(u - u_h, u - v_h) \quad (\text{Galerkin Orthogonality}) \\ &\leq \gamma \|u - u_h\| \cdot \|u - v_h\| \quad (\text{Boundedness})\end{aligned}$$

- ▶ As a result

$$\|u - u_h\| \leq \frac{\gamma}{\alpha} \inf_{v_h \in V_h} \|u - v_h\|$$

- ▶ Up to a constant, the error of the Galerkin approximation is the error of the best approximation of the solution in the subspace V_h .

From the Galerkin method to the matrix equation

- ▶ Let $\phi_1 \dots \phi_n$ be a set of basis functions of V_h .
- ▶ Then, we have the representation $u_h = \sum_{j=1}^n u_j \phi_j$
- ▶ In order to search $u_h \in V_h$ such that

$$a(u_h, v_h) = f(v_h) \quad \forall v_h \in V_h$$

it is actually sufficient to require

$$\begin{aligned} a(u_h, \phi_i) &= f(\phi_i) \quad (i = 1 \dots n) \\ a\left(\sum_{j=1}^n u_j \phi_j, \phi_i\right) &= f(\phi_i) \quad (i = 1 \dots n) \\ \sum_{j=1}^n a(\phi_j, \phi_i) u_j &= f(\phi_i) \quad (i = 1 \dots n) \end{aligned}$$

$$AU = F$$

with $A = (a_{ij})$, $a_{ij} = a(\phi_i, \phi_j)$, $F = (f_i)$, $f_i = F(\phi_i)$, $U = (u_i)$.

- ▶ Matrix dimension is $n \times n$. Matrix sparsity ?

Obtaining a finite dimensional subspace

- ▶ Let $\Omega = (a, b) \subset \mathbb{R}^1$
- ▶ Let $a(u, v) = \int_{\Omega} \lambda(x) \nabla u \nabla v dx$.
- ▶ Analysis I provides a finite dimensional subspace: the space of sin/cos functions up to a certain frequency \Rightarrow *spectral method*
- ▶ Ansatz functions have global support \Rightarrow full $n \times n$ matrix
- ▶ OTOH: rather fast convergence for smooth data
- ▶ Generalization to higher dimensions possible
- ▶ Big problem in irregular domains: we need the eigenfunction basis of some operator. . .
- ▶ Spectral methods are successful in cases where one has regular geometry structures and smooth/constant coefficients – e.g. “Spectral Einstein Code”

Definition of a Finite Element (Ciarlet)

Triplet $\{K, P, \Sigma\}$ where

- ▶ $K \subset \mathbb{R}^d$: compact, connected Lipschitz domain with non-empty interior
- ▶ P : finite dimensional vector space of functions $p : K \rightarrow \mathbb{R}$
- ▶ $\Sigma = \{\sigma_1 \dots \sigma_s\} \subset \mathcal{L}(P, \mathbb{R})$: set of linear forms defined on P called *local degrees of freedom* such that the mapping

$$\begin{aligned}\Lambda_\Sigma : P &\rightarrow \mathbb{R}^s \\ p &\mapsto (\sigma_1(p) \dots \sigma_s(p))\end{aligned}$$

is bijective, i.e. Σ is a basis of $\mathcal{L}(P, \mathbb{R})$.

Local shape functions

- ▶ Due to bijectivity of Λ_Σ , for any finite element $\{K, P, \Sigma\}$, there exists a basis $\{\theta_1 \dots \theta_s\} \subset P$ such that

$$\sigma_i(\theta_j) = \delta_{ij} \quad (1 \leq i, j \leq s)$$

- ▶ Elements of such a basis are called *local shape functions*

Unisolvence

- ▶ Bijectivity of Λ_Σ is equivalent to the condition

$$\forall (\alpha_1 \dots \alpha_s) \in \mathbb{R}^s \exists! p \in P \text{ such that } \sigma_i(p) = \alpha_i \quad (1 \leq i \leq s)$$

i.e. for any given tuple of values $a = (\alpha_1 \dots \alpha_s)$ there is a unique polynomial $p \in P$ such that $\Lambda_\Sigma(p) = a$.

