Simple finite element methods in Python

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1 Heat equation

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ be the computational domain. We suppose to have a disjoined partition of its boundary: $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$. We consider the parabolic equation for the temperature T, heat flux $\vec{q}$ and heat release $\dot{q}$

Heat equation (strong formulation)

$$
\begin{cases}
\vec{q} = -k\nabla T & \\
\rho C_p \dfrac{\partial T}{\partial t} + \operatorname{div}(\vec{v}T) + \operatorname{div}\vec{q} = \dot{q} & \text{in } \Omega \\
T = T^D & \text{in } \Gamma_D \\
k\dfrac{\partial T}{\partial n} = q^N & \text{in } \Gamma_N \\
c_R T + k\dfrac{\partial T}{\partial n} = q^R & \text{in } \Gamma_R
\end{cases}
\tag{1.1}
$$

Heat equation (weak formulation)

Let $H^1_f := \left\{ u \in H^1(\Omega) \,\middle|\, T_{|_{\Gamma_D}} = f \right\}$. The standard weak formulation looks for $T \in H^1_{T^D}$ such that for all $\phi \in H^1_0(\Omega)$

$$
\int_\Omega \rho C_p \frac{\partial T}{\partial t}\phi - \int_\Omega \vec{v}T\cdot\nabla\phi + \int_\Omega k\nabla T\cdot\nabla\phi + \int_{\Gamma_R} c_R T\phi + \int_{\Gamma_R\cup\Gamma_N} \vec{v}_n T\phi = \int_\Omega \dot{q}\phi + \int_{\Gamma_R} q^R\phi \tag{1.2}
$$

We can derive (1.2) from (1.1) by the divergence theorem

$$
\int_\Omega \operatorname{div}\vec{F} = \int_{\partial\Omega} \vec{F}_n \quad \overset{F\to F\phi}{\Longrightarrow} \quad \int_\Omega (\operatorname{div}\vec{F})\phi = -\int_\Omega \vec{F}\cdot\nabla\phi + \int_{\partial\Omega} \vec{F}_n\phi,
$$

which gives with $\vec{F} = \vec{v} + \vec{q}$

$$
\int_\Omega \operatorname{div}(\vec{v}+\vec{q})\,\phi = -\int_\Omega \vec{v}\cdot\nabla\phi + \int_\Omega k\nabla T\cdot\nabla\phi + \int_{\partial\Omega} \vec{F}_n\phi.
$$

Using that ϕ vanishes on Γ_D we have

$$
\int_{\partial\Omega} \vec{F}_n\phi = \int_{\Gamma_N\cup\Gamma_R} \vec{F}_n\phi = \int_{\Gamma_N\cup\Gamma_R} \vec{v}_n\phi + \int_{\Gamma_N\cup\Gamma_R} \vec{q}_n\phi,
$$

and then with the different boundary conditions, we find

$$
\int_{\Gamma_N\cup\Gamma_R} \vec{q}_n\phi = \int_{\Gamma_D} q^N\phi + \int_{\Gamma_R} \left(q^R - c_R T\right)\phi
$$

1.1 Computation of the matrices for $\mathcal{P}^1_h\Omega$

For the convection, we suppose that $\vec{v} \in \mathcal{RT}^0_h(\Omega)$ and let for given $K \in \mathcal{K}_h$ $\vec{v} = \sum_{k=1}^{d+1} v_k\Phi_k$. Using

$$
x_k = x^K_{S_k}, \quad h_k = h^K_{S_k}, \quad \sigma_k = \sigma^K_{S_k}, n_k = n_{S_k}
$$

we compute

$$\int_K \lambda_j \vec{v} \cdot \nabla \lambda_i = \sum_{k=1}^{d+1} \nu_k \int_K \lambda_j \Phi_k \cdot \nabla \lambda_i$$

$$\int_K \lambda_j \Phi_k \cdot \nabla \lambda_i = -\frac{\sigma_k \sigma_i}{h_k h_i} \int_K \lambda_j (x - x_k) \cdot n_i = -\frac{\sigma_k \sigma_i}{h_k h_i} \sum_{l=1}^{d+1} (x_l - x_k) \cdot n_i \int_K \lambda_j \lambda_l$$

