

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 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: $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R \cup \Gamma_P$, the outward unit normal is denoted by \mathbf{n} . We denote by $\pi_{\mathbf{n}^\perp} := (\mathbf{I} - \mathbf{n}\mathbf{n}^\top) \in \mathbb{R}^{(d-1) \times d}$ the projection on the tangent plane.

$$\left\{ \begin{array}{l} -\operatorname{div}(\mu \nabla \mathbf{v}) + \nabla \mathbf{p} = \mathbf{f} \quad \text{in } \Omega \\ \operatorname{div} \mathbf{v} = g \quad \text{in } \Omega \\ \mathbf{v} = \mathbf{v}^D \quad \text{in } \Gamma_D, \\ \left\{ \begin{array}{l} \pi_{\mathbf{n}^\perp} \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} = 0 \\ \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \mathbf{n} - \mathbf{p} = -\mathbf{p}^N \end{array} \right\} \quad \text{in } \Gamma_N, \\ \left\{ \begin{array}{l} \mathbf{v}_n = \mathbf{v}_n^R \\ \pi_{\mathbf{n}^\perp} \left(\lambda_R \mathbf{v} + \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \right) = \pi_{\mathbf{n}^\perp} \mathbf{g}^R \end{array} \right\} \quad \text{in } \Gamma_R, \\ \left\{ \begin{array}{l} \pi_{\mathbf{n}^\perp} \mathbf{v} = \pi_{\mathbf{n}^\perp} \mathbf{v}^P \\ \left(\mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \mathbf{n} - \mathbf{p} \right) = -\mathbf{p}^P \end{array} \right\} \quad \text{in } \Gamma_P. \end{array} \right. \quad (2.1)$$

We can express the equations by means of the Cauchy stress tensor

$$\sigma := 2\mu \mathbf{D}(\mathbf{v}) + \lambda \operatorname{div}(\mathbf{v}) \mathbf{I} - \mathbf{p} \mathbf{I}, \quad \mathbf{D}(\mathbf{v}) = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^\top). \quad (2.2)$$

Due to $\operatorname{div} \mathbf{v} = 0$, the bulk viscosity λ is neglected.

Then the momentum balance is (with the row-wise divergence operator)

$$-\operatorname{div} \sigma = \mathbf{f} \quad \text{in } \Omega.$$

The weak formulation (2.4) is based on the non-symmetric

$$\tilde{\sigma} := \mu \nabla \mathbf{v} - \mathbf{p} \mathbf{I}, \quad (2.3)$$

which is equivalent to using σ for volume integrals since $\mathbf{A} : \mathbf{B} = \frac{\mathbf{A} + \mathbf{A}^\top}{2} : \mathbf{B}$ for all symmetric $\mathbf{B} \in \mathbb{R}^{d \times d}$ and any $\mathbf{A} \in \mathbb{R}^{d \times d}$.

Using σ in a weak formulation will in general generate different boundary conditions.

2.1 Weak formulation

The standard weak formulation reads

$$\left\{ \begin{array}{l} \mathbf{V}_{\mathbf{v}^D, \mathbf{v}_n^R, \mathbf{v}^P} := \left\{ \mathbf{v} \in H^1(\Omega, \mathbb{R}^d) \mid \mathbf{v}|_{\Gamma_D} = \mathbf{v}^D \text{ \& } \mathbf{v}_n|_{\Gamma_R} \text{ \& } \pi_{\mathbf{n}^\perp} \mathbf{v}|_{\Gamma_P} = \pi_{\mathbf{n}^\perp} \mathbf{v}^P \right\} \\ Q := L^2(\Omega) \quad (Q := L^2(\Omega)/\mathbb{R} \text{ if } |\Gamma_N \cup \Gamma_P| = 0) \\ (\mathbf{v}, \mathbf{p}) \in \mathbf{V}_{\mathbf{v}^D, \mathbf{v}_n^R, \mathbf{v}^P} \times Q : \quad \mathbf{a}_\Omega(\mathbf{v}, \mathbf{p}; \phi, \xi) = \mathbf{l}_\Omega(\phi, \xi) \quad \forall (\phi, \xi) \in \mathbf{V}_{0,0,0} \times Q \\ \mathbf{a}_\Omega(\mathbf{v}, \mathbf{p}; \phi, \xi) := \int_\Omega \mu \nabla \mathbf{v} : \nabla \phi - \int_\Omega \mathbf{p} \operatorname{div} \phi + \int_\Omega \operatorname{div} \mathbf{v} \xi + \lambda_R \int_{\Gamma_R} (\mathbf{v} \cdot \phi - \mathbf{v}_n \phi_n), \\ \mathbf{l}_\Omega(\phi, \xi) := \int_\Omega \mathbf{f} \cdot \phi + \int_\Omega g \xi + \int_{\Gamma_R} (\mathbf{g}^R \cdot \phi - \mathbf{g}_n^R \phi_n) - \int_{\Gamma_N} \mathbf{p}^N \phi_n - \int_{\Gamma_P} \mathbf{p}^P \phi_n. \end{array} \right. \quad (2.4)$$