- ▶ Equivalent to *unisolvence*:

$$\begin{cases} \dim P = |\Sigma| = s \\ \forall p \in P : \sigma_i(p) = 0 (i = 1 \dots s) \Rightarrow p = 0 \end{cases}$$

Lagrange finite elements

- ▶ A finite element $\{K, P, \Sigma\}$ is called *Lagrange* finite element (or *nodal* finite element) if there exist a set of points $\{a_1 \dots a_s\} \subset K$ such that

$$\sigma_i(p) = p(a_i) \quad 1 \leq i \leq s$$

- ▶ $\{a_1 \dots a_s\}$: *nodes* of the finite element
- ▶ nodal basis: $\{\theta_1 \dots \theta_s\} \subset P$ such that

$$\theta_j(a_i) = \delta_{ij} \quad (1 \leq i, j \leq s)$$

Local interpolation operator

- ▶ Let $\{K, P, \Sigma\}$ be a finite element with shape function bases $\{\theta_1 \dots \theta_s\}$. Let $V(K)$ be a normed vector space of functions $v : K \rightarrow \mathbb{R}$ such that
 - ▶ $P \subset V(K)$
 - ▶ The linear forms in Σ can be extended to be defined on $V(K)$
- ▶ *local interpolation operator*

$$\mathcal{I}_K : V(K) \rightarrow P$$

$$v \mapsto \sum_{i=1}^s \sigma_i(v) \theta_i$$

- ▶ P is invariant under the action of \mathcal{I}_K , i.e. $\forall p \in P, \mathcal{I}_K(p) = p$:
 - ▶ Let $p = \sum_{j=1}^s \alpha_j \theta_j$ Then,

$$\begin{aligned} \mathcal{I}_K(p) &= \sum_{i=1}^s \sigma_i(p) \theta_i = \sum_{i=1}^s \sum_{j=1}^s \alpha_j \sigma_i(\theta_j) \theta_i \\ &= \sum_{i=1}^s \sum_{j=1}^s \alpha_j \delta_{ij} \theta_i = \sum_{j=1}^s \alpha_j \theta_j \end{aligned}$$

Local Lagrange interpolation operator

- ▶ Let $V(K) = (C^0(K))$

$$\mathcal{I}_K : V(K) \rightarrow P$$

$$v \mapsto I_K v = \sum_{i=1}^s v(a_i) \theta_i$$

Simplices

- ▶ Let $\{a_0 \dots a_d\} \subset \mathbb{R}^d$ such that the d vectors $a_1 - a_0 \dots a_d - a_0$ are linearly independent. Then the convex hull K of $a_0 \dots a_d$ is called *simplex*, and $a_0 \dots a_d$ are called *vertices* of the simplex.
- ▶ *Unit simplex*: $a_0 = (0 \dots 0)$, $a_1 = (0, 1 \dots 0) \dots a_d = (0 \dots 0, 1)$.

$$K = \left\{ x \in \mathbb{R}^d : x_i \geq 0 \ (i = 1 \dots d) \text{ and } \sum_{i=1}^d x_i \leq 1 \right\}$$

- ▶ A general simplex can be defined as an image of the unit simplex under some affine transformation
- ▶ F_i : face of K opposite to a_i
- ▶ \mathbf{n}_i : outward normal to F_i

Barycentric coordinates

- ▶ Let K be a simplex.
- ▶ Functions λ_i ($i = 0 \dots d$):

$$\lambda_i : \mathbb{R}^d \rightarrow \mathbb{R}$$

$$x \mapsto \lambda_i(x) = 1 - \frac{(x - a_j) \cdot \mathbf{n}_i}{(a_j - a_i) \cdot \mathbf{n}_i}$$

where a_j is any vertex of K situated in F_i .

