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 Python implementation

We suppose to have a `class SimplexMesh` contaning 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' $\tilde{\vec{n}}$ is the measure of of the face

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

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.

[0] 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 Finite elements on simplices

B.1 Simplices

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

$$|K| = \frac{1}{d!}\det(x_1 - x_0, \ldots, x_d - x_0) = \frac{1}{d!}\det(1, x_0, x_1 \ldots, x_d) \quad 1 = (1, \ldots, 1)^{T1}. \tag{B.1}$$

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 $P_{S_k} x_k = x_k + h_k \vec{n}_k$ and $S_k = \left\{x \in \mathbb{R}^d \;\middle|\; \vec{n}_k^T x = h_k\right\}$ and

$$0 = \int_K \operatorname{div}(\vec{c}) = \sum_{i=0}^{d} \int_{S_i} \vec{c} \cdot \vec{n}_i = \vec{c} \cdot \sum_{i=0}^{d} |S_i|\, \vec{n}_i \quad \Rightarrow \quad \sum_{i=0}^{d} |S_i|\, \vec{n}_i = 0$$

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

Height formula

$$h_k = d\frac{|K|}{|S_k|}$$

B.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

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

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

$$\int_K \lambda^\alpha = |K| \frac{d!\alpha!}{(|\alpha| + d)!} \tag{B.3}$$

see **[EisenbergMalvern73]**, **[VermolenSegal18]**.

Gradient of λ_i

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

[1] https://en.wikipedia.org/wiki/Simplex#Volume

B.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 $\pi_h^k : L^2(\Omega) \to \mathcal{D}_h^k(\Omega)$.

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

$$\nabla\lambda_S^K = -\frac{\sigma_S^K}{h_S^K} n_S, \qquad \frac{1}{|K|}\int_K \lambda_S^K = \frac{1}{d+1}. \tag{B.4}$$

For the computation of matrices we use (B.3), 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

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

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

$$\int_K \lambda_{i_1}\cdots\lambda_{i_k} = \frac{|K|\alpha!}{(d+k)\cdots(d+1)}, \quad \alpha_l = \#\left\{j \in [\![0,d]\!] \mid i_j = l\right\}, \quad 1 \leqslant l \leqslant k. \tag{B.6}$$

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

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

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

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

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

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

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

$$\mathcal{RT}_h^k(\Omega) := \left\{ v \in D_h^k(\Omega, \mathbb{R}^d) \oplus X_h^k \,\middle|\, \int_S [v_n]\, p = 0 \; \forall S \in \mathcal{S}_h^{\mathrm{int}}, \forall p \in P^k(S) \right\} \tag{B.9}$$

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

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

Formulae for $\mathcal{RT}^0$

$$\Phi_{S|_K} := \sigma_S^K \frac{x - x_S^K}{h_S^K}, \qquad \int_K \operatorname{div} \Phi_{S|_K} = \sigma_S^K \frac{d|K|}{h_S^K} = \sigma_S^K |S|, \qquad \frac{1}{|K|} \int_K \Phi_S = \sigma_S^K \frac{x_K - x_S^K}{h_S^K}. \tag{B.10}$$

For the `pyhon` implementation of the projection on $\mathcal{D}_h^0(\Omega, \mathbb{R}^d)$ we have with the height formula

$$\pi_h(\vec{v})_{|_K} = \sum_{i=1}^d v_i \frac{1}{|K|} \int_K \Phi_i(x) = \sum_{i=1}^d v_i \sigma_i^K (x_K - x_{S_i}) \frac{|S_i|}{d\,|K|}$$

The `pyhon` implementation reads

```
```

C Discreization of the transport equation

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

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

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 $C^k_h(\Omega)$ is denoted by $\mathcal{D}^k_h(\Omega)$ and the $L^2(\Omega)$-projection by $\pi^k_h : L^2(\Omega) \to \mathcal{D}^k_h(\Omega)$.

Suppose u satisfies

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

From the integration by parts formula

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

it then follows that u satisfies

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

with

$$a(u, v) := \int_\Omega \mathrm{div}(\beta)uv + \int_\Omega (\beta \cdot \nabla u)v - \int_{\partial\Omega} \beta^-_n uv, \quad l(v) := \int_\Omega fv - \int_{\partial\Omega} \beta^-_n u^D v. \tag{C.4}$$

We also have

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

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

Let $K \in \mathcal{K}_h$, $\beta_K = \pi_K\beta$, x_K be the barycenter of K and $x^\sharp_K \in \partial K$ such that with $\delta_K \geqslant 0$

$$x^\sharp_K = x_K + \delta_K\beta_K \tag{C.5}$$

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

$$\lambda_i(x^\sharp_K) = \lambda_i(x_K) + \delta_K \nabla\lambda_i{}^T\beta_K = \frac{1}{d+1} - \delta_K\frac{\vec{n}_i^T\beta_K}{h_i} = \frac{1}{d+1} - \delta_K\frac{\vec{n}_i^T\beta_K\,|S_i|}{d\,|K|}$$

It follows that

$$\delta_K = \max\left\{ \frac{d\,|K|}{(d+1)\,|S_i|\left(\vec{n}_i^T\beta_K\right)^+} \;\middle|\; 0 \leqslant i \leqslant d \right\}. \tag{C.6}$$

The stabilized bilinear form is

$$a^{\mathrm{supg}}(u, v) := \int_\Omega (\beta \cdot \nabla u)v - \int_{\partial\Omega} \beta^-_n uv + \int_\Omega \delta(\beta \cdot \nabla u)(\beta \cdot \nabla v) \tag{C.7}$$

Then we have

$$a^{\mathrm{supg}}(u, v) =$$