Lemma 2.1. *A regular solution of the formulation (2.4) satisfies (2.1).*

Proof. By integration by parts we have, together with $\mathbf{v} \cdot \boldsymbol{\phi} - \mathbf{v}_n \phi_n = \pi_{n^\perp} \mathbf{v} \cdot \boldsymbol{\phi}$

$$\mathbf{a}_\Omega(\mathbf{v}, \mathbf{p}; \boldsymbol{\phi}, \xi) = \int_\Omega (-\mu \Delta \mathbf{v} + \nabla \mathbf{p}) \cdot \boldsymbol{\phi} + \int_{\partial\Omega} \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \boldsymbol{\phi} - \int_{\partial\Omega} \mathbf{p} \phi_n + \int_\Omega \operatorname{div} \mathbf{v} \xi + \lambda_R \int_{\Gamma_R} \pi_{n^\perp} \mathbf{v} \cdot \boldsymbol{\phi}$$

Then the (regular) weak solution satisfies

$$\int_\Omega (-\mu \Delta \mathbf{v} + \nabla \mathbf{p} - \mathbf{f}) \cdot \boldsymbol{\phi} + \int_\Omega (\operatorname{div} \mathbf{v} - g) \xi = \int_{\partial\Omega} \mathbf{p} \phi_n - \int_{\partial\Omega} \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \boldsymbol{\phi} - \int_{\Gamma_N} \mathbf{p}^N \phi_n - \int_{\Gamma_P} \mathbf{p}^P \phi_n + \int_{\Gamma_R} \pi_{n^\perp} (g^R - \lambda_R \mathbf{v}) \cdot \boldsymbol{\phi}$$

Taking $\boldsymbol{\phi} \in H_0^1(\Omega, \mathbb{R}^d)$, the right-hand side vanishes and the density of this space in $L^2(\Omega)$ gives us

$$-\mu \Delta \mathbf{v} + \nabla \mathbf{p} = \mathbf{f}, \quad \operatorname{div} \mathbf{v} = g \quad \text{a.e. in } \Omega.$$

But this means that for general $\boldsymbol{\phi} \in V_{0,0,0}$

$$\int_{\partial\Omega} \mathbf{p} \phi_n - \int_{\partial\Omega} \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \boldsymbol{\phi} - \int_{\Gamma_N} \mathbf{p}^N \phi_n - \int_{\Gamma_P} \mathbf{p}^P \phi_n + \int_{\Gamma_R} \pi_{n^\perp} (g^R - \lambda_R \mathbf{v}) \cdot \boldsymbol{\phi} = 0$$

Decomposing the test function as

$$\boldsymbol{\phi} = \phi_n \mathbf{n} + \pi_{n^\perp} \boldsymbol{\phi}$$

and using the definition of $V_{0,0,0}$ we find

$$\int_{\Gamma_N} \left((\mathbf{p} - \mathbf{p}^N) \mathbf{n} - \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \right) \cdot \boldsymbol{\phi} + \int_{\Gamma_P} (\mathbf{p} - \mathbf{p}^P - \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \mathbf{n}) \phi_n + \int_{\Gamma_R} \pi_{n^\perp} (g^R - \lambda_R \mathbf{v} - \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}}) \cdot \boldsymbol{\phi} = 0$$