- ▶ For $x \in K$, one has

$$\begin{aligned} 1 - \frac{(x - a_j) \cdot \mathbf{n}_i}{(a_j - a_i) \cdot \mathbf{n}_i} &= \frac{(a_j - a_i) \cdot \mathbf{n}_i - (x - a_j) \cdot \mathbf{n}_i}{(a_j - a_i) \cdot \mathbf{n}_i} \\ &= \frac{(a_j - x) \cdot \mathbf{n}_i}{(a_j - a_i) \cdot \mathbf{n}_i} = \frac{\text{dist}(x, F_i)}{\text{dist}(a_i, F_i)} \\ &= \frac{\text{dist}(x, F_i) |F_i| / d}{\text{dist}(a_i, F_i) |F_i| / d} \\ &= \frac{\text{dist}(x, F_i) |F_i|}{|K|} \end{aligned}$$

i.e. $\lambda_i(x)$ is the ratio of the volume of the simplex $K_i(x)$ made up of x and the vertices of F_i to the volume of K .

Barycentric coordinates II

- ▶ $\lambda_i(a_j) = \delta_{ij}$
- ▶ $\lambda_i(x) = 0 \forall x \in F_i$
- ▶ $\sum_{i=0}^d \lambda_i(x) = 1 \forall x \in \mathbb{R}^d$
(just sum up the volumes)
- ▶ $\sum_{i=0}^d \lambda_i(x)(x - a_i) = 0 \forall x \in \mathbb{R}^d$
(due to $\sum \lambda_i(x)x = x$ and $\sum \lambda_i a_i = x$ as the vector of linear coordinate functions)
- ▶ Unit simplex:
 - ▶ $\lambda_0(x) = 1 - \sum_{i=1}^d x_i$
 - ▶ $\lambda_i(x) = x_i$ for $1 \leq i \leq d$

Polynomial space \mathbb{P}_k

- ▶ Space of polynomials in $x_1 \dots x_d$ of total degree $\leq k$ with real coefficients $\alpha_{i_1 \dots i_d}$:

$$\mathbb{P}_k = \left\{ p(x) = \sum_{\substack{0 \leq i_1 \dots i_d \leq k \\ i_1 + \dots + i_d \leq k}} \alpha_{i_1 \dots i_d} x_1^{i_1} \dots x_d^{i_d} \right\}$$

- ▶ Dimension:

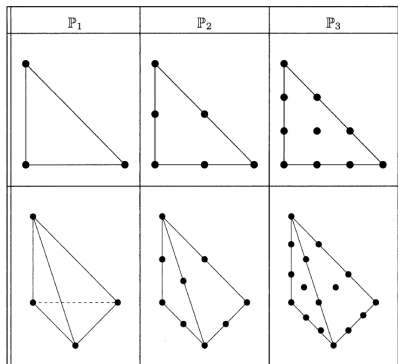
$$\dim \mathbb{P}_k = \binom{d+k}{k} = \begin{cases} k+1, & d=1 \\ \frac{1}{2}(k+1)(k+2), & d=2 \\ \frac{1}{6}(k+1)(k+2)(k+3), & d=3 \end{cases}$$

$$\dim \mathbb{P}_1 = d+1$$

$$\dim \mathbb{P}_2 = \begin{cases} 3, & d=1 \\ 6, & d=2 \\ 10, & d=3 \end{cases}$$

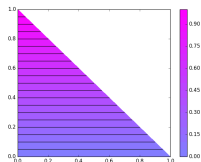
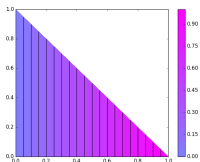
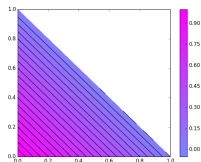
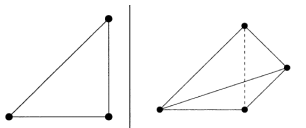
\mathbb{P}_k simplex finite elements

- ▶ K : simplex spanned by $a_0 \dots a_d$ in \mathbb{R}^d
- ▶ $P = \mathbb{P}_k$, such that $s = \dim P_k$
- ▶ For $0 \leq i_0 \dots i_d \leq k$, $i_0 + \dots + i_d = k$, let the set of nodes be defined by the points $a_{i_1 \dots i_d; k}$ with barycentric coordinates $(\frac{i_0}{k} \dots \frac{i_d}{k})$. Define Σ by $\sigma_{i_1 \dots i_d; k}(p) = p(a_{i_1 \dots i_d; k})$.



