

Simple finite element methods in Python

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November 21, 2020

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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 disjointed 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)

$$\left\{ \begin{array}{ll} \vec{q} = -k\nabla T \\ \rho C_p \frac{\partial T}{\partial t} + \text{div}(\vec{v}T) + \text{div} \vec{q} = \dot{q} & \text{in } \Omega \\ T = T^D & \text{in } \Gamma_D \\ k \frac{\partial T}{\partial n} = q^N & \text{in } \Gamma_N \\ c_R T + k \frac{\partial T}{\partial n} = q^R & \text{in } \Gamma_R \end{array} \right. \quad (1.1)$$

Heat equation (weak formulation)

Let $H_f^1 := \{u \in H^1(\Omega) \mid T|_{\Gamma_D} = f\}$. The standard weak formulation looks for $T \in H_{T^D}^1$ such that for all $\phi \in H_0^1(\Omega)$

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

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

$$\int_{\Omega} \text{div} \vec{F} = \int_{\partial\Omega} \vec{F}_n \quad \xLeftrightarrow{F \rightarrow F\phi} \quad \int_{\Omega} (\text{div} \vec{F}) \phi = - \int_{\Omega} \vec{F} \cdot \nabla \phi + \int_{\partial\Omega} \vec{F}_n \phi,$$

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

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

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

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

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

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

$$x_k = x_{S_k}^K, \quad h_k = h_{S_k}^K, \quad \sigma_k = \sigma_{S_k}^K, \quad n_k = n_{S_k}$$

we compute

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

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

A Finite elements on simplices

A.1 Simplices

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

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

The $d+1$ sides S_k (co-dimension one, $d-1$ -simplices or facets) are defined by $S_k = (x_0, \dots, x_k, \dots, x_d)$. 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

$$h_k = d \frac{|K|}{|S_k|}, \quad d|K| = \int_K \operatorname{div}(x) = \sum_{i=0}^d \int_{S_i} x \cdot \vec{n}_i$$

A.2 Barycentric coordinates

The barycentric coordinate of a point $x \in \mathbb{R}^d$ give the coefficients in the affine combination of $x = \sum_{i=0}^d \lambda_i x_i$ ($\sum_{i=0}^d \lambda_i = 1$) and can be expressed by means of the outer unit normal \vec{n}_i of S_i or the signed distance d^s as

$$\lambda_i(x) = \frac{\vec{n}_i^T(x_j - x)}{\vec{n}_i^T(x_j - x_i)} \quad (j \neq i), \quad \lambda_i(x) = \frac{d^s(x, H)}{h_i}. \quad (\text{A.2})$$

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

$$\int_K \lambda^\alpha = |K| \frac{d! \alpha!}{(|\alpha| + d)!} \quad (\text{A.3})$$

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^∂ , 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 $S \in \mathcal{S}_h^\partial$.

¹<https://en.wikipedia.org/wiki/Simplex#Volume>

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

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

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

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

$$\nabla \lambda_S^K = -\frac{\sigma_S^K}{h_S^K} n_S, \quad \frac{1}{|K|} \int_K \lambda_S^K = \frac{1}{d+1}. \quad (\text{A.4})$$

For the computation of matrices we use (A.3), for example for $i, j \in \llbracket 0, d \rrbracket$

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

so

$$\int_K \lambda_i \lambda_j = \frac{|K|}{(d+2)(d+1)} (1 + \delta_{ij}) \quad (\text{A.5})$$

More generally, we have for $i_l \in \llbracket 0, d \rrbracket$ with $1 \leq l \leq k$

$$\int_K \lambda_{i_1} \cdots \lambda_{i_k} = \frac{|K| \alpha!}{(d+k) \cdots (d+1)}, \quad \alpha_l = \# \{j \in \llbracket 0, d \rrbracket \mid i_j = l\}, \quad 1 \leq l \leq k. \quad (\text{A.6})$$

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

$$\mathcal{CR}_h^k(\Omega) := \left\{ q \in \mathcal{D}_h^k(\Omega) \mid \int_S [q] p = 0 \quad \forall S \in \mathcal{S}_h^{\text{int}}, \forall p \in P^{k-1}(S) \right\}. \quad (\text{A.7})$$

