Simple finite element methods in Python

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1 Heat equation

Let $\Omega \subset \mathbb{R}^d$, d=2,3 be the computational domain. We suppose to have a disjoined partition of its boundary: $\partial \Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$. We consider the parabolic equation for the temperature T, heat flux \vec{q} and heat release \dot{q}

Heat equation (strong formulation)

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

Heat equation (weak formulation)

Let $H^1_f:=\Big\{u\in H^1(\Omega)\ \Big|\ T_{|_{\Gamma_D}}=f\Big\}$. The standard weak formulation looks for $T\in H^1_{T^D}$ such that for all $\varphi\in H^1_0(\Omega)$

$$\int_{\Omega} \rho C_{p} \frac{\partial T}{\partial t} \varphi - \int_{\Omega} \vec{v} T \cdot \nabla \varphi + \int_{\Omega} k \nabla T \cdot \nabla \varphi + \int_{\Gamma_{R}} c_{R} T \varphi + \int_{\Gamma_{R} \cup \Gamma_{N}} \vec{v}_{n} T \varphi = \int_{\Omega} \dot{q} \varphi + \int_{\Gamma_{R}} q^{R} \varphi \quad (1.2)$$

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

$$\int_{\Omega} \operatorname{div} \vec{F} = \int_{\partial \Omega} \vec{F}_{n} \quad \stackrel{F \to F \varphi}{\Longrightarrow} \quad \int_{\Omega} (\operatorname{div} \vec{F}) \varphi = -\int_{\Omega} \vec{F} \cdot \nabla \varphi + \int_{\partial \Omega} \vec{F}_{n} \varphi,$$

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

$$\int_{\Omega} \operatorname{div} \left(\vec{v} + \vec{q} \right) \varphi = - \int_{\Omega} \vec{v} \cdot \nabla \varphi + \int_{\Omega} k \nabla T \cdot \nabla \varphi + \int_{\partial \Omega} \vec{F}_n \varphi.$$

Using that ϕ vanishes on Γ_D we have

$$\int_{\partial\Omega} \vec{F}_n \varphi = \int_{\Gamma_N \cup \Gamma_R} \vec{F}_n \varphi = \int_{\Gamma_N \cup \Gamma_R} \vec{v}_n \varphi + \int_{\Gamma_N \cup \Gamma_R} \vec{q}_n \varphi,$$

and then with the different boundary conditions, we find

$$\int_{\Gamma_{N}\cup\Gamma_{R}}\vec{q}_{n}\varphi=\int_{\Gamma_{D}}q^{N}\varphi+\int_{\Gamma_{R}}\left(q^{R}-c_{R}T\right)\varphi$$

1.1 Boundary conditions

1.1.1 Nitsche's method

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

$$(1.3)$$

Let $-\operatorname{div}(\mu \nabla z) = 0$ and $z_{|_{\Gamma_{\!_{\rm D}}}} = 1$ and $z_{|_{\Gamma_{\!_{\rm N}}}} = 0$. 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 $z - z_h \in H_0^1(\Omega)$

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

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

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

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

we compute

$$\begin{split} \int_{K} \lambda_{j} \vec{v} \cdot \nabla \lambda_{i} &= \sum_{k=1}^{d+1} \nu_{k} \int_{K} \lambda_{j} \Phi_{k} \cdot \nabla \lambda_{i} \\ \int_{K} \lambda_{j} \Phi_{k} \cdot \nabla \lambda_{i} &= -\frac{\sigma_{k} \sigma_{i}}{h_{k} h_{i}} \int_{K} \lambda_{j} (x - x_{k}) \cdot n_{i} = -\frac{\sigma_{k} \sigma_{i}}{h_{k} h_{i}} \sum_{l=1}^{d+1} (x_{l} - x_{k}) \cdot n_{i} \int_{K} \lambda_{j} \lambda_{l} \end{split}$$

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: $\partial \Omega = \Gamma_D \cup \Gamma_N$.

$$\begin{cases} -\operatorname{div}\left(\mu\nabla\nu\right) + \nabla p = f & \text{in } \Omega \\ \operatorname{div}\nu = g & \text{in } \Omega \end{cases} \\ \nu = \nu^{D} & \text{in } \Gamma_{D} \end{cases}$$

$$\mu \frac{\partial \nu}{\partial n} - p n = -p^{N} n & \text{in } \Gamma_{N}$$

$$(2.1)$$

2.1 Weak formulation

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

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

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

Proof. By integration by parts we have

$$\alpha_{\Omega}(\nu,p;\varphi,\xi) = \int_{\Omega} \left(-\mu \Delta \nu + \nabla p \right) \cdot \varphi + \int_{\partial\Omega} \mu \frac{\partial\nu}{\partial n} \cdot \varphi - \int_{\partial\Omega} p \varphi_n + \int_{\Omega} \operatorname{div} \nu \xi$$