\mathbb{P}_1 simplex finite elements

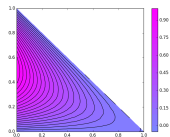
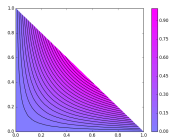
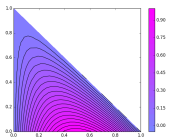
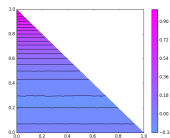
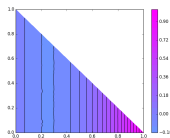
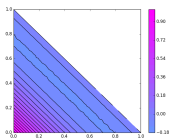
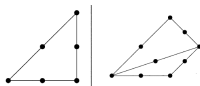
- ▶ K : simplex spanned by $a_0 \dots a_d$ in \mathbb{R}^d
- ▶ $P = \mathbb{P}_1$, such that $s = d + 1$
- ▶ Nodes \equiv vertices
- ▶ Basis functions \equiv barycentric coordinates



\mathbb{P}_2 simplex finite elements

- ▶ K : simplex spanned by $a_0 \dots a_d$ in \mathbb{R}^d
- ▶ $P = \mathbb{P}_2$, Nodes \equiv vertices + edge midpoints
- ▶ Basis functions:

$$\lambda_i(2\lambda_i - 1), (0 \leq i \leq d); \quad 4\lambda_i\lambda_j, \quad (0 \leq i < j \leq d) \quad (\text{"edge bubbles"})$$



General finite elements

- ▶ Simplicial finite elements can be defined on triangulations of polygonal domains. During the course we will stick to this case.
- ▶ For vector PDEs, one can define finite elements for vector valued functions
- ▶ A curved domain Ω may be approximated by a polygonal domain Ω_h which is then triangulated. During the course, we will ignore this difference.
- ▶ As we have seen, more general elements are possible: cuboids, but also prismatic elements etc.
- ▶ Curved geometries are possible. Isoparametric finite elements use the polynomial space to define a mapping of some polyhedral reference element to an element with curved boundary

Conformal triangulations

- ▶ Let \mathcal{T}_h be a subdivision of the polygonal domain $\Omega \subset \mathbb{R}^d$ into non-intersecting compact simplices K_m , $m = 1 \dots n_e$:

$$\bar{\Omega} = \bigcup_{m=1}^{n_e} K_m$$

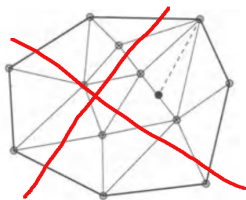
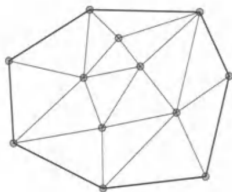
- ▶ Each simplex can be seen as the image of a affine transformation of a reference (e.g. unit) simplex \hat{K} :

$$K_m = T_m(\hat{K})$$

- ▶ We assume that it is conformal, i.e. if K_m, K_n have a $d - 1$ dimensional intersection $F = K_m \cap K_n$, then there is a face \hat{F} of \hat{K} and renumberings of the vertices of K_n, K_m such that $F = T_m(\hat{F}) = T_n(\hat{F})$ and $T_m|_{\hat{F}} = T_n|_{\hat{F}}$

Conformal triangulations II

- ▶ $d = 1$: Each intersection $F = K_m \cap K_n$ is either empty or a common vertex
- ▶ $d = 2$: Each intersection $F = K_m \cap K_n$ is either empty or a common vertex or a common edge



- ▶ $d = 3$: Each intersection $F = K_m \cap K_n$ is either empty or a common vertex or a common edge or a common face
- ▶ Delaunay triangulations are conformal