□

Proposition 2.2. *If we use the weak formulation based on the stress tensor*

$$\mathbf{a}_\Omega(\mathbf{v}, \mathbf{p}; \boldsymbol{\phi}, \xi) := \int_\Omega \boldsymbol{\sigma} : \nabla \boldsymbol{\phi} + \int_\Omega \operatorname{div} \mathbf{v} \xi + \lambda_R \int_{\Gamma_R} \mathbf{v}_{n^\perp} \boldsymbol{\phi}_{n^\perp}, \quad (2.5)$$

the resulting boundary conditions are

$$\left\{ \begin{array}{ll} \mathbf{v} = \mathbf{v}^D & \text{in } \Gamma_D, \\ \boldsymbol{\sigma} \mathbf{n} = -\mathbf{p}^N \mathbf{n} & \text{in } \Gamma_N, \\ \left\{ \begin{array}{l} \pi_{n^\perp} \mathbf{v} = \pi_{n^\perp} \mathbf{v}^P \\ (\mathbf{I} - \pi_{n^\perp}) \boldsymbol{\sigma} \mathbf{n} = -\mathbf{p}^P \end{array} \right\} & \text{in } \Gamma_P, \\ \left\{ \begin{array}{l} \mathbf{v}_n = \mathbf{v}_n^R \\ \pi_{n^\perp} (\lambda_R \mathbf{v} + \boldsymbol{\sigma} \mathbf{n}) = \pi_{n^\perp} g^R \end{array} \right\} & \text{in } \Gamma_R. \end{array} \right. \Leftrightarrow \left\{ \begin{array}{ll} \mathbf{v} = \mathbf{v}^D & \text{in } \Gamma_D, \\ \boldsymbol{\sigma} \mathbf{n} = -\mathbf{p}^N \mathbf{n} & \text{in } \Gamma_N, \\ \left\{ \begin{array}{l} \pi_{n^\perp} \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} - \mu \omega \mathbf{n} = 0 \\ \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \mathbf{n} - \mathbf{p} = -\mathbf{p}^N \end{array} \right\} & \text{in } \Gamma_N, \\ \left\{ \begin{array}{l} \pi_{n^\perp} \mathbf{v} = \pi_{n^\perp} \mathbf{v}^P \\ \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \mathbf{n} - \mathbf{p} = -\mathbf{p}^P \end{array} \right\} & \text{in } \Gamma_P, \\ \left\{ \begin{array}{l} \mathbf{v}_n = \mathbf{v}_n^R \\ \pi_{n^\perp} \left(\lambda_R \mathbf{v} + \mu \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \right) - \mu \omega \mathbf{n} = \pi_{n^\perp} g^R \end{array} \right\} & \text{in } \Gamma_R. \end{array} \right. \quad (2.6)$$

Proof. Using now

$$\int_{\Omega} \sigma : \nabla \phi = - \int_{\Omega} \operatorname{div} \sigma \cdot \phi + \int_{\partial \Omega} \sigma \mathbf{n} \cdot \phi \quad (2.7)$$

we get in similar way as before

$$\int_{\Gamma_N} (\mathbf{p}^N \mathbf{n} + \sigma \mathbf{n}) \cdot \phi + \int_{\Gamma_P} (\mathbf{I} - \pi_{\mathbf{n}^\perp}) (\mathbf{p}^P \mathbf{n} + \sigma \mathbf{n}) \cdot \phi + \int_{\Gamma_R} \pi_{\mathbf{n}^\perp} (\lambda_R \mathbf{v} + \sigma \mathbf{n} - \mathbf{g}^R) \cdot \phi = 0$$

