Simple finite element methods in Python

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Contents

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)

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

Heat equation (weak formulation)

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

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

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 Boundary conditions

1.1.1 Nitsche's method

$$
\begin{cases}
u_h \in V_h : \quad a_\Omega(u_h,\phi) + a_{\partial\Omega}(u_h,\phi) = l_\Omega(\phi) + l_{\partial\Omega}(\phi) \quad \forall \phi \in V_h \\
a_\Omega(v,\phi) := \int_\Omega \mu \nabla u \cdot \nabla \phi \\
a_{\partial\Omega}(v,\phi) := \int_{\Gamma_D} \frac{\gamma\mu}{h} u\phi - \int_{\Gamma_D} \mu \left(\frac{\partial u}{\partial n}\phi + u \frac{\partial \phi}{\partial n} \right) \\
l_\Omega(\phi) := \int_\Omega f\phi, \quad l_{\partial\Omega}(\phi) = \int_{\Gamma_D} \mu u^D \left(\frac{\gamma}{h}\phi - \frac{\partial\phi}{\partial n} \right)
\end{cases}
\tag{1.3}
$$

Let $-\operatorname{div}(\mu\nabla z) = 0$ and $z\big|_{\Gamma_D} = 1$ and $z\big|_{\Gamma_N} = 0$. Then

$$
\int_\Omega \mu \nabla u \cdot \nabla z - \int_\Omega fz = \int_\Omega (\mu\nabla u \cdot \nabla z + \operatorname{div}(\mu\nabla u) z) = \int_{\Gamma_D} \mu \frac{\partial u}{\partial n}.
$$

Now, if $z_h \in V_h$ such that $z - z_h \in H^1_0(\Omega)$

$$
\begin{aligned}
\int_\Omega \mu\nabla(u-u_h)\cdot\nabla(z-z_h) &= \int_\Omega f(z-z_h) - \int_\Omega \mu\nabla u_h \cdot \nabla(z-z_h) \\
&= \int_\Omega fz - \int_\Omega \mu\nabla u_h\cdot\nabla z + \int_\Omega \mu\nabla u_h \cdot\nabla(z-z_h) - \int_\Omega f z_h \\
&= -\int_{\Gamma_D} \mu\frac{\partial u}{\partial n} + \int_\Omega \mu\nabla(u-u_h)\cdot\nabla z + \int_{\Gamma_D} \mu(u^D-u_h)\left(\frac{\gamma}{h} z_h - \frac{\partial z_h}{\partial n}\right) + \int_{\Gamma_D} \mu \frac{\partial u_h}{\partial n} \\
&= \int_{\Gamma_D} \mu\frac{\partial u_h}{\partial n} + \int_{\Gamma_D} (u^D - u_h)\frac{\mu\gamma}{h} - \int_{\Gamma_D} \mu\frac{\partial u}{\partial n} + \int_{\Gamma_D} \mu(u-u_h)\frac{\partial(z-z_h)}{\partial n},
\end{aligned}
$$

so we get a possibly second-order approximation of the flux by

$$
F_h := \int_{\Gamma_D} \mu\frac{\partial u_h}{\partial n} + \int_{\Gamma_D} (u^D - u_h)\frac{\mu\gamma}{h}. \tag{1.4}
$$

1.2 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

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

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

2 Stokes problem

Let $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ be the computational domain. We suppose to have a disjoined partition of its boundary: $\partial\Omega = \Gamma_D \cup \Gamma_N$.

$$\begin{cases} -\operatorname{div}(\mu\nabla v) + \nabla p = f & \text{in } \Omega \\ \operatorname{div} v = g & \text{in } \Omega \\ v = v^D & \text{in } \Gamma_D \\ \mu\dfrac{\partial v}{\partial n} - pn = -p^N n & \text{in } \Gamma_N \end{cases} \tag{2.1}$$