Global interpolation operator \mathcal{I}_h

- ▶ Let $\{K, P_K, \Sigma_K\}_{K \in \mathcal{T}_h}$ be a triangulation of Ω .
- ▶ Domain:

$$D(\mathcal{I}_h) = \{v \in (L^1(\Omega)) \text{ such that } \forall K \in \mathcal{T}_h, v|_K \in V(K)\}$$

- ▶ For all $v \in D(\mathcal{I}_h)$, define $\mathcal{I}_h v$ via

$$\mathcal{I}_h v|_K = \mathcal{I}_K(v|_K) = \sum_{i=1}^s \sigma_{K,i}(v|_K) \theta_{K,i} \quad \forall K \in \mathcal{T}_h,$$

Assuming $\theta_{K,i} = 0$ outside of K , one can write

$$\mathcal{I}_h v = \sum_{K \in \mathcal{T}_h} \sum_{i=1}^s \sigma_{K,i}(v|_K) \theta_{K,i},$$

mapping $D(\mathcal{I}_h)$ to the *approximation space*

$$W_h = \{v_h \in (L^1(\Omega)) \text{ such that } \forall K \in \mathcal{T}_h, v_h|_K \in P_K\}$$

H^1 -Conformal approximation using Lagrangian finite elements

- ▶ Conformal subspace of W_h with zero jumps at element faces:

$$V_h = \{v_h \in W_h : \forall n, m, K_m \cap K_n \neq \emptyset \Rightarrow (v_h|_{K_m})_{K_m \cap K_n} = (v_h|_{K_n})_{K_m \cap K_n}\}$$

- ▶ Then: $V_h \subset H^1(\Omega)$.

Zero jump at interfaces with Lagrangian finite elements

- ▶ Assume geometrically conformal mesh
- ▶ Assume all faces of \hat{K} have the same number of nodes s^∂
- ▶ For any face $F = K_1 \cap K_2$ there are renumberings of the nodes of K_1 and K_2 such that for $i = 1 \dots s^\partial$, $a_{K_1,i} = a_{K_2,i}$
- ▶ Then, $v_h|_{K_1}$ and $v_h|_{K_2}$ match at the interface $K_1 \cap K_2$ if and only if they match at the common nodes

$$v_h|_{K_1}(a_{K_1,i}) = v_h|_{K_2}(a_{K_2,i}) \quad (i = 1 \dots s^\partial)$$

Global degrees of freedom

- ▶ Let $\{a_1 \dots a_N\} = \bigcup_{K \in \mathcal{T}_h} \{a_{K,1} \dots a_{K,s}\}$
- ▶ Degree of freedom map

$$j : \mathcal{T}_h \times \{1 \dots s\} \rightarrow \{1 \dots N\}$$

$(K, m) \mapsto j(K, m)$ the global degree of freedom number

- ▶ Global shape functions $\phi_1, \dots, \phi_N \in W_h$ defined by

$$\phi_i|_K(a_{K,m}) = \begin{cases} \delta_{mn} & \text{if } \exists n \in \{1 \dots s\} : j(K, n) = i \\ 0 & \text{otherwise} \end{cases}$$

- ▶ Global degrees of freedom $\gamma_1, \dots, \gamma_N : V_h \rightarrow \mathbb{R}$ defined by

$$\gamma_i(v_h) = v_h(a_i)$$

Lagrange finite element basis

- ▶ $\{\phi_1, \dots, \phi_N\}$ is a basis of V_h , and $\gamma_1 \dots \gamma_N$ is a basis of $\mathcal{L}(V_h, \mathbb{R})$.

