SimFem

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Contents

1 Geometry and finite elements

1.1 Simplices

We consider an arbitrary non-degenerate simplex $K = (x_0, x_1, \ldots, x_d)$. The (signed) volume of K is given by

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

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 $d_k = |P_{S_k} x_k - x_k|$, where P_S is the orthogonal projection on the hyperplane associated to S. We have

$$d_k = d\frac{|K|}{|S_k|} \qquad \text{(and for } d = 3\ |S_k| = \tfrac{1}{2}|u \times v|)$$

1.2 Finite elements

The $d+1$ basis functions of the Courant element are the barycentric coordinates λ_i defined as being affine with respect to the coordinates and $\lambda_i(x_j) = \delta_{ij}$. The constant gradient is given by

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

The relation with the $d+1$ Crouzeix-Raviart basis functions ψ_i is given by

$$\psi_i = 1 - d\lambda_i$$

Finally the $d+1$ Raviart-Thomas basis functions ξ_i, associated to side S_i, i.e. the opposite node x_i, are given by

$$\xi_i = \frac{x - x_i}{d_i} = \frac{1}{d_i}\sum_{\substack{j=0\\ i\neq j}}^{d} x_j\lambda_j$$

1.3 Numerical integration

Any polynomial in the barycentric coordinates can be integrates exactly.

$$\int_K \prod_{i=1}^{d+1} \lambda_i^{n_i}\,dv = d!|K|\frac{\prod\limits_{i=1}^{d+1} n_i!}{\left(\sum\limits_{i=1}^{d+1} n_i + d\right)!} \tag{2}$$

see [EisenbergMalvern73], [VermolenSegal18].

Let $V = \mathrm{Vect}(\phi)$. For a smooth function f and $u = \sum_j u_j\phi_j$ we use and approximation based on $\mathrm{Vect}(\psi)$ such that $\psi_l(x_k- = \delta_{kl}$ and

$$f(u) \approx \sum_k f(u(x_k))\psi_k = \sum_k f(\sum_j u_j\phi_j(x_k))\psi_k$$

Then

$$\int_K f(u)\phi_i \approx \sum_k f_k \int_K \psi_k\phi_i, \quad f_k = f(\sum_l u_l\phi_l(x_k))$$

$$\int_K f'(u)(\phi_j)\phi_i \approx \sum_k f'_{k,j} \int_K \psi_k\phi_i, \quad f'_{k,j} = f'(\sum_l u_l\phi_l(x_k))\phi_j(x_k)$$

For $\psi = \phi$ this becomes considerably cheaper:

$$\int_K f(u)\phi_i \approx \sum_k f_k \int_K \phi_k\phi_i, \quad f_k = f(u_k)$$

$$\int_K f'(u)(\phi_j)\phi_i \approx f'_j \int_K \phi_j\phi_i, \quad f'_k = f'(u_k)$$

1.4 Element matrices for C^1

1.4.1 Mass matrix

$$M_{ij} = \begin{cases} \frac{2d!|K|}{(2+d)!} & i{=}j \\ \frac{d!|K|}{(2+d)!} & i{\neq}j \end{cases} \quad M^{1D} = |K| \begin{bmatrix} \frac{1}{3} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{3} \end{bmatrix}, \; M^{2D} = |K| \begin{bmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{6} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{6} \end{bmatrix}, \; M^{3D} = |K| \begin{bmatrix} \frac{1}{10} & \frac{1}{20} & \frac{1}{20} & \frac{1}{20} \\ \frac{1}{20} & \frac{1}{10} & \frac{1}{20} & \frac{1}{20} \\ \frac{1}{20} & \frac{1}{20} & \frac{1}{10} & \frac{1}{20} \\ \frac{1}{20} & \frac{1}{20} & \frac{1}{20} & \frac{1}{10} \end{bmatrix}$$

Lumped mass

$$\tilde{M}_{ij} = \begin{cases} \frac{|K|}{(1+d)} & i{=}j \\ 0 & i{\neq}j \end{cases}$$

2 Test problems

2.1 Advection-Diffusion-Reaction

$$\operatorname{div}(\beta u) - \operatorname{div}(k\nabla u) + \psi(u) = f \quad \text{in } \Omega, \qquad u = u^D \text{on } \Gamma_D, \qquad k\frac{\partial u}{\partial n} = q^D \text{on } \Gamma_N \tag{3}$$

2.1.1 Courant element

$$\int_\Omega \psi(u)v + \int_\Omega k\nabla u \cdot \nabla v - \int_\Omega u\beta \cdot \nabla v + \int_{\partial\Omega} \beta_n^+ uv = \int_\Omega fv + \int_{\partial\Omega} |\beta_n^-| u^D v$$