2.1 Weak formulation

Supposing $|\Gamma_N| > 0$, we have

$$\begin{cases} V := H^1(\Omega, \mathbb{R}^d) \quad Q := L^2(\Omega) \\ (v, p) \in V \times Q : \quad a_\Omega(v, p; \phi\xi) + a_{\partial\Omega}(v, p; \phi, \xi) = l_\Omega(\phi, \xi) + l_{\partial\Omega}(\phi, \xi) \quad \forall(\phi, \xi) \in V \times Q \\ a_\Omega(v, p; \phi, \xi) := \displaystyle\int_\Omega \mu\nabla v : \nabla\phi - \int_\Omega p \operatorname{div}\phi + \int_\Omega \operatorname{div} v\xi \\ a_{\partial\Omega}(v, p; \phi, \xi) := \displaystyle\int_{\Gamma_D} \frac{\gamma\mu}{h} v\cdot\phi - \int_{\Gamma_D} \mu\left(\frac{\partial v}{\partial n}\cdot\phi + v\cdot\frac{\partial\phi}{\partial n}\right) + \int_{\Gamma_D}(p\phi_n - v_n\xi) \\ l_\Omega(\phi, \xi) := \displaystyle\int_\Omega f\cdot\phi + \int_\Omega g\xi, \quad l_{\partial\Omega}(\phi, \xi) = \int_{\Gamma_D}\mu v^D\cdot\left(\frac{\gamma}{h}\phi - \frac{\partial\phi}{\partial n}\right) - \int_{\Gamma_D} v_n^D\xi - \int_{\Gamma_N} p^N\phi_n. \end{cases} \tag{2.2}$$

Lemma 2.1. *A regular solution of the formulation (2.2) satisfies (2.1).*

Proof. By integration by parts we have

$$a_\Omega(v, p; \phi, \xi) = \int_\Omega(-\mu\Delta v + \nabla p)\cdot\phi + \int_{\partial\Omega}\mu\frac{\partial v}{\partial n}\cdot\phi - \int_{\partial\Omega}p\phi_n + \int_\Omega \operatorname{div} v\xi$$

and therefore with $a := a_\Omega + a_{\partial\Omega}$ and $l := l_\Omega + l_{\partial\Omega}$

$$\begin{aligned} a(v, p; \phi\xi) - l(v, p; \phi\xi) = &\int_\Omega(-\mu\Delta v + \nabla p - f)\cdot\phi + \int_\Omega(\operatorname{div} v - g)\xi + \int_{\Gamma_N}\left(\mu\frac{\partial v}{\partial n} - pn + p^N n\right)\cdot\phi \\ &+ \int_{\Gamma_D}\frac{\gamma\mu}{h}v\cdot\phi - \int_{\Gamma_D}\mu(v - v^D)\cdot\left(\frac{\gamma}{h}\phi - \frac{\partial\phi}{\partial n}\right) - \int_{\Gamma_D}(v - v^D)\cdot n\xi \end{aligned}$$

□

Alternatively, we can write the system as

$$\begin{cases} (v, p) \in V \times Q : \quad a(v, p; \phi\xi) + b(v, \xi) - b(\phi, p) = l_\Omega(\phi, \xi) + l_{\partial\Omega}(\phi, \xi) \quad \forall(\phi, \xi) \in V \times Q \\ a(v, p; \phi, \xi) := \displaystyle\int_\Omega \mu\nabla v : \nabla\phi + \int_{\Gamma_D}\frac{\gamma\mu}{h}v\cdot\phi - \int_{\Gamma_D}\mu\left(\frac{\partial v}{\partial n}\cdot n\phi + vn\cdot\frac{\partial\phi}{\partial n}\right) \\ b(v, \xi) := \displaystyle\int_\Omega \operatorname{div} v\xi - \int_{\Gamma_D} v_n\xi \end{cases} \tag{2.3}$$

2.2 Implementations of Dirichlet condition

We write the discrete velocity space V_h as a direct sum $V_h = V_h^{\mathrm{int}} \oplus V_h^{\mathrm{dir}}$, with V_h^{dir} corresponding to the discrete functions not vanishing on Γ_D. Splitting the matrix and right-hand side vector correspondingly, and letting $u_h^D \in V_h^{\mathrm{dir}}$ be an approximation of the Dirichlet data v^D we have the traditional way to implement Dirichlet boundary conditions:

$$\begin{bmatrix} A^{\mathrm{int}} & 0 & -{B^{\mathrm{int}}}^T \\ 0 & I & 0 \\ B^{\mathrm{int}} & 0 & 0 \end{bmatrix} \begin{bmatrix} v_h^{\mathrm{int}} \\ v_h^{\mathrm{dir}} \\ p_h \end{bmatrix} = \begin{bmatrix} f^{\mathrm{int}} - A^{\mathrm{int,dir}} v_h^D \\ v_h^D \\ g - B^{\mathrm{dir}} v_h^D \end{bmatrix}. \tag{2.4}$$