Proof:

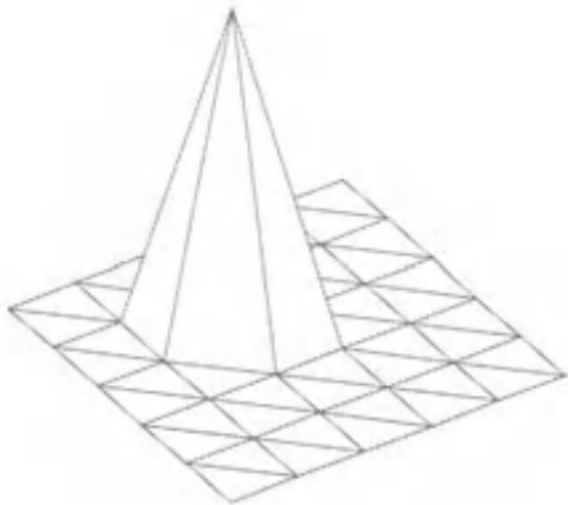
- ▶ $\{\phi_1, \dots, \phi_N\}$ are linearly independent: if $\sum_{j=1}^N \alpha_j \phi_j = 0$ then evaluation at $a_1 \dots a_N$ yields that $\alpha_1 \dots \alpha_N = 0$.
- ▶ Let $v_h \in V_h$. It is single valued in $a_1 \dots a_N$. Let $w_h = \sum_{j=1}^N v_h(a_j) \phi_j$. Then for all $K \in \mathcal{T}_h$, $v_h|_K$ and $w_h|_K$ coincide in the local nodes $a_{K,1} \dots a_{K,2}$, and by unisolvence, $v_h|_K = w_h|_K$.

Finite element approximation space

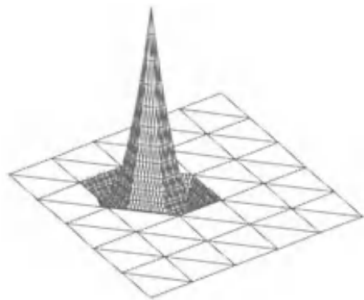
- ▶ $P_{c,h}^k = P_h^k = \{v_h \in C^0(\bar{\Omega}_h) : \forall K \in \mathcal{T}_h, v_k \circ T_K \in \mathbb{P}^k\}$
- ▶ 'c' for continuity across mesh interfaces. There are also discontinuous FEM spaces which we do not consider here.

d	k	$N = \dim P_h^k$
1	1	N_v
1	2	$N_v + N_{el}$
1	3	$N_v + 2N_{el}$
2	1	N_v
2	2	$N_v + N_{ed}$
2	3	$N_v + 2N_{ed} + N_{el}$
3	1	N_v
3	2	$N_v + N_{ed}$
3	3	$N_v + 2N_{ed} + N_f$

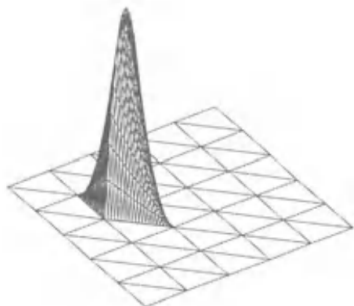
P^1 global shape functions



P^2 global shape functions



Node based



Edge based

Global Lagrange interpolation operator

Let $V_h = P_h^k$

$$\mathcal{I}_h : C^0(\bar{\Omega}_h) \rightarrow V_h$$
$$v \mapsto \sum_{i=1}^N v(\mathbf{a}_i) \phi_i$$

Quadrature rules

- ▶ *Quadrature rule:*

$$\int_K g(x) \, d\mathbf{x} \approx |K| \sum_{l=1}^{l_q} \omega_l g(\xi_l)$$

- ▶ ξ_l : *nodes, Gauss points*
- ▶ ω_l : *weights*
- ▶ The largest number k such that the quadrature is exact for polynomials of order k is called *order* k_q of the quadrature rule, i.e.

$$\forall k \leq k_q, \forall p \in \mathbb{P}^k \int_K p(x) \, d\mathbf{x} = |K| \sum_{l=1}^{l_q} \omega_l p(\xi_l)$$

- ▶ *Error estimate:*

$$\forall \phi \in C^{k_q+1}(K), \left| \frac{1}{|K|} \int_K \phi(x) \, d\mathbf{x} - \sum_{l=1}^{l_q} \omega_l \phi(\xi_l) \right| \leq ch_K^{k_q+1} \sup_{x \in K, |\alpha|=k_q+1} |\partial^\alpha \phi(x)|$$

