

Simple finite element methods in Python

Roland Becker

May 17, 2021

Contents

1	Heat equation	2
1.1	Boundary conditions	3
1.1.1	Nitsche's method	3
1.2	Computation of the matrices for $\mathcal{P}_h^1(\Omega)$	3
2	Stokes problem	4
2.1	Weak formulation	4
2.2	Implementations of Dirichlet condition	5
2.2.1	Pressure mean	5
3	Beam problem	6
3.1	Weak formulation	6
3.2	Lowest order approximation	7
A	Python implementation	9
B	Finite elements on simplices	10
B.1	Simplices	10
B.2	Barycentric coordinates	10
B.3	Finite elements	11
B.3.1	$\mathcal{P}_h^1(\Omega)$	11
B.3.2	$\mathcal{CR}_h^1(\Omega)$	12
B.3.3	$\mathcal{RT}_h^0(\Omega)$	12
B.3.4	Moving a point to the boundary	12
C	Discretization of the transport equation	14
C.1	$\mathcal{D}_h^k(\Omega)$	14
C.2	$\mathcal{D}_h^1(\Omega)$	16
C.3	$\mathcal{P}_h^1(\Omega)$	16

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)

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

Heat equation (weak formulation)

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

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

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 Boundary conditions

1.1.1 Nitsche's method

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

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

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

Now, if $z_h \in V_h$ such that $z - z_h \in H_0^1(\Omega)$

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

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

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

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

For the convection, we suppose that $\vec{v} \in \mathcal{R}_h^0(\Omega)$ 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

$$\begin{aligned} \int_K \lambda_j \vec{v} \cdot \nabla \lambda_i &= \sum_{k=1}^{d+1} v_k \int_K \lambda_j \Phi_k \cdot \nabla \lambda_i \\ \int_K \lambda_j \Phi_k \cdot \nabla \lambda_i &= - \frac{\sigma_k \sigma_i}{h_k h_i} \int_K \lambda_j (x - x_k) \cdot n_i = - \frac{\sigma_k \sigma_i}{h_k h_i} \sum_{l=1}^{d+1} (x_l - x_k) \cdot n_i \int_K \lambda_j \lambda_l \end{aligned}$$

2 Stokes problem

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

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

2.1 Weak formulation

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

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

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 $l := l_\Omega + l_{\partial\Omega}$

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

□

Alternatively, we can write the system as

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

2.2 Implementations of Dirichlet condition

We write the discrete velocity space V_h as a direct sum $V_h = V_h^{\text{int}} \oplus V_h^{\text{dir}}$, 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 $u_h^D \in V_h^{\text{dir}}$ be an approximation of the Dirichlet data v^D we have the traditional way to implement Dirichlet boundary conditions:

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

As for the Poisson problem, we obtain an alternative formulation

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

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 $(1, nc)$

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

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

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

3 Beam problem

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

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.

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

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

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

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

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

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

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

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 $EI \frac{d^2 w}{dx^2}(0) = 0$. Finally for $0 = x_f$ we find the free end conditions by (3.4). \square

3.2 Lowest order approximation

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

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

$$u \in C^1(\Omega) \quad \Leftrightarrow \quad \int_{\Omega} (u' \phi'_i + u'' \phi_i) = 0 \quad \forall 1 \leq i < N, \quad (3.5)$$

we define

$$V_h := \left\{ v \in \mathcal{P}_h^2 \mid \int_{\Omega} (v' \phi'_i + v'' \phi_i) = 0 \quad \forall 0 \leq i \leq N \right\} \cap H_0^1(\Omega). \quad (3.6)$$

and the discrete problem is

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

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

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

Then the discrete system reads

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

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

$$\begin{aligned} \psi_i'(x) &= \frac{(x_{i-\frac{1}{2}} - x)}{h_i^2}, \quad \psi_i''(x) = \frac{-1}{h_i^2}, \\ B_{ii} &= \int_{x_{i-1}}^{x_i} \phi_i' \psi_i' + \phi_i \psi_i'' = \int_{x_{i-1}}^{x_i} \phi_i \psi_i'' = \frac{-1}{2h_i}, \quad B_{i,i+1} = \frac{-1}{2h_{i+1}}, \quad D_{ii} = \frac{EI_i}{h_i^3} \\ &\quad \left\{ \begin{aligned} X_{i,i-1} &= \frac{h_i}{4EI_i} \\ X_{i,i} &= \frac{h_i}{4EI_i} + \frac{h_{i+1}}{4EI_{i+1}} \\ X_{i,i+1} &= \frac{h_{i+1}}{4EI_{i+1}} \end{aligned} \right. \end{aligned}$$

A 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((
    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 $K = (x_0, x_1, \dots, x_d)$. The volume of K is given by

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

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 $P_{S_k} x_k = x_k + h_k \vec{n}[k]$ and $S_k = \{x \in \mathbb{R}^d \mid \vec{n}[k]^T x = h_k\}$ and

$$\begin{aligned} 0 &= \int_K \operatorname{div}(\vec{c}) = \sum_{i=0}^d \int_{S_i} \vec{c} \cdot \vec{n}[i] = \vec{c} \cdot \sum_{i=0}^d |S_i| \vec{n}[i] \Rightarrow \sum_{i=0}^d |S_i| \vec{n}[i] = 0 \\ d|K| &= \int_K \operatorname{div}(x) = \sum_{i=0}^d \int_{S_i} x \cdot \vec{n}[i] = \sum_{i=0}^d |S_i| h_i \end{aligned}$$