As for the Poisson problem, we obtain an alternative formulation

$$\begin{bmatrix} A^{\mathrm{int}} & 0 & -{B^{\mathrm{int}}}^T \\ 0 & A^{\mathrm{dir}} & 0 \\ B^{\mathrm{int}} & 0 & 0 \end{bmatrix} \begin{bmatrix} v_h^{\mathrm{int}} \\ v_h^{\mathrm{dir}} \\ p_h \end{bmatrix} = \begin{bmatrix} f^{\mathrm{int}} - A^{\mathrm{int,dir}} v_h^D \\ A^{\mathrm{dir}} v_h^D \\ g - B^{\mathrm{dir}} v_h^D \end{bmatrix}. \tag{2.5}$$

2.2.1 Pressure mean

If all boundary conditions are Dirichlet, the pressure is only determined up to a constant. In order to impose the zero mean on the pressure, let C the matrix of size $(1, nc)$

$$\begin{bmatrix} A & -B^T & 0 \\ B & 0 & C^T \\ 0 & C & 0 \end{bmatrix} \begin{bmatrix} v \\ p \\ \lambda \end{bmatrix} = \begin{bmatrix} f \\ g \\ 0 \end{bmatrix}. \tag{2.6}$$

Let us considered solution of (2.6) with $S = BA^{-1}B^T$, $T = CS^{-1}C^T$

$$\begin{cases} A\tilde{v} & = f \\ S\tilde{p} & = g - B\tilde{v} \\ T\lambda & = -C\tilde{p} \\ S(p - \tilde{p}) & = C^T\lambda \\ A(v - \tilde{v}) & = B^T p \end{cases} \tag{2.7}$$

2.2.2 Iterative solution

We have to solve (2.6) with

$$\mathcal{A} = \begin{bmatrix} A & -B^T & 0 \\ B & 0 & C^T \\ 0 & C & 0 \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ BA^{-1} & I & 0 \\ 0 & CS^{-1} & I \end{bmatrix} \begin{bmatrix} A & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & T \end{bmatrix} \begin{bmatrix} I & -A^{-1}B^T & 0 \\ 0 & I & S^{-1}C^T \\ 0 & 0 & I \end{bmatrix}$$

where $S = BA^{-1}B^T$, $T = -CS^{-1}C^T$. We have

$$\mathcal{A}^{-1} = \begin{bmatrix} I & A^{-1}B^T & 0 \\ 0 & I & -S^{-1}C^T \\ 0 & 0 & I \end{bmatrix} \begin{bmatrix} A^{-1} & 0 & 0 \\ 0 & S^{-1} & 0 \\ 0 & 0 & T^{-1} \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ -BA^{-1} & I & 0 \\ 0 & -CS^{-1} & I \end{bmatrix}$$

We construct our preconditioner by approximations of A, S, and T. The preconditioner $(y_{v},_{p}, y_\lambda) \to (x_v, x_p, x_\lambda)$has the steps

$$\begin{cases} Ax'_v &= y_v \\ Sx'_p &= y_p - Bx'_v \\ Tx_\lambda &= y_\lambda - Cx'_p \\ Sx''_p &= C^T x_\lambda \\ x_p &= x'_p - x''_p \\ Ax''_v &= B^T x_p \\ x_v &= x'_v + x''_v \end{cases}$$

3 Beam problem

$$\begin{cases} & \frac{d^2}{dx^2}(EI\frac{d^2w}{dx^2})(x) = q(x) \quad \Omega =]0;L[\\ w(x) = \frac{dw}{dx}(x) = 0 & \text{(clamped end)} \\ w(x) = \frac{d^2w}{dx^2}(x) = 0 & \text{(simply supported end)} \\ \frac{d^2w}{dx^2}(x) = \frac{\alpha}{EI}, \frac{d^3w}{dx^3}(x) = \frac{\beta}{EI} & \text{(free end with forces)} \end{cases} \tag{3.1}$$

