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 $K \in \mathcal{K}_h$ $\vec{v} = \sum_{k=1}^{d+1} \nu_k\Phi_k$. 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

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

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

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 [1], [2].

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

A.3.1 $\mathcal{P}_h^1(\Omega)$

We have $\mathcal{P}_h^1(\Omega) = \mathcal{D}_h^1(\Omega) \cap C(\overline{\Omega})$, but the FEM definition also provides a basis. The restrictions of the basis functions of $\mathcal{P}_h^1(\Omega)$ to the simplex K are the barycentric coordinates λ_S^K associated to the node opposite to S in K.

Formulae for $\mathcal{P}_h^1(\Omega)$

$$\nabla\lambda_S^K = -\frac{\sigma_S^K}{h_S^K} n_S, \qquad \frac{1}{|K|}\int_K \lambda_S^K = \frac{1}{d+1}. \tag{A.3}$$

For the computation of matrices we use (A.2), for example for $i, j \in [\![0, d]\!]$

$$\int_K \lambda_i \lambda_j = |K| \frac{d!\alpha!}{(|\alpha| + d)!} \quad \text{with} \quad \begin{cases} \alpha = (1, 1, 0, \cdots, 0) & (i \neq j) \\ \alpha = (2, 0, \cdots, 0) & (i = j) \end{cases}$$

so

$$\int_K \lambda_i \lambda_j = \frac{|K|}{(d+2)(d+1)}(1 + \delta_{ij}) \tag{A.4}$$

More generally, we have for $i_l \in [\![0, d]\!]$ with $1 \leqslant l \leqslant k$

$$\int_K \lambda_{i_1} \cdots \lambda_{i_k} = \frac{|K|\alpha!}{(d+k)\cdots(d+1)}, \quad \alpha_l = \#\left\{j \in [\![0, d]\!] \;\middle|\; i_j = l\right\}, \quad 1 \leqslant l \leqslant k. \tag{A.5}$$

A.3.2 $\mathcal{CR}_h^1(\Omega)$

$$\mathcal{CR}_h^k(\Omega) := \left\{ q \in \mathcal{D}_h^k(\Omega) \;\middle|\; \int_S [q]\, p = 0 \;\forall S \in \mathcal{S}_h^{\text{int}}, \forall p \in P^{k-1}(S) \right\}. \tag{A.6}$$

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

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

$$\psi_{S|_K} = 1 - d\lambda_S^K, \quad \nabla\psi_{S|_K} = \frac{|S|\sigma_S^K}{|K|} n_S, \quad \frac{1}{|K|}\int_K \psi_S = \frac{1}{d+1}. \tag{A.7}$$

A.3.3 $\mathcal{RT}_h^0(\Omega)$

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

$$\mathcal{RT}_h^k(\Omega) := \left\{ v \in D_h^k(\Omega, \mathbb{R}^d) \oplus X_h^k \;\middle|\; \int_S [v_n]\, p = 0 \;\forall S \in \mathcal{S}_h^{\text{int}}, \forall p \in P^k(S) \right\} \tag{A.8}$$

where $X_h^k := \left\{ xp \mid p_{|_K} \in P_{\text{hom}}^k(K) \;\forall K \in \mathcal{K}_h \right\}$ with $P_{\text{hom}}^k(K)$ the space of k-th order homogenous polynomials.

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

Formulae for $\mathcal{RT}^0$

$$\Phi_{S|_K} := \sigma_S^K \frac{x - x_S^K}{h_S^K}, \quad \int_K \operatorname{div} \Phi_{S|_K} = \sigma_S^K \frac{d|K|}{h_S^K} = \sigma_S^K |S|, \quad \frac{1}{|K|}\int_K \Phi_S = \sigma_S^K \frac{x_K^* - x_S^K}{h_S^K}. \tag{A.9}$$

References Section A

[1] 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.

[2] F. J. Vermolen and A. Segal. “On an integration rule for products of barycentric coordinates over simplexes in $\mathbb{R}^n$”. In: *J. Comput. Appl. Math.* 330 (2018), pp. 289–294.

B Discreization of the transport equation

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 $\mathrm{div}_h : \mathcal{C}_h^l(\Omega, \mathbb{R}^d) \to \mathcal{C}_h^{l-1}(\Omega)$. We frequently use the piecewise Stokes formula

$$\int_\Omega \nabla_h q v + \int_\Omega q \,\mathrm{div}_h\, v = \int_{\mathcal{S}_h^{\mathrm{int}}} [q v_n] + \int_{\mathcal{S}_h^\partial} q v_n, \tag{B.1}$$

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 $C_h^k(\Omega)$ is denoted by $\mathcal{D}_h^k(\Omega)$ and the $L^2(\Omega)$-projection by $\pi_h^k : L^2(\Omega) \to \mathcal{D}_h^k(\Omega)$.

Suppose u satisfies

$$\mathrm{div}(\beta u) = f \quad \text{in } \Omega, \qquad \beta_n^-(u - u^D) = 0 \quad \text{on } \partial\Omega. \tag{B.2}$$

From the integration by parts formula

$$\int_\Omega \mathrm{div}(\beta u) v = -\int_\Omega \beta u \cdot \nabla v + \int_{\partial\Omega} \beta_n u v \tag{B.3}$$

it then follows that u satisfies

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

with

$$a(u, v) := -\int_\Omega u\beta \cdot \nabla v + \int_{\partial\Omega} \beta_n^+ u v, \quad l(v) := \int_\Omega f v - \int_{\partial\Omega} \beta_n^- u^D v. \tag{B.4}$$

We also have

$$\begin{aligned} a(u, v) =& -\frac{1}{2}\int_\Omega u\beta \cdot \nabla v + \frac{1}{2}\int_\Omega \mathrm{div}(\beta u) v - \frac{1}{2}\int_{\partial\Omega} \beta_n u v + \int_{\partial\Omega} \beta_n^+ u v \\ =& \frac{1}{2}\int_\Omega \mathrm{div}(\beta) u v + \frac{1}{2}\left(\int_\Omega \beta \cdot \nabla u v - \int_\Omega u\beta \cdot \nabla v\right) + \frac{1}{2}\int_{\partial\Omega} |\beta_n| u v \end{aligned}$$

B.1 $\mathcal{P}_h^1(\Omega)$

Let $K \in \mathcal{K}_h$, $\beta_K = \pi_K \beta$, x_K be the barycenter of K and $x_K^{\mathrm{up}} \in \partial K$ such that $x_K - x_K^{\mathrm{up}}$ is aligned with β_K.