We have

$$\mathbf{n}^\top (\nabla \mathbf{v})^\top \mathbf{n} = (\nabla \mathbf{v} \mathbf{n})^\top \mathbf{n} = \frac{\partial \mathbf{v}^\top}{\partial \mathbf{n}} \mathbf{n} = \mathbf{n}^\top \frac{\partial \mathbf{v}}{\partial \mathbf{n}} = \mathbf{n}^\top (\nabla \mathbf{v}) \mathbf{n}$$

and therefore

$$\begin{aligned} \mathbf{n}^\top \sigma \mathbf{n} &= \mathbf{n}^\top \tilde{\sigma} \mathbf{n} \Rightarrow (\mathbf{I} - \pi_{\mathbf{n}^\perp}) \sigma \mathbf{n} = (\mathbf{I} - \pi_{\mathbf{n}^\perp}) \tilde{\sigma} \mathbf{n}, \\ \pi_{\mathbf{n}^\perp} \sigma \mathbf{n} &= (\mathbf{I} - \mathbf{n} \mathbf{n}^\top) \sigma \mathbf{n} = \sigma \mathbf{n} - \mathbf{n} \mathbf{n}^\top \tilde{\sigma} \mathbf{n} = \pi_{\mathbf{n}^\perp} \tilde{\sigma} \mathbf{n} + (\sigma - \tilde{\sigma}) \mathbf{n} = \pi_{\mathbf{n}^\perp} \tilde{\sigma} \mathbf{n} + \mu \omega \mathbf{n} \end{aligned}$$

with $\omega := \frac{1}{2}(\nabla \mathbf{v}^\top - \nabla \mathbf{v})$. □

2.2 Discretization

We use finite element spaces V_h for the velocity and Q_h for the pressure. One main difficulty is to obtain a stable approximation of the pressure gradient, which requires the inf-sup condition

$$\inf_{\mathbf{p} \in Q_h \setminus \{0\}} \sup_{\mathbf{v} \in V_h \setminus \{0\}} \frac{\int_{\Omega} \mathbf{p} \operatorname{div} \mathbf{v}}{\|\mathbf{v}\|_V \|\mathbf{p}\|_Q} \geq \gamma > 0. \quad (2.8)$$

To this end, we use the classical spaces $V_h = \mathcal{R}_h^1(\Omega, \mathbb{R}^d)$ and $Q_h = \mathcal{D}_h^0$.

2.3 Implementations of Boundary condition

2.3.1 Strong implementation 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 $\mathbf{u}_h^D \in V_h^{\text{dir}}$ be an approximation of the Dirichlet data \mathbf{v}^D we have the traditional way to implement Dirichlet boundary conditions:

$$\begin{bmatrix} A^{\text{int}} & 0 & -B^{\text{int}\top} \\ 0 & I & 0 \\ B^{\text{int}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}_h^{\text{int}} \\ \mathbf{v}_h^{\text{dir}} \\ \mathbf{p}_h \end{bmatrix} = \begin{bmatrix} \mathbf{f}^{\text{int}} - A^{\text{int,dir}} \mathbf{v}_h^D \\ \mathbf{v}_h^D \\ \mathbf{g} - B^{\text{dir}} \mathbf{v}_h^D \end{bmatrix}. \quad (2.9)$$

As for the Poisson problem, we obtain an alternative formulation

$$\begin{bmatrix} A^{\text{int}} & 0 & -B^{\text{int}\top} \\ 0 & A^{\text{dir}} & 0 \\ B^{\text{int}} & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{v}_h^{\text{int}} \\ \mathbf{v}_h^{\text{dir}} \\ \mathbf{p}_h \end{bmatrix} = \begin{bmatrix} \mathbf{f}^{\text{int}} - A^{\text{int,dir}} \mathbf{v}_h^D \\ A^{\text{dir}} \mathbf{v}_h^D \\ \mathbf{g} - B^{\text{dir}} \mathbf{v}_h^D \end{bmatrix}. \quad (2.10)$$

2.3.2 Weak implementation (Nitsche's method)

Instead of modifying the discrete velocity space, we add additional terms to the bilinear and linear forms.