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

Formulae for \mathcal{CR}_h^1

$$\psi_{S|_K} = 1 - d \lambda_S^K, \quad \nabla \psi_{S|_K} = \frac{|S| \sigma_S^K}{|K|} n_S, \quad \frac{1}{|K|} \int_K \psi_S = \frac{1}{d+1}. \quad (\text{A.8})$$

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

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

$$\mathcal{RT}_h^k(\Omega) := \left\{ v \in D_h^k(\Omega, \mathbb{R}^d) \oplus X_h^k \mid \int_S [v_n] p = 0 \quad \forall S \in \mathcal{S}_h^{\text{int}}, \forall p \in P^k(S) \right\} \quad (\text{A.9})$$

where $X_h^k := \{xp \mid p|_K \in P_{\text{hom}}^k(K) \forall K \in \mathcal{K}_h\}$ 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

$$\Phi_{S|_K} := \sigma_S^K \frac{x - x_S^K}{h_S^K}, \quad \int_K \text{div } \Phi_{S|_K} = \sigma_S^K \frac{d|K|}{h_S^K} = \sigma_S^K |S|, \quad \frac{1}{|K|} \int_K \Phi_S = \sigma_S^K \frac{x_K - x_S^K}{h_S^K}. \quad (\text{A.10})$$

For the projection on $\mathcal{D}_h^0(\Omega, \mathbb{R}^d)$ we have

$$\sum_{i=1}^d v_i \frac{1}{|K|} \int_K \Phi_i(x)$$

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 $\nabla_h : \mathcal{C}_h^l(\Omega) \rightarrow \mathcal{C}_h^{l-1}(\Omega, \mathbb{R}^d)$ ($l \in \mathbb{N}$) by $\nabla_h q|_K := \nabla(q|_K)$ for $q \in \mathcal{C}_h^l(\Omega)$ and similarly for $\text{div}_h : \mathcal{C}_h^l(\Omega, \mathbb{R}^d) \rightarrow \mathcal{C}_h^{l-1}(\Omega)$. We frequently use the piecewise Stokes formula

$$\int_{\Omega} \nabla_h q v + \int_{\Omega} q \text{div}_h v = \int_{S_h^{\text{int}}} [q v_n] + \int_{S_h^{\partial}} q v_n, \quad (\text{B.1})$$

where $\int_{S_h} = \sum_{S \in \mathcal{S}_h} \int_S$ 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 $\pi_h^k : L^2(\Omega) \rightarrow \mathcal{D}_h^k(\Omega)$.

Suppose u satisfies

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

From the integration by parts formula

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

it then follows that u satisfies

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

with

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

We also have

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

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 $x_K^\# \in \partial K$ such that with $\delta_K \geq 0$

$$x_K^\# = x_K + \delta_K \beta_K \quad (\text{B.5})$$

If we know $\vec{n}_i^T \beta_K$, we can compute $x_K^\#$ as follows.

$$\lambda_i(x_K^\#) = \lambda_i(x_K) + \delta_K \nabla \lambda_i^T \beta_K = \frac{1}{d+1} - \delta_K \frac{\vec{n}_i^T \beta_K}{h_i}$$

It follows that

$$\delta_K = \max \left\{ \frac{(\vec{n}_i^T \beta_K)^+}{3h_i} \mid 0 \leq i \leq d \right\}. \quad (\text{B.6})$$

C Python implementation

We suppose to have a `class SimplexMesh` containing the following elements

```
class SimplexMesh():
    dimension, nnodes, ncells, nfaces
    simplices # np.array((ncells, dimension+1))
    faces     # np.array((nfaces, dimension))
    points, pointsc, pointsf # np.array((nnodes,3)), np.array((ncells,3)
    ), np.array((nfaces,3))
    normals, sigma # np.array((nfaces,dimension)), np.array((ncells,
    dimension+1))
    dV            # np.array((ncells))
    bdrylabels    # dictionary(keys: colors, values: id's of boundary
    faces)
```

The norm of the 'normals' $\widetilde{\vec{n}}$ is the measure of of the face

$$\widetilde{\vec{n}}_i = |S_i| \vec{n}_i$$