Some common quadrature rules

Nodes are characterized by the barycentric coordinates

d	k_q	l_q	Nodes	Weights
1	1	1	$(\frac{1}{2}, \frac{1}{2})$	1
	1	2	$(1, 0), (0, 1)$	$\frac{1}{2}, \frac{1}{2}$
	3	2	$(\frac{1}{2} + \frac{\sqrt{3}}{6}, \frac{1}{2} - \frac{\sqrt{3}}{6}), (\frac{1}{2} - \frac{\sqrt{3}}{6}, \frac{1}{2} + \frac{\sqrt{3}}{6})$	$\frac{1}{2}, \frac{1}{2}$
	5	3	$(\frac{1}{2}, \frac{1}{2}), (\frac{1}{2} + \sqrt{\frac{3}{20}}, \frac{1}{2} - \sqrt{\frac{3}{20}}), (\frac{1}{2} - \sqrt{\frac{3}{20}}, \frac{1}{2} + \sqrt{\frac{3}{20}})$	$\frac{8}{18}, \frac{5}{18}, \frac{5}{18}$
2	1	1	$(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$	1
	1	3	$(1, 0, 0), (0, 1, 0), (0, 0, 1)$	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$
	2	3	$(\frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, 0, \frac{1}{2}), (0, \frac{1}{2}, \frac{1}{2})$	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$
	3	4	$(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}), (\frac{1}{5}, \frac{1}{5}, \frac{3}{5}), (\frac{1}{5}, \frac{3}{5}, \frac{1}{5}), (\frac{3}{5}, \frac{1}{5}, \frac{1}{5})$	$\frac{9}{16}, \frac{25}{48}, \frac{25}{48}, \frac{25}{48}$
3	1	1	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	1
	1	4	$(1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1)$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
	2	4	$(\frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5+3\sqrt{5}}{20}), \dots$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Weak formulation of homogeneous Dirichlet problem

- ▶ Search $u \in V = H_0^1(\Omega)$ such that

$$\int_{\Omega} \kappa \nabla u \nabla v \, d\mathbf{x} = \int_{\Omega} f v \, d\mathbf{x} \quad \forall v \in H_0^1(\Omega)$$

- ▶ Then,

$$a(u, v) := \int_{\Omega} \kappa \nabla u \nabla v \, d\mathbf{x}$$

is a self-adjoint bilinear form defined on the Hilbert space $H_0^1(\Omega)$.

Galerkin ansatz

- ▶ Let $V_h \subset V$ be a finite dimensional subspace of V
- ▶ “Discrete” problem \equiv Galerkin approximation:
Search $u_h \in V_h$ such that

$$a(u_h, v_h) = f(v_h) \quad \forall v_h \in V_h$$

- ▶ E.g. V_h is the space of P1 Lagrange finite element approximations

Stiffness matrix for Laplace operator for P1 FEM

- ▶ Element-wise calculation:

$$a_{ij} = a(\phi_i, \phi_j) = \int_{\Omega} \nabla \phi_i \nabla \phi_j \, d\mathbf{x} = \int_{\Omega} \sum_{K \in \mathcal{T}_h} \nabla \phi_i|_K \nabla \phi_j|_K \, d\mathbf{x}$$

- ▶ Standard assembly loop:

```
for  $i, j = 1 \dots N$  do
```

```
  | set  $a_{ij} = 0$ 
```

```
end
```

```
for  $K \in \mathcal{T}_h$  do
```

```
  | for  $m, n = 0 \dots d$  do
```

```
    |  $s_{mn} = \int_K \nabla \lambda_m \nabla \lambda_n \, d\mathbf{x}$ 
```

```
    |  $a_{j_{\text{dof}}(K, m), j_{\text{dof}}(K, n)} = a_{j_{\text{dof}}(K, m), j_{\text{dof}}(K, n)} + s_{mn}$ 
```

```
  | end
```

```
end
```

- ▶ Local stiffness matrix:

$$S_K = (s_{K; m, n}) = \int_K \nabla \lambda_m \nabla \lambda_n \, d\mathbf{x}$$