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

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

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

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

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^{∂} , 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

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

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

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

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

For the computation of matrices we use (B.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

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

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

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

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

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

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

Formulae for \mathcal{CR}_h^1

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

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

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

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

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

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

For the [python](#) 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 [python](#) implementation reads

B.3.4 Moving a point to the boundary

Let K be a simplex and $x \in K = \text{conv}\{a_i \mid 0 \leq i \leq d\}$ 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

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

The condition $x_\beta \in \partial K$ amounts to $0 \leq \mu_i \leq 1$, $\sum_{i=0}^d \mu_i = 1$, 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

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

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

$$\left\{ \begin{array}{l} 0 \leq \lambda_i + \delta b_i \leq 1 \\ 0 \leq \sum_{i=1}^d (\lambda_i + \delta b_i) \leq 1 \end{array} \right\} \Leftrightarrow \left\{ \begin{array}{l} -\lambda_i \leq \delta b_i \leq 1 - \lambda_i \quad \forall 1 \leq i \leq d, \\ \delta \sum_{i=1}^d b_i \leq \lambda_0 \end{array} \right.$$

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

$$\max \left\{ \delta \left| \begin{array}{l} -\lambda_i \leq \delta b_i \leq 1 - \lambda_i \quad \forall 1 \leq i \leq d, \\ \delta \sum_{i=1}^d b_i \leq \lambda_0 \end{array} \right. \right\} \quad (B.12)$$

is

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

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

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

C Discretization 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

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

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

Suppose u satisfies

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

From the integration by parts formula

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

it then follows that u satisfies

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

with

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

Lemma C.1.

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

Proof. We also have

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

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

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

Let

$$\begin{cases} a_h(u, v) := \int_{\Omega} \text{div}_h(\beta u) v - \int_{\partial\Omega} \beta_n^- u v - \int_{S_h} [u] \beta_S^\#(v) \\ \beta_S^\#(v) := \beta_{n_S}^- v^{\text{in}} + \beta_{n_S}^+ v^{\text{ex}} = \beta_{n_S} \{v\} - \frac{|\beta_{n_S}|}{2} [v] \end{cases} \quad (\text{C.6})$$

Lemma C.2. *We have*

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

and

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

Proof.

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

We get (C.7) with

$$\begin{aligned} \beta_{n_S} [uv] - [u] \beta_S^\#(v) &= \beta_{n_S} ([u] \{v\} + \{u\} [v]) - [u] \beta_{n_S} \{v\} + \frac{|\beta_{n_S}|}{2} [u] [v] \\ &= \beta_{n_S} \{u\} [v] + \frac{|\beta_{n_S}|}{2} [u] [v] = \beta_S^b(u) [v]. \end{aligned}$$

Finally for (C.8)

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

□

Corollary C.3.

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

Proof.

$$\begin{aligned} 2a_h(u, u) &= \int_{\Omega} \text{div}_h(\beta u) u - \int_{\partial\Omega} \beta_n^- uu - \int_{S_h} \beta_S^\#(u) [u] - \int_{\Omega} u(\beta \cdot \nabla_h u) + \int_{\partial\Omega} \beta_n^+ uu + \int_{S_h} [u] \beta_S^b(u) \\ &= \int_{\Omega} \text{div}_h(\beta) u^2 + \int_{\partial\Omega} |\beta_n| u^2 + \int_{S_h} [u] (\beta_S^b(u) - \beta_S^\#(u)) \end{aligned}$$

$$\beta_S^b(u) - \beta_S^\#(u) = \beta_{n_S}^+ u^{\text{in}} + \beta_{n_S}^- u^{\text{ex}} - \beta_{n_S}^- u^{\text{in}} - \beta_{n_S}^+ u^{\text{ex}} = |\beta_{n_S}| u^{\text{in}} - |\beta_{n_S}| u^{\text{ex}}$$

□

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

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

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

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

satisfies monotonicity: $l \geq 0$ implies $u \geq 0$

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

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

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

$$\int_{\mathcal{S}_h} \frac{|\beta_n|}{2} [u] [v] + \int_{\mathcal{S}_h} \frac{\beta_n}{2} (u^{\text{ex}} v^{\text{in}} - u^{\text{in}} v^{\text{ex}}) = \int_{\mathcal{S}_h} \frac{|\beta_n|}{2} (u^{\text{in}} v^{\text{in}} + u^{\text{ex}} v^{\text{ex}}) + \int_{\mathcal{S}_h} (\beta_n^- u^{\text{ex}} v^{\text{in}} - \beta_n^+ u^{\text{in}} v^{\text{ex}}) \quad (\text{C.11})$$

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

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

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

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

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

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

$$x_K^\# = x_K + \delta_K \beta_K \quad (\text{C.12})$$

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

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

It follows that

$$\delta_K = \max \left\{ \frac{d|K|}{(d+1)|S_i| \left(\vec{n}[i]^T \beta_K \right)^+} \mid 0 \leq i \leq d \right\}. \quad (\text{C.13})$$

The stabilized bilinear form is

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

Then we have

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