and therefore with $\mathfrak{a}:=\mathfrak{a}_\Omega+\mathfrak{a}_{\partial\Omega}$ and $\mathfrak{l}:=\mathfrak{l}_\Omega+\mathfrak{l}_{\partial\Omega}$

$$\begin{split} \alpha(\nu,p;\varphi\xi) - l(\nu,p;\varphi\xi) = & \int_{\Omega} \left(-\mu\Delta\nu + \nabla p - f \right) \cdot \varphi + \int_{\Omega} (\operatorname{div}\nu - g)\xi + \int_{\Gamma_{N}} \left(\mu\frac{\partial\nu}{\partial n} - pn + p^{N}n \right) \cdot \varphi \\ & + \int_{\Gamma_{D}} \frac{\gamma\mu}{h}\nu \cdot \varphi - \int_{\Gamma_{D}} \mu(\nu - \nu^{D}) \cdot \left(\frac{\gamma}{h}\varphi - \frac{\partial\varphi}{\partial n} \right) - \int_{\Gamma_{D}} (\nu - \nu^{D}) \cdot n\xi \end{split}$$

Alternatively, we can write the system as

$$\begin{cases} (\nu,p) \in V \times Q : & a(\nu,p;\varphi\xi) + b(\nu,\xi) - b(\varphi,p) = l_{\Omega}(\varphi,\xi) + l_{\partial\Omega}(\varphi,\xi) & \forall (\varphi,\xi) \in V \times Q \\ a(\nu,p;\varphi,\xi) := \int_{\Omega} \mu \nabla \nu : \nabla \varphi + \int_{\Gamma_{D}} \frac{\gamma \mu}{h} \nu \cdot \varphi - \int_{\Gamma_{D}} \mu \left(\frac{\partial \nu}{\partial n} \cdot n\varphi + \nu n \cdot \frac{\partial \varphi}{\partial n} \right) \\ b(\nu,\xi) := \int_{\Omega} \operatorname{div} \nu \xi - \int_{\Gamma_{D}} \nu_{n} \xi \end{cases} \tag{2.3}$$

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2.2 Implementations of Dirichlet condition

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

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

As for the Poisson problem, we obtain an alternative formulation

$$\begin{bmatrix} A^{\text{int}} & 0 & -B^{\text{int}}^{\mathsf{T}} \\ 0 & A^{\text{dir}} & 0 \\ B^{\text{int}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}_{h}^{\text{int}} \\ \mathbf{v}_{h}^{\text{dir}} \\ \mathbf{p}_{h} \end{bmatrix} = \begin{bmatrix} f^{\text{int}} - A^{\text{int}, \text{dir}} \mathbf{v}_{h}^{D} \\ A^{\text{dir}} \mathbf{v}_{h}^{D} \\ g - B^{\text{dir}} \mathbf{v}_{h}^{D} \end{bmatrix}.$$
(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)

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

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

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

$$(2.7)$$

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

$$\frac{d^2}{dx^2}(EI\frac{d^2w}{dx^2})(x) = q(x) \quad \Omega =]0; L[$$

$$\begin{cases} w(x) = \frac{dw}{dx}(x) = 0 & \text{(clamped end)} \\ w(x) = \frac{d^2w}{dx^2}(x) = 0 & \text{(simply supported end)} \\ \frac{d^2w}{dx^2}(x) = \frac{\alpha}{EI}, \frac{d^3w}{dx^3}(x) = \frac{\beta}{EI} & \text{(free end with forces)} \end{cases}$$
(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.

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

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

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

$$\begin{split} \int_{\Omega} \mathsf{E}\mathsf{I} \frac{\mathrm{d}^2 w}{\mathrm{d} x^2} \frac{\mathrm{d}^2 v}{\mathrm{d} x^2} &= -\int_{\Omega} \frac{\mathrm{d}}{\mathrm{d} x} (\mathsf{E}\mathsf{I} \frac{\mathrm{d}^2 w}{\mathrm{d} x^2}) \frac{\mathrm{d} v}{\mathrm{d} x} + \left[\mathsf{E}\mathsf{I} \frac{\mathrm{d}^2 w}{\mathrm{d} x^2} \frac{\mathrm{d} v}{\mathrm{d} x} \right]_0^{\mathsf{L}} \\ &= \int_{\Omega} \frac{\mathrm{d}^2}{\mathrm{d} x^2} (\mathsf{E}\mathsf{I} \frac{\mathrm{d}^2 w}{\mathrm{d} x^2}) v + \left[\mathsf{E}\mathsf{I} \frac{\mathrm{d}^2 w}{\mathrm{d} x^2} \frac{\mathrm{d} v}{\mathrm{d} x} \right]_0^{\mathsf{L}} - \left[\mathsf{E}\mathsf{I} \frac{\mathrm{d}^3 w}{\mathrm{d} x^3} v \right]_0^{\mathsf{L}} \end{split}$$