3.1 Weak formulation

Let $\Gamma_C \subset \partial\Omega$, $\Gamma_S \subset \partial\Omega$, and $\Gamma_F \subset \partial\Omega$ be the points where the clamped, simply supported and fixed boundary conditions hold.

$$V := \left\{ v \in H^2(\Omega) \,\middle|\, v(x_c) = \frac{dv}{dx}(x_c) = 0, \quad v(x_s) = 0, \quad x_c \in \Gamma_C, x_s \in \Gamma_S \right\} \tag{3.2}$$

For $a \in L^2(\Omega)$

$$w \in V: \quad \int_\Omega EI\frac{d^2w}{dx^2}\frac{d^2v}{dx^2} = \int_\Omega qv + \int_{\Gamma_F}(\alpha\frac{dv}{dx} + \beta v) =: l(v) \quad \forall v \in V. \tag{3.3}$$

Lemma 3.1. *(3.3) has a unique solution if $\Gamma_C \neq \emptyset$ and the solution satisfies a weak version of (3.1).*

Proof. Existence and uniqueness follow from the Lax-Milgram lemma and Poincaré's inequality, for which we need the boundary condition.

If w is smooth enough, integration by parts gives

$$\begin{aligned} \int_\Omega EI\frac{d^2w}{dx^2}\frac{d^2v}{dx^2} &= -\int_\Omega \frac{d}{dx}(EI\frac{d^2w}{dx^2})\frac{dv}{dx} + \left[EI\frac{d^2w}{dx^2}\frac{dv}{dx}\right]_0^L \\ &= \int_\Omega \frac{d^2}{dx^2}(EI\frac{d^2w}{dx^2})v + \left[EI\frac{d^2w}{dx^2}\frac{dv}{dx}\right]_0^L - \left[EI\frac{d^3w}{dx^3}v\right]_0^L \end{aligned}$$

Taking $v \in H_0^2(\Omega) \subset V$, we have $\frac{d^2}{dx^2}(EI\frac{d^2w}{dx^2})(x) = q(x)$ a.e. For arbitrary $v \in V$ we then have

$$\left[EI\frac{d^2w}{dx^2}\frac{dv}{dx}\right]_0^L - \left[EI\frac{d^3w}{dx^3}v\right]_0^L = 0 \tag{3.4}$$

find the boundary conditions. First of $0 = x_c$ we have the boundary conditions by the definition of V and the corresponding boundary terms in (3.4) vanish. If $0 = x_s$ we have by definition of V $w(0) = 0$ and the remaining term in (3.4) yields $EI\frac{d^2w}{dx^2}(0) = 0$. Finally for $0 = x_f$ we find the free end conditions by (3.4) . □

3.2 Lowest order approximation

We use a mesh $h : 0 = x_0 < x_1 < \cdots < x_N = L$ and the spaces of quadratic B-splines, writing them as the subspace of quadratic finite elements of class C^1. Let $(\phi_i)_{0 \leqslant i \leqslant N}$ be the canonical bases $\mathcal{P}^1_h$ and $\psi_i(x) := \frac{(x-x_{i-1})(x_i-x)}{2h_i^2}$, $1 \leqslant i \leqslant N$. In addition let $h_i := x_i - x_{i-1}$ and $x_{i-\frac{1}{2}} := \frac{x_{i-1}+x_i}{2}$, $1 \leqslant i \leqslant N$.

We consider the case of a left and right clamped beam. Noticing that, with u' the piecewise derivative of $u \in \mathcal{P}^2_h$, we have

$$u \in C^1(\Omega) \quad \Leftrightarrow \quad \int_\Omega \left(u'\phi_i' + u''\phi_i\right) = 0 \quad \forall 1 \leqslant i < N, \tag{3.5}$$

we define

$$V_h := \left\{ v \in \mathcal{P}^2_h \;\middle|\; \int_\Omega \left(v'\phi_i' + v''\phi_i\right) = 0 \quad \forall 0 \leqslant i \leqslant N \right\} \cap H^1_0(\Omega). \tag{3.6}$$

and the discrete problem is

$$\inf \left\{ \frac{1}{2} \int_\Omega EI \left(\frac{d^2 w}{dx^2}\right)^2 - l(w) \;\middle|\; w \in V_h \right\}. \tag{3.7}$$