Appendices

A Finite elements on simplices

A.1 Simplices

We consider an arbitrary non-degenerate simplex $K = (x_0, x_1, \ldots, x_d)$. The (signed) volume of K is given by

$$|K| = \frac{1}{d!}\det(x_1 - x_0, \ldots, x_d - x_0) = \frac{1}{d!}\det(1, x_0, x_1 \ldots, x_d) \quad 1 = (1, \ldots, 1)^T. \tag{A.1}$$

The $d{+}1$ sides S_k (co-dimension one, $d{-}1$-simplices or facets) are defined by $S_k = (x_0, \ldots, \cancel{x_k}, \ldots, x_d)$. The height is $h_k = |P_{S_k}x_k - x_k|$, where P_S is the orthogonal projection on the hyperplane associated to S_k. We have

$$h_k = d\frac{|K|}{|S_k|} \qquad (\text{and for } d = 3\ |S_k| = \tfrac{1}{2}|u \times v|)$$

A.2 Barycentric coordinates

Any polynomial in the barycentric coordinates can be integrated exactly. For $\alpha \in \mathbb{N}_0^{d+1}$ we let $\alpha! = \prod_{i=0}^{d}\alpha_i!$, $|\alpha| = \sum_{i=0}^{d}\alpha_i$, and $\lambda^\alpha = \prod_{i=0}^{d}\lambda_i^{\alpha_i}$

Integration on K

$$\int_K \lambda^\alpha = |K|\frac{d!\alpha!}{(|\alpha| + d)!} \tag{A.2}$$

see [0], [0].

Gradient of λ_i

$$\nabla\lambda_i = -\frac{1}{h_i}\vec{n_i}.$$

A.3 Finite elements

We consider a family $\mathcal{H}$ of regular simplicial meshes h on a polyhedral domain $\Omega \subset \mathbb{R}^d$. The set of simplices of $h \in \mathcal{H}$ is denoted by $\mathcal{K}_h$, and its $d-1$-dimensional sides by $\mathcal{S}_h$, divided into interior and boundary sides $\mathcal{S}_h^{\text{int}}$ and $\mathcal{S}_h^{\partial}$, respectively. The set of $d+1$ sides of $K \in \mathcal{K}_h$ is $\mathcal{S}_h(K)$. To any side $S \in \mathcal{S}_h$ we associate a unit normal vector n_S, which coincides with the unit outward normal vector $n_{\partial\Omega}$ if $S \in \mathcal{S}_h^{\partial}$.

For $K \in \mathcal{K}_h$ and $S \in \mathcal{S}_h$, or $S \in \mathcal{S}_h(K)$ we denote

x_K :	barycenter of K	x_S :	barycenter of S
x_S^K :	vertex opposite to S in K	h_S^K :	distance of x_S^K to S
$\sigma_S^K := \begin{cases} +1 & \text{if } n_S = n_K, \\ -1 & \text{if } n_S = -n_K. \end{cases}$		λ_S^K :	barycentric coordinates of K

For $k \in \mathbb{N}_0$ we denote by $\mathcal{C}_h^k(\Omega)$ the space of piecewise k-times differential functions with respect to $\mathcal{K}_h$, and piecewise differential operators $\nabla_h : \mathcal{C}_h^l(\Omega) \to \mathcal{C}_h^{l-1}(\Omega, \mathbb{R}^d)$ ($l \in \mathbb{N}$) by $\nabla_h q_{|K} := \nabla\left(q_{|K}\right)$ for $q \in \mathcal{C}_h^l(\Omega)$ and similarly for $\operatorname{div}_h : \mathcal{C}_h^l(\Omega, \mathbb{R}^d) \to \mathcal{C}_h^{l-1}(\Omega)$. We frequently use the piecewise Stokes formula

$$\int_\Omega \nabla_h q v + \int_\Omega q \operatorname{div}_h v = \int_{\mathcal{S}_h^{\text{int}}} [q v_n] + \int_{\mathcal{S}_h^{\partial}} q v_n, \tag{A.3}$$

where $\int_{\mathcal{S}_h} = \sum_{S\in\mathcal{S}_h}\int_S$ and n in the sum stands for n_S.