$$\left\{ \begin{array}{l} (v, p) \in V_h \times Q_h : \quad a_\Omega(v, p; \phi, \xi) + a_{\partial\Omega}(v, p; \phi, \xi) = l_\Omega(\phi, \xi) + l_{\partial\Omega}(\phi, \xi) \quad \forall (\phi, \xi) \in V_h \times Q_h \\ a_{\partial\Omega}(v, p; \phi, \xi) := \int_{\Gamma_D \cup \Gamma_P} \frac{\gamma\mu}{h} v \cdot \phi - \int_{\Gamma_D \cup \Gamma_P} \mu \left(\frac{\partial v}{\partial n} \cdot \phi + v \cdot \frac{\partial \phi}{\partial n} \right) \\ \quad + \int_{\Gamma_R} \frac{\gamma\mu}{h} v_n \phi_n - \int_{\Gamma_R} \mu \left(\frac{\partial v}{\partial n} \cdot n \phi_n + v_n \frac{\partial \phi}{\partial n} \cdot n \right) \\ \quad - \int_{\Gamma_P} \frac{\gamma\mu}{h} v_n \phi_n + \int_{\Gamma_P} \mu \left(\frac{\partial v}{\partial n} \cdot n \phi_n + v_n \frac{\partial \phi}{\partial n} \cdot n \right) \\ \quad + \int_{\Gamma_D \cup \Gamma_R} (p \phi_n - v_n \xi) \\ l_{\partial\Omega}(\phi, \xi) = \int_{\Gamma_D} \mu v^D \cdot \left(\frac{\gamma}{h} \phi - \frac{\partial \phi}{\partial n} \right) - \int_{\Gamma_D} v_n^D \xi + \int_{\Gamma_R} \mu v_n^R \cdot \left(\frac{\gamma}{h} \phi_n - \frac{\partial \phi}{\partial n} \cdot n \right) - \int_{\Gamma_R} v_n^R \xi \\ \quad + \int_{\Gamma_P} \mu \pi_{n^\perp} v^P \cdot \pi_{n^\perp} \left(\frac{\gamma}{h} \phi - \frac{\partial \phi}{\partial n} \right). \end{array} \right. \quad (2.11)$$

Lemma 2.3. *A regular continuous solution of the formulation (2.4) satisfies (2.11).*

Proof. We have already seen that a regular continuous solution satisfies for $(\phi, \xi) \in V_h \times Q_h$

$$a_\Omega(v, p; \phi, \xi) - l_\Omega(\phi, \xi) = \int_{\Gamma_D} \left(\mu \frac{\partial v}{\partial n} - p n \right) \cdot \phi + \int_{\Gamma_R} \left(\mu \frac{\partial v}{\partial n} \cdot n - p \right) \phi_n + \int_{\Gamma_P} \pi_{n^\perp} \mu \frac{\partial v}{\partial n} \cdot \phi$$

Thanks to the boundary conditions we also have

$$\begin{aligned} \int_{\Gamma_D} \mu (v^D - v) \cdot \left(\frac{\gamma}{h} \phi - \frac{\partial \phi}{\partial n} \right) - \int_{\Gamma_D} (v_n^D - v_n) \xi &= 0 \\ \int_{\Gamma_R} \mu (v_n^R - v_n) \left(\frac{\gamma}{h} \phi_n - \frac{\partial \phi}{\partial n} \cdot n \right) - \int_{\Gamma_R} (v_n^R - v_n) \xi &= 0 \\ \int_{\Gamma_P} \mu \pi_{n^\perp} (v^P - v) \cdot \left(\frac{\gamma}{h} \phi - \frac{\partial \phi}{\partial n} \right) &= 0 \end{aligned}$$

Adding these terms we get

$$\begin{aligned}
a_{\Omega}(v, p; \phi, \xi) - l_{\Omega}(\phi, \xi) &= - \int_{\Gamma_D} \frac{\gamma \mu}{h} v \cdot \phi + \int_{\Gamma_D} \mu \left(\frac{\partial v}{\partial n} \cdot \phi + v \cdot \frac{\partial \phi}{\partial n} \right) - \int_{\Gamma_D} (p \phi_n - v_n \xi) \\
&\quad + \int_{\Gamma_D} \mu v^D \cdot \left(\frac{\gamma}{h} \phi - \frac{\partial \phi}{\partial n} \right) - \int_{\Gamma_D} v_n^D \xi \\
&\quad - \int_{\Gamma_R} \frac{\gamma \mu}{h} v_n \phi_n + \int_{\Gamma_R} \mu \left(\frac{\partial v}{\partial n} \cdot n \phi_n + v_n \frac{\partial \phi}{\partial n} \cdot n \right) - \int_{\Gamma_R} (p \phi_n - v_n \xi) \\
&\quad + \int_{\Gamma_R} \mu v_n^R \cdot \left(\frac{\gamma}{h} \phi_n - \frac{\partial \phi}{\partial n} \cdot n \right) - \int_{\Gamma_R} v_n^R \xi \\
&\quad - \int_{\Gamma_P} \frac{\gamma \mu}{h} \pi_{n^\perp} v \cdot \pi_{n^\perp} \phi + \int_{\Gamma_P} \mu \left(\pi_{n^\perp} \frac{\partial v}{\partial n} \cdot \pi_{n^\perp} \phi + \pi_{n^\perp} v \cdot \pi_{n^\perp} \frac{\partial \phi}{\partial n} \right) \\
&\quad + \int_{\Gamma_P} \mu \pi_{n^\perp} v^P \cdot \pi_{n^\perp} \left(\frac{\gamma}{h} \phi - \frac{\partial \phi}{\partial n} \right) \\
&= l_{\partial\Omega}(\phi, \xi) - a_{\partial\Omega}(v, p; \phi, \xi)
\end{aligned}$$