For the implementation we consider (3.7) as a constrained minimization and use the representation in terms of the indicated basis and a lagrange multiplier

$$w = \sum_{j=0}^N \alpha_j \phi_j + \sum_{j=1}^N \beta_j \psi_j, \quad \lambda := \sum_{j=0}^N \gamma_j \phi_j. \tag{3.8}$$

Then the discrete system reads

$$\begin{bmatrix} 0 & 0 & A^T & C^T \\ 0 & D & B^T & 0 \\ A & B & 0 & 0 \\ C & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{bmatrix} = \begin{bmatrix} a \\ b \\ 0 \\ 0 \end{bmatrix}, \quad \left\{ \begin{aligned} a_i := l(\phi_i), \quad b_i := l(\psi_i) \\ D_{ij} = \int_\Omega EI\psi_i''\psi_j'', \quad A_{ij} = \int_\Omega \phi_i'\phi_j', \\ B_{ij} = \int_\Omega \phi_i'\psi_j' + \phi_i\psi_j'', \\ C_{ij} = \phi_j(x_i) \quad x_i \in \{0; L\}. \end{aligned} \right. \tag{3.9}$$

Since D is a regular diagonal matrix we can easily eliminate β:

$$\begin{bmatrix} 0 & A^T & C^T \\ A & X & 0 \\ C & 0 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \gamma \\ \delta \end{bmatrix} = \begin{bmatrix} a \\ BD^{-1}b \\ 0 \end{bmatrix}, \quad X := -BD^{-1}B^T$$

We have

$$\psi_i'(x) = \frac{(x_{i-\frac{1}{2}} - x)}{h_i^2}, \quad \psi_i''(x) = \frac{-1}{h_i^2},$$

$$B_{ii} = \int_{x_{i-1}}^{x_i} \phi_i'\psi_i' + \phi_i\psi_i'' = \int_{x_{i-1}}^{x_i} \phi_i\psi_i'' = \frac{-1}{2h_i}, \quad B_{i,i+1} = \frac{-1}{2h_{i+1}}, \quad D_{ii} = \frac{EI_i}{h_i^3}$$

$$\begin{cases} X_{i,i-1} = \dfrac{h_i}{4EI_i} \\ X_{i,i} = \dfrac{h_i}{4EI_i} + \dfrac{h_{i+1}}{4EI_{i+1}} \\ X_{i,i+1} = \dfrac{h_{i+1}}{4EI_{i+1}} \end{cases}$$

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((
  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

$$\widetilde{\vec{n}[i]} = |S_i|\, \vec{n}[i]$$

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]**.

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

Gradient of λ_i

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

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

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

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 $1 \leqslant l \leqslant k$

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

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

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

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

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

$$\psi_S\big|_K = 1 - d\lambda^K_S, \quad \nabla\psi_S\big|_K = \frac{|S|\sigma^K_S}{|K|} n_S, \quad \frac{1}{|K|}\int_K \psi_S = \frac{1}{d+1}. \tag{B.8}$$

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

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

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

where $X^k_h := \left\{ xp \mid p\big|_K \in P^k_{\mathrm{hom}}(K)\; \forall K \in \mathcal{K}_h \right\}$ 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 $\mathcal{RT}^0$

$$\Phi_S\big|_K := \sigma^K_S \frac{x - x^K_S}{h^K_S}, \quad \int_K \operatorname{div}\Phi_S\big|_K = \sigma^K_S \frac{d|K|}{h^K_S} = \sigma^K_S |S|, \quad \frac{1}{|K|}\int_K \Phi_S = \sigma^K_S \frac{x_K - x^K_S}{h^K_S}. \tag{B.10}$$

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

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

The `pyhon` implementation reads

B.3.4 Moving a point to the boundary

Let K be a simplex and $x \in K = \operatorname{conv}\{a_i \mid 0 \leqslant i \leqslant d\}$ given, i.e.

$$x = \sum_{i=0}^d \lambda_i a_i = a_0 + \sum_{i=1}^d \lambda_i (a_i - a_0)$$

Given $\beta \in \mathbb{R}^d$ we wish to find $x_\beta \in \partial K$ such that

$$x_\beta = \sum_{i=0}^d \mu_i a_i, \quad x_\beta = x + \delta\beta, \quad \delta > 0. \tag{B.11}$$

