

~

P1 finite elements: time dependent problems

Scientific Computing Winter 2016/2017

Lecture 22

Jürgen Fuhrmann

juergen.fuhrmann@wias-berlin.de



~

Recap

Global interpolation error estimate for Lagrangian finite elements, $k = 1$

- ▶ Assume $v \in H^2(\Omega)$

$$\|v - \mathcal{I}_h^k v\|_{0,\Omega} + h|v - \mathcal{I}_h^k v|_{1,\Omega} \leq ch^2|v|_{2,\Omega}$$

$$|v - \mathcal{I}_h^k v|_{1,\Omega} \leq ch|v|_{2,\Omega}$$

$$\lim_{h \rightarrow 0} \left(\inf_{v_h \in V_h^k} |v - v_h|_{1,\Omega} \right) = 0$$

- ▶ If $v \in H^2(\Omega)$ cannot be guaranteed, estimates become worse. Example: L-shaped domain.
- ▶ These results immediately can be applied in Cea's lemma.

Error estimates for homogeneous Dirichlet problem

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

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

- ▶ Then, $\lim_{h \rightarrow 0} \|u - u_h\|_{1,\Omega} = 0$.
- ▶ If $u \in H^2(\Omega)$ (e.g. convex domain, smooth coefficients), then

$$\|u - u_h\|_{1,\Omega} \leq ch|u|_{2,\Omega} \leq c'h|f|_{0,\Omega}$$

$$\|u - u_h\|_{0,\Omega} \leq ch^2|u|_{2,\Omega} \leq c'h^2|f|_{0,\Omega}$$

and (“Aubin-Nitsche-Lemma”)

$$\|u - u_h\|_{0,\Omega} \leq ch|u|_{1,\Omega}$$

H^2 -Regularity

- ▶ $u \in H^2(\Omega)$ may be *not* fulfilled e.g.
 - ▶ if Ω has re-entrant corners
 - ▶ if on a smooth part of the domain, the boundary condition type changes
 - ▶ if problem coefficients (λ) are discontinuous
- ▶ Situations differ as well between two and three space dimensions
- ▶ Delicate theory, ongoing research in functional analysis
- ▶ Consequence for simulations
 - ▶ Deterioration of convergence rate
 - ▶ Remedy: local refinement of the discretization mesh
 - ▶ using a priori information
 - ▶ using a posteriori error estimators + automatic refinement of discretization mesh

Higher regularity

- ▶ If $u \in H^s(\Omega)$ for $s > 2$, convergence order estimates become even better for P^k finite elements of order $k > 1$.
- ▶ Depending on the regularity of the solution the combination of grid adaptation and higher order ansatz functions may be successful

More complicated integrals

- ▶ Assume non-constant right hand side f , space dependent heat conduction coefficient κ .
- ▶ Right hand side integrals

$$f_i = \int_K f(x) \lambda_i(x) dx$$

- ▶ P^1 stiffness matrix elements

$$a_{ij} = \int_K \kappa(x) \nabla \lambda_i \nabla \lambda_j dx$$

- ▶ P^k stiffness matrix elements created from higher order ansatz functions

Quadrature rules

- ▶ *Quadrature rule:*

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

- ▶ 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.

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

- ▶ *Error estimate:*

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

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	$(\frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5+3\sqrt{5}}{20}) \dots$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Matching of approximation order and quadrature order

- ▶ “Variational crime”: instead of

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

we solve

$$a_h(u_h, v_h) = f_h(v_h) \quad \forall v_h \in V_h$$

where a_h, f_h are derived from their exact counterparts by quadrature

- ▶ For P^1 finite elements, zero order quadrature for volume integrals and first order quadrature for surface integrals is sufficient to keep the convergence order estimates stated before
- ▶ The rule of thumb for the volume quadrature is that the highest order terms must be evaluated exactly if the coefficients of the PDE are constant.

