Simple finite element methods in Python

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Contents

1 Heat equation **2**

1.1 Boundary conditions . . . 2

1.1.1 Nitsche's method . . . 2

1.2 Computation of the matrices for $\mathcal{P}^1_h(\Omega)$ . . . 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 . . . 6

A Python implementation **8**

B Finite elements on simplices **9**

B.1 Simplices . . . 9

B.2 Barycentric coordinates . . . 9

B.3 Finite elements . . . 10

B.3.1 $\mathcal{P}^1_h(\Omega)$ . . . 10

B.3.2 $\mathcal{CR}^1_h(\Omega)$ . . . 10

B.3.3 $\mathcal{RT}^0_h(\Omega)$ . . . 11

B.3.4 Moving a point to the boundary . . . 11

C Discreization of the transport equation **12**

C.1 $\mathcal{P}^1_h(\Omega)$ . . . 12

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 Boundary conditions

1.1.1 Nitsche's method

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

Let $-\operatorname{div}(\mu\nabla z) = 0$ and $z_{|\Gamma_D} = 1$ and $z_{|\Gamma_N} = 0$. 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 $z - z_h \in H^1_0(\Omega)$

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

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

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

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

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 $V_h = V_h^{\text{int}} \oplus V_h^{\text{dir}}$, 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:

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

As for the Poisson problem, we obtain an alternative formulation

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

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 $S = BA^{-1}B^T$, $T = CS^{-1}C^T$

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

References Section 2

[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.

3 Beam problem

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

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 $\mathcal{P}_h^1$ 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 $u \in \mathcal{P}_h^2$, 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

$$V_h := \left\{ v \in \mathcal{P}_h^2 \;\middle|\; \int_\Omega \left(v'\phi_i' + v''\phi_i\right) = 0 \quad \forall 0 \leqslant i \leqslant N \right\} \cap H_0^1(\Omega). \tag{3.6}$$

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

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

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((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

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

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

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

[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

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

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 $C_h^k(\Omega)$ 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 $\mathcal{CR}_h^1(\Omega)$

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

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

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

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

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

Formulae for $\mathcal{RT}^0$

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

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

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.

$$0 \leqslant \lambda_i + \delta b_i \leqslant 1 \quad \Leftrightarrow \quad -\lambda_i \leqslant \delta b_i \leqslant 1 - \lambda_i \quad \forall 1 \leqslant i \leqslant d.$$

The maximization of δ under these constraints has the solution

$$\delta = \max\left\{ \max\left\{ \frac{1-\lambda_i}{b_i} \;\middle|\; b_i > 0 \right\}, \max\left\{ \frac{\lambda_i}{-b_i} \;\middle|\; b_i < 0 \right\} \right\}. \tag{B.12}$$

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

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