The condition $x_\beta \in \partial K$ amounts to $0 \leqslant \mu_i \leqslant 1$, $\sum_{i=0}^{d} \mu_i = 1$, and δ to be maximal. We get the solution in two steps. First we find b_i such that

$$\beta = \sum_{i=1}^{d} b_i(a_i - a_0),$$

which gives

$$\sum_{i=1}^{d} (\mu_i - \lambda_i - \delta b_i)(a_i - a_0) = 0 \quad \Rightarrow \quad \mu_i = \lambda_i + \delta b_i \quad \forall 1 \leqslant i \leqslant d.$$

Now δ has to be chosen, such that the point x_β lies inside K, i.e.

$$\begin{cases} 0 \leqslant \lambda_i + \delta b_i \leqslant 1 \\ 0 \leqslant \displaystyle\sum_{i=1}^{d} (\lambda_i + \delta b_i) \leqslant 1 \end{cases} \Leftrightarrow \quad \begin{cases} -\lambda_i \leqslant \delta b_i \leqslant 1 - \lambda_i \quad \forall 1 \leqslant i \leqslant d, \\ \delta \displaystyle\sum_{i=1}^{d} b_i \leqslant \lambda_0 \end{cases}$$

Lemma B.1. *Let* $0 \leqslant \lambda_i \leqslant 1$. *Then the solution of*

$$\max \left\{ \delta \;\middle|\; -\lambda_i \leqslant \delta b_i \leqslant 1 - \lambda_i \quad \forall 1 \leqslant i \leqslant d, \quad \delta \sum_{i=1}^{d} b_i \leqslant \lambda_0 \right\} \tag{B.12}$$

is

$$\delta = \min \left\{ \min \left\{ \frac{1 - \lambda_i}{b_i} \;\middle|\; b_i > 0 \right\}, \min \left\{ \frac{-\lambda_i}{b_i} \;\middle|\; b_i < 0 \right\}, \frac{\lambda_0}{\sum_{i=1}^{d} b_i} \right\} \quad \textit{if} \quad \sum_{i=1}^{d} b_i > 0 \tag{B.13}$$

Proof. For $b_i > 0$ we have $\delta \leqslant \frac{1-\lambda_i}{b_i}$, so $0 \leqslant \delta b_i + \lambda_i \leqslant 1$.

For $b_i < 0$ we have $\delta \leqslant \frac{-\lambda_i}{b_i}$, so $0 \leqslant \lambda_i + \delta b_i \leqslant \lambda_i \leqslant 1$. □

C 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 $\nabla_h q\big|_K := \nabla\left(q\big|_K\right)$ 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

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

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 $C_h^k(\Omega)$ 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

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

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

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

Lemma C.1.

$$a(u,u) = \int_\Omega \frac{\mathrm{div}(\beta)}{2}u^2 + \int_{\partial\Omega} \frac{|\beta_n|}{2}u^2. \tag{C.5}$$

Proof. We also have

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

such that the result follows with $v = u$. □

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

Let

$$\begin{cases}
a_h(u,v) := \displaystyle\int_\Omega \mathrm{div}_h(\beta u)v - \int_{\partial\Omega} \beta_n^- uv - \int_{\mathcal{S}_h} [u]\, \beta_S^\sharp(v) \\
\beta_S^\sharp(v) := \beta_{n_S}^- v^{\mathrm{in}} + \beta_{n_S}^+ v^{\mathrm{ex}} = \beta_{n_S}\{v\} - \dfrac{|\beta_{n_S}|}{2}[v]
\end{cases} \tag{C.6}$$

Lemma C.2. *We have*

$$\begin{cases} a_h(u,v) = -\int_\Omega u(\beta\cdot\nabla_h v) + \int_{\partial\Omega} \beta_n^+ uv + \int_{\mathcal{S}_h} \beta_S^\flat(u)\,[v]\,, \\ \beta_S^\flat(u) := \beta_{n_S}^+ u^{\text{in}} + \beta_{n_S}^- u^{\text{ex}} = -(-\beta_S)^\sharp(u) = \beta_{n_S}\{v\} + \frac{|\beta_{n_S}|}{2}[v] \end{cases} \tag{C.7}$$

and

$$a_h(u,v) = \frac{1}{2}\int_\Omega (\operatorname{div}_h(\beta u)v - u(\beta\cdot\nabla_h v)) + \int_{\partial\Omega}\frac{|\beta_n|}{2}uv + \int_{\mathcal{S}_h}\frac{|\beta_n|}{2}[u]\,[v] + \int_{\mathcal{S}_h}\frac{\beta_n}{2}\left(u^{\text{ex}}v^{\text{in}} - u^{\text{in}}v^{\text{ex}}\right) \tag{C.8}$$