The subspace of piecewise polynomial functions of order $k \in \mathbb{N}_0$ in $C^k_h(\Omega)$ is denoted by $\mathcal{D}^k_h(\Omega)$ and the $L^2(\Omega)$-projection by $\pi^k_h : L^2(\Omega) \to \mathcal{D}^k_h(\Omega)$.

The subspaces of continuous and nonconforming piecewise-polynmial functions are for $k \in \mathbb{N}$

$$\mathcal{P}^k_h(\Omega) := \mathcal{D}^k_h(\Omega) \cap C(\overline{\Omega}), \quad \mathcal{CR}^k_h(\Omega) := \left\{ q \in \mathcal{D}^k_h(\Omega) \;\middle|\; \int_S [q]\, p = 0 \;\forall S \in \mathcal{S}^{\mathrm{int}}_h, \forall p \in P^{k-1}(S) \right\}. \tag{A.4}$$

The standard finite element theory provides canonical basis functions and interpolation operators, which however need special care in the nonconforming case for even k.

The restrictions of the basis functions of $\mathcal{P}^1_h(\Omega)$ to the simplex K are the barycentric coordinates λ^K_S associated to the node opposite to S in K.

Formulae for $\mathcal{P}^1_h$

$$\nabla\lambda^K_S = -\frac{\sigma^K_S}{h^K_S} n_S, \quad \frac{1}{|K|}\int_K \lambda^K_S = \frac{1}{d+1}. \tag{A.5}$$

Denote in addition the basis of $\mathcal{CR}^1_h(\Omega)$ by ψ_S, we have

Formulae for $\mathcal{CR}^1_h$

$$\psi_{S|_K} = 1 - d\lambda^K_S, \quad \nabla\psi_{S|_K} = \frac{|S|\sigma^K_S}{|K|} n_S, \quad \frac{1}{|K|}\int_K \psi_S = \frac{1}{d+1}. \tag{A.6}$$

The Raviart-Thomas space for $k \geqslant 0$ is given by

$$\mathcal{RT}^k_h(\Omega) := \left\{ v \in D^k_h(\Omega, \mathbb{R}^d) \oplus X^k_h \;\middle|\; \int_S [v_n]\, p = 0 \;\forall S \in \mathcal{S}^{\mathrm{int}}_h, \forall p \in P^k(S) \right\} \tag{A.7}$$

where $X^k_h := \left\{ xp \mid p_{|K} \in P^k_{\mathrm{hom}}(K) \;\forall K \in \mathcal{K}_h \right\}$ with $P^k_{\mathrm{hom}}(K)$ the space of k-th order homogenous polynomials.

Then the Raviart-Thomas basis function of lowest order is given by

Formulae for $\mathcal{RT}^0$

$$\Phi_{S|_K} := \sigma^K_S \frac{x - x^K_S}{h^K_S}, \quad \int_K \operatorname{div}\Phi_{S|_K} = \sigma^K_S \frac{d|K|}{h^K_S} = \sigma^K_S |S|, \quad \frac{1}{|K|}\int_K \Phi_S = \sigma^K_S \frac{x^*_K - x^K_S}{h^K_S}. \tag{A.8}$$

References Section A

[0] M. A. Eisenberg and L. E. Malvern. "On finite element integration in natural co-ordinates". In: *Int. J. of Numer. Meth. in Engrg.* 7 (1973), pp. 574–575.

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