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

$$\left[EI \frac{d^2 w}{dx^2} \frac{dv}{dx} \right]_0^L - \left[EI \frac{d^3 w}{dx^3} v \right]_0^L = 0$$
 (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 $\mathrm{EI} \frac{\mathrm{d}^2 w}{\mathrm{d} x^2}(0)=0$. 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 $(\varphi_i)_{0\leqslant i\leqslant N}$ 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 \mathfrak{u}' the piecewise derivative of $\mathfrak{u} \in \mathcal{P}^2_h$, we have

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

we define

$$V_{h} := \left\{ v \in \mathcal{P}_{h}^{2} \mid \int_{\Omega} \left(v' \varphi_{i}' + v'' \varphi_{i} \right) = 0 \quad \forall 0 \leqslant i \leqslant N \right\} \cap H_{0}^{1}(\Omega). \tag{3.6}$$

and the discrete problem is

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

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

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

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

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

We have

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

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

$$|K| = \frac{1}{d!} \det(x_1 - x_0, \dots, x_d - x_0) = \frac{1}{d!} \det(1, x_0, x_1, \dots, x_d) \quad 1 = (1, \dots, 1)^{\mathsf{T}_1}.$$
 (B.1)

The d+1 sides S_k (co-dimension one, d-1-simplices or facets) are defined by $S_k = (x_0, \dots, y_k, \dots, x_d)$. 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 $P_{S_k}x_k = x_k + h_k\vec{\pi}_k$ and $S_k = \left\{x \in \mathbb{R}^d \mid \vec{\pi}_k^\mathsf{T} x = h_k\right\}$ 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

$$\lambda_{i}(x) = \frac{\vec{\pi}_{i}^{\mathsf{T}}(x_{j} - x)}{\vec{\pi}_{i}^{\mathsf{T}}(x_{j} - x_{i})} \quad (j \neq i), \qquad \lambda_{i}(x) = \frac{d^{s}(x, H)}{h_{i}}. \tag{B.2}$$

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

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

see [EisenbergMalvern73], [VermolenSegal18].

Gradient of λ_i

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

¹https://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 $\mathcal S_h^{int}$ 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 $\mathfrak n_S$, which coincides with the unit outward normal vector $\mathfrak n_{\partial\Omega}$ 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

 $\sigma_S^K := \begin{cases} +1 & \text{if } n_S = n_K, \\ -1 & \text{if } n_S = -n_K. \end{cases} \qquad \lambda_S^K : \text{ barycentric coordinates of } K$

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 . 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 $\pi^k_h: L^2(\Omega) \to \mathcal{D}^k_h(\Omega)$.

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 $\mathcal{P}^1_{h}(\Omega)$

$$\nabla \lambda_{S}^{K} = -\frac{\sigma_{S}^{K}}{h_{S}^{K}} n_{S}, \quad \frac{1}{|K|} \int_{K} \lambda_{S}^{K} = \frac{1}{d+1}. \tag{B.4}$$

For the computation of matrices we use (B.3), for example for $i, j \in [0, d]$

$$\int_{\mathsf{K}} \lambda_{\mathbf{i}} \lambda_{\mathbf{j}} = |\mathsf{K}| \frac{d!\alpha!}{(|\alpha|+d)!} \quad \text{with} \quad \begin{cases} \alpha = (1,1,0,\cdots,0) & (\mathbf{i} \neq \mathbf{j}) \\ \alpha = (2,0,\cdots,0) & (\mathbf{i} = \mathbf{j}) \end{cases}$$

so

$$\int_{K} \lambda_{i} \lambda_{j} = \frac{|K|}{(d+2)(d+1)} (1 + \delta_{ij})$$
(B.5)

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

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

B.3.2 $\mathfrak{CR}^1_{\mathsf{h}}(\Omega)$

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

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

Formulae for \mathbb{CR}^1

$$\psi_{S|_{K}} = 1 - d\lambda_{S}^{K}, \quad \nabla \psi_{S|_{K}} = \frac{|S|\sigma_{S}^{K}}{|K|} n_{S}, \quad \frac{1}{|K|} \int_{K} \psi_{S} = \frac{1}{d+1}.$$
 (B.8)