□

Alternatively, we can write the system as

$$\left\{ \begin{array}{l} (v, p) \in V_h \times Q_h : \quad a(v, p; \phi, \xi) + b(v, \xi) - b(\phi, p) = l_{\Omega}(\phi, \xi) + l_{\partial\Omega}(\phi, \xi) \quad \forall (\phi, \xi) \in V_h \times Q_h \\ a(v, p; \phi, \xi) := \int_{\Omega} \mu \nabla v : \nabla \phi + \lambda_R \int_{\Gamma_R} (v \cdot \phi - v_n \phi_n) + \int_{\Gamma_D \cup \Gamma_P} \frac{\gamma \mu}{h} v \cdot \phi - \int_{\Gamma_D \cup \Gamma_P} \mu \left(\frac{\partial v}{\partial n} \cdot n \phi + v_n \cdot \frac{\partial \phi}{\partial n} \right) \\ \quad + \int_{\Gamma_R} \frac{\gamma \mu}{h} v_n \phi_n - \int_{\Gamma_R} \mu \left(\frac{\partial v}{\partial n} \cdot n \phi_n + v_n \frac{\partial \phi}{\partial n} \cdot n \right) - \int_{\Gamma_P} \frac{\gamma \mu}{h} v_n \phi_n + \int_{\Gamma_P} \mu \left(\frac{\partial v}{\partial n} \cdot n \phi_n + v_n \frac{\partial \phi}{\partial n} \cdot n \right) \\ b(v, \xi) := \int_{\Omega} \operatorname{div} v \xi - \int_{\Gamma_D} v_n \xi \end{array} \right. \quad (2.12)$$

2.4 Computation of boundary forces

Suppose $\psi \in \mathbb{R}^d$ is a vector field which equals $\vec{d} \in \mathbb{R}^d$ on a given part $\Gamma \subset \partial\Omega$ of the boundary and vanishes on its complement. Then we get the sum of the forces on Γ in direction \vec{d} by means of the integration by parts formula (2.7), supposed the weak solution is sufficiently smooth, as

$$\begin{aligned}
\int_{\Gamma} n^T \sigma \vec{d} &= \int_{\partial\Omega} n^T \sigma \psi = \int_{\Omega} \sigma : \nabla \psi + \int_{\Omega} \operatorname{div} \sigma \cdot \psi = \int_{\Omega} \sigma : \nabla \psi - \int_{\Omega} f \cdot \psi \\
&= a_{\Omega}(v, p; \psi, 0) - l_{\Omega}(\psi, 0) - \lambda_R \int_{\Gamma_R} (v \cdot \psi - v_n \psi_n) + \int_{\Gamma_R} (g^R \cdot \psi - g_n^R \psi_n) - \int_{\Gamma_N} p^N \psi_n - \int_{\Gamma_P} p^P \psi_n
\end{aligned}$$