Proof.

$$\int_\Omega \operatorname{div}_h(\beta u)v = -\int_\Omega u(\beta\cdot\nabla_h v) + \int_{\partial\Omega}\beta_n uv + \int_{\mathcal{S}_h}\beta_{n_S}\,[uv]$$

We get (C.7) with

$$\begin{aligned} \beta_{n_S}\,[uv] - [u]\,\beta_S^\sharp(v) =& \beta_{n_S}\left([u]\{v\} + \{u\}[v]\right) - [u]\,\beta_{n_S}\{v\} + \frac{|\beta_{n_S}|}{2}[u]\,[v] \\ =& \beta_{n_S}\{u\}[v] + \frac{|\beta_{n_S}|}{2}[u]\,[v] = \beta_S^\flat(u)\,[v]\,. \end{aligned}$$

Finally for (C.8)

$$\begin{aligned} \beta_S^\flat(u)\,[v] - [u]\,\beta_S^\sharp(v) &= |\beta_n|\,[u]\,[v] + \beta_{n_S}\{u\}[v] - [u]\,\beta_{n_S}\{v\} \\ \beta_{n_S}\{u\}[v] - [u]\,\beta_{n_S}\{v\} &= \frac{\beta_n}{2}\left(u^{\text{ex}}v^{\text{in}} - u^{\text{in}}v^{\text{ex}}\right) \end{aligned}$$

□

Corollary C.3.

$$a_h(u,u) = \int_\Omega \frac{\operatorname{div}_h(\beta)}{2}u^2 + \int_{\partial\Omega}\frac{|\beta_n|}{2}u^2 + \int_{\mathcal{S}_h}\frac{|\beta_{n_S}|}{2}[u]^2 \tag{C.9}$$

Proof.

$$\begin{aligned} 2a_h(u,u) =& \int_\Omega \operatorname{div}_h(\beta u)u - \int_{\partial\Omega}\beta_n^- uu - \int_{\mathcal{S}_h}\beta_S^\sharp(u)\,[u] - \int_\Omega u(\beta\cdot\nabla_h u) + \int_{\partial\Omega}\beta_n^+ uu + \int_{\mathcal{S}_h}[u]\,\beta_S^\flat(u) \\ =& \int_\Omega \operatorname{div}_h(\beta)u^2 + \int_{\partial\Omega}|\beta_n|\,u^2 + \int_{\mathcal{S}_h}[u]\left(\beta_S^\flat(u) - \beta_S^\sharp(u)\right) \end{aligned}$$

$$\beta_S^\flat(u) - \beta_S^\sharp(u) = \beta_{n_S}^+ u^{\text{in}} + \beta_{n_S}^- u^{\text{ex}} - \beta_{n_S}^- u^{\text{in}} - \beta_{n_S}^+ u^{\text{ex}} = |\beta_{n_S}|\,u^{\text{in}} - |\beta_{n_S}|\,u^{\text{ex}}$$

□

We suppose $\beta \in \mathcal{RT}_h^1$ with $\operatorname{div}\beta = 0$. Then $\beta \in D_h^0$ and we have

$$\int_\Omega u(\beta\cdot\nabla_h v) = \int_\Omega \pi_h u(\beta\cdot\nabla_h v) = \int_{\partial\Omega}\beta_n(\pi_h u)v + \int_{\mathcal{S}_h}\beta_n\,[\pi_h u]\,v$$