Practical realization of integrals

- ▶ Integral over barycentric coordinate function

$$\int_K \lambda_i(x) dx = \frac{1}{3}|K|$$

- ▶ Right hand side integrals. Assume $f(x)$ is given as a piecewise linear function with given values in the nodes of the triangulation

$$f_i = \int_K f(x)\lambda_i(x) dx \approx \frac{1}{3}|K|f(a_i)$$

- ▶ Integral over space dependent heat conduction coefficient: Assume $\kappa(x)$ is given as a piecewise linear function with given values in the nodes of the triangulation

$$a_{ij} = \int_K \kappa(x) \nabla \lambda_i \nabla \lambda_j dx = \frac{1}{3}(\kappa(a_0) + \kappa(a_1) + \kappa(a_2)) \int_K \kappa(x) \nabla \lambda_i \nabla \lambda_j dx$$

Practical realization of boundary conditions


- ▶ Robin boundary value problem

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

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

$$\int_{\Omega} \kappa \nabla u \nabla v \, dx + \int_{\partial\Omega} \alpha u v \, ds = \int_{\Omega} f v \, dx + \int_{\partial\Omega} \alpha g v \, ds \quad \forall v \in H^1(\Omega)$$

- ▶ In 2D, for P^1 FEM, boundary integrals can be calculated by trapezoidal rule without sacrificing approximation order



Time dependent problems

Time dependent Robin boundary value problem

- ▶ Choose final time $T > 0$. Regard functions $(x, t) \rightarrow \mathbb{R}$.

$$\begin{aligned}\partial_t u - \nabla \cdot \kappa \nabla u &= f && \text{in } \Omega \times [0, T] \\ \kappa \nabla u + \alpha(u - g) &= 0 && \text{on } \partial\Omega \times [0, T] \\ u(x, 0) &= u_0(x) && \text{in } \Omega\end{aligned}$$

- ▶ This is an initial boundary value problem
- ▶ This problem has a weak formulation in the Sobolev space $L^2([0, T], H^1(\Omega))$, which then allows for a Galerkin approximation in a corresponding subspace
- ▶ We will proceed in a simpler manner: first, perform a finite difference discretization in time, then perform a finite element (finite volume) discretization in space.
 - ▶ Rothe method: first discretize in time, then in space
 - ▶ Method of lines: first discretize in space, get a huge ODE system

Time discretization

- ▶ Choose time discretization points $0 = t_0 < t_1 \cdots < t_N = T$, let

$$\tau_i = t_i - t_{i-1}$$

For $i = 1 \dots N$, solve

$$\begin{aligned} \frac{u_i - u_{i-1}}{\tau_i} - \nabla \cdot \kappa \nabla u_\theta &= f \quad \text{in } \Omega \times [0, T] \\ \kappa \nabla u_\theta + \alpha(u_\theta - g) &= 0 \quad \text{on } \partial\Omega \times [0, T] \end{aligned}$$

where $u_\theta = \theta u_i + (1 - \theta)u_{i-1}$

- ▶ $\theta = 1$: backward (implicit) Euler method
- ▶ $\theta = \frac{1}{2}$: Crank-Nicolson scheme
- ▶ $\theta = 0$: forward (explicit) Euler method
- ▶ Note that the explicit Euler method does not involve the solution of a PDE system. What do we have to pay for this ?

Weak formulation

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

$$\begin{aligned} \frac{1}{\tau_i} \int_{\Omega} u_i v \, dx + \theta \left(\int_{\Omega} \kappa \nabla u_i \nabla v \, dx + \int_{\partial\Omega} \alpha u_i v \, ds \right) = \\ \frac{1}{\tau_i} \int_{\Omega} u_{i-1} v \, dx + (1 - \theta) \left(\int_{\Omega} \kappa \nabla u_{i-1} \nabla v \, dx + \int_{\partial\Omega} \alpha u_{i-1} v \, ds \right) \\ + \int_{\Omega} f v \, dx + \int_{\partial\Omega} \alpha g v \, ds \quad \forall v \in H^1(\Omega) \end{aligned}$$

- ▶ Matrix formulation (in case of constant coefficients, $A_i = A$)

$$\frac{1}{\tau_i} M u_i + \theta A_i u_i = \frac{1}{\tau_i} M u_{i-1} + (1 - \theta) A_i u_{i-1} + F$$

- ▶ M : mass matrix, A : stiffness matrix