Supposing ψ is a discrete vector field (in general we have to approximate it), for the strong implementation, we can retrieve the last expression by the parts of the matrix eliminated. For the weak

implementation we have, since ψ is now an admissible test function

$$\begin{aligned}
\int_{\Gamma} \mathbf{n}^T \sigma \vec{d} &= a_{\Omega}(v, p; \psi, 0) - l_{\Omega}(\psi, 0) - \lambda_R \int_{\Gamma_R} (v \cdot \psi - v_n \psi_n) + \int_{\Gamma_R} (g^R \cdot \psi - g_n^R \psi_n) - \int_{\Gamma_N} p^N \psi_n - \int_{\Gamma_P} p^P \psi_n \\
&= l_{\partial\Omega}(\psi, 0) - a_{\partial\Omega}(v, p; \psi, 0) - \lambda_R \int_{\Gamma_R} (v \cdot \psi - v_n \psi_n) + \int_{\Gamma_R} (g^R \cdot \psi - g_n^R \psi_n) - \int_{\Gamma_N} p^N \psi_n - \int_{\Gamma_P} p^P \psi_n \\
&= \int_{\Gamma_D} \mu v^D \cdot \frac{\gamma}{h} \psi + \int_{\Gamma_R} \mu v_n^R \cdot \frac{\gamma}{h} \psi_n + \int_{\Gamma_P} \mu \pi_{n^\perp} v^P \cdot \pi_{n^\perp} \frac{\gamma}{h} \psi \\
&\quad - \int_{\Gamma_D \cup \Gamma_P} \frac{\gamma \mu}{h} v \cdot \psi + \int_{\Gamma_D \cup \Gamma_P} \mu \frac{\partial v}{\partial n} \cdot \psi \\
&\quad - \int_{\Gamma_R} \frac{\gamma \mu}{h} v_n \psi_n - \int_{\Gamma_R} \mu \frac{\partial v}{\partial n} \cdot n \psi_n \\
&\quad + \int_{\Gamma_P} \frac{\gamma \mu}{h} v_n \psi_n + \int_{\Gamma_P} \mu \frac{\partial v}{\partial n} \cdot n \psi_n \\
&\quad - \lambda_R \int_{\Gamma_R} (v \cdot \psi - v_n \psi_n) + \int_{\Gamma_R} (g^R \cdot \psi - g_n^R \psi_n) - \int_{\Gamma_N} p^N \psi_n - \int_{\Gamma_P} p^P \psi_n \\
\int_{\Gamma} \mathbf{n}^T \sigma \vec{d} &= \begin{cases} \int_{\Gamma} \left(\mu \frac{\partial v}{\partial n} - p n \right) \cdot d + \int_{\Gamma} \frac{\gamma \mu}{h} (v^D - v) \cdot d & \Gamma \subset \Gamma_D \\ \int_{\Gamma} \mu \left(\frac{\partial v}{\partial n} \cdot n \phi_n \right) - \int_{\Gamma} p \phi_n + \int_{\Gamma} \mu (v_n^R - v_n) \cdot \left(\frac{\gamma}{h} \phi_n - \frac{\partial \phi}{\partial n} \cdot n \right) & \Gamma \subset \Gamma_R \end{cases} \quad (2.13)
\end{aligned}$$

2.5 Pressure mean

If no boundary conditions is Neumann, 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 $(1, nc)$

$$\begin{bmatrix} A & -B^T & 0 \\ B & 0 & C^T \\ 0 & C & 0 \end{bmatrix} \begin{bmatrix} v \\ p \\ \lambda \end{bmatrix} = \begin{bmatrix} f \\ g \\ 0 \end{bmatrix}. \quad (2.14)$$

Let us considered solution of (2.14) with $S = BA^{-1}B^T$, $T = CS^{-1}C^T$

$$\begin{cases} A\tilde{v} &= f \\ S\tilde{p} &= g - B\tilde{v} \\ T\lambda &= -C\tilde{p} \\ S(p - \tilde{p}) &= C^T\lambda \\ A(v - \tilde{v}) &= B^T p \end{cases} \quad (2.15)$$

2.5.1 Iterative solution

We have to solve (2.14) 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 $(y_v, y_p, y_\lambda) \rightarrow (x_v, x_p, x_\lambda)$ 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

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

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

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

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

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

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

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

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

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

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

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

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 $-x - |x| = -2x^+$

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

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

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 $\delta_K \geq 0$

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

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

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

The stabilized bilinear form is

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

Then we have

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