Piecewise constant approximation for k

$$\int_K \nabla\lambda_i \cdot \nabla\lambda_j = |K| \frac{n_i}{d_i} \cdot \frac{n_j}{d_j} = |K| \frac{|S_i|}{d|K|} \frac{|S_j|}{d|K|} n_i \cdot n_j = \frac{1}{d^2|K|} \tilde{n}_i \cdot \tilde{n}_j$$

$$-\int_K u\beta \cdot \nabla\lambda_i = u(x_K)|K|\beta \cdot \frac{n_i}{d_i} = u(x_K)\frac{1}{d}\beta \cdot \tilde{n}_i$$

$$-\int_S f\frac{\partial v_i}{\partial n} = -f(x_S)|S|\nabla v_i \cdot n = f(x_S)|S|\frac{1}{d_i} n_i \cdot n = f(x_S)|S|\frac{|S_i|}{d|K|} n_i \cdot n = f(x_S)\frac{\tilde{n}_i \cdot \tilde{n}}{d|K|}$$

2.2 Turing

We consider a reaction-diffusion system on $\Omega =]-1,+1[^d$

$$\begin{cases} \dfrac{\partial u}{\partial t} - k_u \Delta u = f(u,v) \quad \text{in } \Omega, & \dfrac{\partial u}{\partial n} = 0 \quad \text{on } \partial\Omega, \\ \dfrac{\partial v}{\partial t} - k_v \Delta v = g(u,v) \quad \text{in } \Omega, & \dfrac{\partial v}{\partial n} = 0 \quad \text{on } \partial\Omega, \end{cases} \tag{4}$$

Alan Turing discovered that the astonishing effect of destabilization by diffusion [Turing52], which leads to pattern formation [1]

$$f(u, v) = (a - u) - \psi(u, v), \qquad g(u, v) = \psi(u, v). \tag{5}$$

An equilibrium point satisfies

$$u^* = a, \qquad \psi(a, v^*) = 0$$

The linear stability analysis is based on the Jacobian

$$\begin{bmatrix} -1 - \psi'_u & -\psi'_v \\ \psi'_u & \psi'_v \end{bmatrix} \quad \Rightarrow \quad tr = \psi'_v - \psi'_u - 1, \quad det = -\psi'_v$$

The brusselator is given by

$$\psi(u, v) = bu - u^2 v \qquad (\psi'_u = b - 2uv, \quad \psi'_v = -u^2). \tag{6}$$

An equilibrium point of (6) necessarily satisfies $u^* = a$ and $v^* = b/a$. We now have

$$tr = -b + 2uv - u^2 - 1, \quad det = u^2$$

and for the equilibrium point

$$tr^* = -1 - b + 2b - a^2 = b - 1 - a^2, \quad det^* = a^2$$

We conclude that a Hopf bifurcation appears if $b > a^2 + 1$.

2.2.1 The influence of diffusion

We consider an expansion into eigenfunctions of the Laplace operator withe eigenvalues $l \geq 0$. The for the frequency l we have the Jacopian

$$\begin{bmatrix} -1 - \psi'_u - k_u l & -\psi'_v \\ \psi'_u & \psi'_v - k_v l \end{bmatrix} \quad \Rightarrow \quad tr = \psi'_v - \psi'_u - 1 - (k_u + k_v)l,$$
$$det = (1 + k_u l)(k_v l - \psi'_v) + k_v l \psi'_u = k_u k_v l^2 + (k_v(\psi'_u + 1) - k_u \psi'_v)l - \psi'_v$$

For the brusselator we have at the eqilubrium

$$det = k_u k_v l^2 + (k_u a^2 - k_v(b - 1))l + a^2.$$

The discriminant is

$$\Delta = (k_u a^2 - k_v(b - 1))^2 - 4a^2 k_u k_v$$

[1] For an introduction and references see `https://en.wikipedia.org/wiki/Reaction-diffusion_system`.

which is positive ($a = 1$) for

$$b \leq b^* = 1 + \frac{k_u}{k_v} + 2\frac{\sqrt{k_u}}{\sqrt{k_v}} \tag{7}$$

The critical frequency is

$$l^* = \frac{k_v(b^* - 1) - k_u}{2k_u k_v} = 2k_u^{-1/2}k_v{-3/2}$$

The data for our test problems are

$$\begin{array}{llllll} \text{(cas 1)} & a = 1.0\ , & b = 2.1, & k_u = 0.0\ , & k_v = 0.0\ , & T = 20.0 \\ \text{(cas 2)} & a = 1.0\ , & b = 1.9, & k_u = 0.0001\ , & k_v = 0.01\ , & T = 20.0 \end{array}$$

$$u_0(x) = \begin{cases} 1 & \text{if for all i } x_i \in [-0.4, 0.0] \\ 0 & \text{else} \end{cases} \qquad v_0(x) = \begin{cases} 1 & \text{if for all i } x_i \in [-0.2, 0.2] \\ 0 & \text{else} \end{cases}$$