Corollary C.4. *For* $k = 0$ *the solution to*

$$u \in \mathcal{D}_h^0 : \quad a_h(u, v) = l(v) \quad \forall v \in \mathcal{D}_h^0 \tag{C.10}$$

satisfies monotonicity: $l \geqslant 0$ *implies* $u \geqslant 0$

Proof. We write $u = u^+ + u^-$ and use $v = u^-$ in (C.10) such that

$$a(u^-, u^-) = a(u, u^-) - a(u^+, u^-) = l(u^-) - a(u^+, u^-) \leqslant -a(u^+, u^-).$$

and since with $x - |x| = 2x^-$ and $-x - |x| = -2x^+$

$$\int_{\mathcal{S}_h} \frac{|\beta_n|}{2} [u] [v] + \int_{\mathcal{S}_h} \frac{\beta_n}{2} \left(u^{\mathrm{ex}} v^{\mathrm{in}} - u^{\mathrm{in}} v^{\mathrm{ex}}\right) = \int_{\mathcal{S}_h} \frac{|\beta_n|}{2} \left(u^{\mathrm{in}} v^{\mathrm{in}} + u^{\mathrm{ex}} v^{\mathrm{ex}}\right) + \int_{\mathcal{S}_h} \left(\beta_n^- u^{\mathrm{ex}} v^{\mathrm{in}} - \beta^+ u^{\mathrm{in}} v^{\mathrm{ex}}\right) \tag{C.11}$$

$$\begin{aligned} a(u^+, u^-) &= \int_{\partial\Omega} \frac{|\beta_n|}{2} u^+ u^- + \int_{\mathcal{S}_h} \frac{|\beta_n|}{2} \left[u^+\right] \left[u^-\right] + \int_{\mathcal{S}_h} \frac{\beta_n}{2} \left(u^{+\mathrm{ex}} u^{-\mathrm{in}} - u^{+\mathrm{in}} u^{-\mathrm{ex}}\right) \\ &= \underbrace{\int_{\partial\Omega} \frac{|\beta_n|}{2} u^+ u^-}_{=0} + \underbrace{\int_{\mathcal{S}_h} \frac{|\beta_n|}{2} \left(u^{+\mathrm{in}} u^{-\mathrm{in}} + u^{+\mathrm{ex}} u^{-\mathrm{ex}}\right)}_{=0} + \underbrace{\int_{\mathcal{S}_h} \left(\beta_n^- u^{+\mathrm{ex}} u^{-\mathrm{in}} - \beta^+ u^{+\mathrm{in}} u^{-\mathrm{ex}}\right)}_{\geqslant 0} \end{aligned}$$

Since $a(u, u)$ is norm on $\mathcal{D}_h^0$, we have $u^- = 0$, i.e. $u \geqslant 0$. □

C.2 $\mathcal{D}_h^1(\Omega)$

We have for $\beta \in \mathcal{RT}_h^0$ with $\operatorname{div} \beta = 0$

$$\int_\Omega (\beta \cdot \nabla_h u) v = \int_\Omega (\beta \cdot \nabla_h u) \pi_h^0 v = \int_{\mathcal{S}_h^{\mathrm{int}}} \beta_n \left[u \pi_h^0 v\right] + \int_{\partial\Omega} u \beta_n \pi_h^0 v$$

C.3 $\mathcal{P}_h^1(\Omega)$

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

$$x_K^\sharp = x_K + \delta_K \beta_K \tag{C.12}$$

If we know $\vec{n}[i]^\mathsf{T} \beta_K$, we can compute $x_K^\sharp$ as follows.

$$\lambda_i(x_K^\sharp) = \lambda_i(x_K) + \delta_K \nabla \lambda_i{}^\mathsf{T} \beta_K = \frac{1}{d+1} - \delta_K \frac{\vec{n}[i]^\mathsf{T} \beta_K}{h_i} = \frac{1}{d+1} - \delta_K \frac{\vec{n}[i]^\mathsf{T} \beta_K |S_i|}{d\,|K|}$$

It follows that

$$\delta_K = \max \left\{ \frac{d\,|K|}{(d+1)\,|S_i| \left(\vec{n}[i]^\mathsf{T} \beta_K\right)^+} \;\middle|\; 0 \leqslant i \leqslant d \right\}. \tag{C.13}$$

The stabilized bilinear form is

$$a^{\mathrm{supg}}(u, v) := \int_\Omega (\beta \cdot \nabla u) v - \int_{\partial\Omega} \beta_n^- u v + \int_\Omega \delta (\beta \cdot \nabla u)(\beta \cdot \nabla v) \tag{C.14}$$

Then we have

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