B.3.3 $\mathfrak{R}_{h}^{0}(\Omega)$

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

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

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

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

Formulae for \mathfrak{R}^0

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

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

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

The pyhon implementation reads

C Discreization of the transport equation

For $k \in \mathbb{N}_0$ we denote by $\mathcal{C}_h^k(\Omega)$ 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 $\nabla_h q_{|_K} := \nabla \left(q_{|_K}\right)$ for $q \in \mathcal{C}_h^l(\Omega)$ and similarly for $\operatorname{div}_h: \mathcal{C}_h^l(\Omega,\mathbb{R}^d) \to \mathcal{C}_h^{l-1}(\Omega)$. We frequently use the piecewise Stokes formula

$$\int_{\Omega} (\nabla_{\mathbf{h}} \mathbf{q}) \mathbf{v} + \int_{\Omega} \mathbf{q}(\operatorname{div}_{\mathbf{h}} \mathbf{v}) = \int_{\mathcal{S}_{\mathbf{h}}^{\text{int}}} [\mathbf{q} \mathbf{v}_{\mathbf{n}}] + \int_{\mathcal{S}_{\mathbf{h}}^{\partial}} \mathbf{q} \mathbf{v}_{\mathbf{n}}, \tag{C.1}$$

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

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

From the integration by parts formula

$$\int_{\Omega} \operatorname{div}(\beta \mathbf{u}) \mathbf{v} = -\int_{\Omega} \beta \mathbf{u} \cdot \nabla \mathbf{v} + \int_{\partial \Omega} \beta_{\mathbf{n}} \mathbf{u} \mathbf{v} \tag{C.3}$$

it then follows that u satisfies

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

with

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

We also have

$$\begin{split} a(\mathbf{u}, \mathbf{v}) = & \frac{1}{2} \int_{\Omega} \operatorname{div}(\beta) \mathbf{u} \mathbf{v} + \frac{1}{2} \int_{\Omega} \operatorname{div}(\beta \mathbf{u}) \mathbf{v} + \frac{1}{2} \int_{\Omega} (\beta \cdot \nabla \mathbf{u}) \mathbf{v} - \int_{\partial \Omega} \beta_{\mathbf{n}}^{-} \mathbf{u} \mathbf{v} \\ = & \frac{1}{2} \int_{\Omega} \operatorname{div}(\beta) \mathbf{u} \mathbf{v} + \frac{1}{2} \int_{\Omega} \left((\beta \cdot \nabla \mathbf{u}) \mathbf{v} - \mathbf{u} (\beta \cdot \nabla \mathbf{v}) \right) + \int_{\partial \Omega} \left(\frac{1}{2} \beta_{\mathbf{n}} - \beta_{\mathbf{n}}^{-} \right) \mathbf{u} \mathbf{v} \\ = & \frac{1}{2} \int_{\Omega} \operatorname{div}(\beta) \mathbf{u} \mathbf{v} + \frac{1}{2} \int_{\Omega} \left((\beta \cdot \nabla \mathbf{u}) \mathbf{v} - \mathbf{u} (\beta \cdot \nabla \mathbf{v}) \right) + \int_{\partial \Omega} \frac{|\beta_{\mathbf{n}}|}{2} \mathbf{u} \mathbf{v} \end{split}$$

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

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

$$x_{K}^{\sharp} = x_{K} + \delta_{K} \beta_{K} \tag{C.5}$$

If we know $\vec{\pi}_i^\mathsf{T} \beta_K$, we can compute x_K^\sharp as follows.

$$\lambda_{i}(\boldsymbol{x}_{K}^{\sharp}) = \lambda_{i}(\boldsymbol{x}_{K}) + \delta_{K} \nabla \lambda_{i}^{\mathsf{T}} \boldsymbol{\beta}_{K} = \frac{1}{d+1} - \delta_{K} \frac{\vec{\pi}_{i}^{\mathsf{T}} \boldsymbol{\beta}_{K}}{h_{i}} = \frac{1}{d+1} - \delta_{K} \frac{\vec{\pi}_{i}^{\mathsf{T}} \boldsymbol{\beta}_{K} |S_{i}|}{d|K|}$$

It follows that

$$\delta_{\mathsf{K}} = \max \left\{ \frac{d \, |\mathsf{K}|}{(d+1) \, |S_{\mathfrak{i}}| \left(\vec{\mathsf{n}}_{\mathfrak{i}}^{\mathsf{T}} \beta_{\mathsf{K}}\right)^{+}} \, \middle| \, 0 \leqslant \mathfrak{i} \leqslant d \right\}. \tag{C.6}$$

The stabilized bilinear form is

$$a^{\text{supg}}(\mathbf{u}, \mathbf{v}) := \int_{\Omega} (\beta \cdot \nabla \mathbf{u}) \mathbf{v} - \int_{\partial \Omega} \beta_{\mathbf{n}}^{-} \mathbf{u} \mathbf{v} + \int_{\Omega} \delta(\beta \cdot \nabla \mathbf{u}) (\beta \cdot \nabla \mathbf{v})$$
 (C.7)

Then we have

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