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Lecture 19

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Practical realization of boundary conditions

- Robin boundary value problem

$$-\nabla \cdot \delta \vec{\nabla} u = f \quad \text{in } \Omega$$
$$\delta \vec{\nabla} u + \alpha(u - g) = 0 \quad \text{on } \partial\Omega$$

- Weak formulation: search $u \in H^1(\Omega)$ such that

$$\int_\Omega \delta \vec{\nabla} u \vec{\nabla} v \, d\vec{x} + \int_{\partial\Omega} \alpha u v \, ds = \int_\Omega f v \, d\vec{x} + \int_{\partial\Omega} \alpha g v \, ds \; \forall v \in H^1(\Omega)$$

- In 2D, for P^1 FEM, boundary integrals can be calculated by trapezoidal rule without sacrificing approximation order
- Use Dirichlet penalty method to handle Dirichlet boundary conditions

More complicated integrals

- Assume non-constant right hand side f, space dependent heat conduction coefficient δ.
- Right hand side integrals

$$f_i = \int_K f(x)\lambda_i(x)\ d\vec{x}$$

- P^1 stiffness matrix elements

$$a_{ij} = \int_K \delta(x)\ \vec{\nabla}\lambda_i\ \vec{\nabla}\lambda_j\ d\vec{x}$$

- P^k stiffness matrix elements created from higher order ansatz functions

Quadrature rules

- *Quadrature rule*:

$$\int_K g(x)\ d\vec{x} \approx |K| \sum_{l=1}^{l_q} \omega_l g(\xi_l)$$

- ξ_l: *nodes, Gauss points*
- ω_l: *weights*
- The largest number k such that the quadrature is exact for polynomials of order k is called *order* k_q of the quadrature rule, i.e.

$$\forall k \leq k_q, \forall p \in \mathbb{P}^k \int_K p(x)\ d\vec{x} = |K| \sum_{l=1}^{l_q} \omega_l p(\xi_l)$$

- Error estimate:

$$\forall \phi \in \mathcal{C}^{k_q+1}(K), \left| \frac{1}{|K|} \int_K \phi(x)\ d\vec{x} - \sum_{l=1}^{l_q} \omega_l g(\xi_l) \right| \leq c h_K^{k_q+1} \sup_{x \in K, |\alpha| = k_q+1} |\partial^\alpha \phi(x)|$$

Some common quadrature rules

Nodes are characterized by the barycentric coordinates

d	k_q	l_q	Nodes	Weights
1	1	1	$(\frac{1}{2}, \frac{1}{2})$	1
	1	2	$(1, 0), (0, 1)$	$\frac{1}{2}, \frac{1}{2}$
	3	2	$(\frac{1}{2} + \frac{\sqrt{3}}{6}, \frac{1}{2} - \frac{\sqrt{3}}{6}), (\frac{1}{2} - \frac{\sqrt{3}}{6}, \frac{1}{2} + \frac{\sqrt{3}}{6})$	$\frac{1}{2}, \frac{1}{2}$
	5	3	$(\frac{1}{2},), (\frac{1}{2} + \sqrt{\frac{3}{20}}, \frac{1}{2} - \sqrt{\frac{3}{20}}), (\frac{1}{2} - \sqrt{\frac{3}{20}}, \frac{1}{2} + \sqrt{\frac{3}{20}})$	$\frac{8}{18}, \frac{5}{18}, \frac{5}{18}$
2	1	1	$(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$	1
	1	3	$(1, 0, 0), (0, 1, 0), (0, 0, 1)$	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$
	2	3	$(\frac{1}{2}, \frac{1}{2}, 0), (\frac{1}{2}, 0, \frac{1}{2}), (0, \frac{1}{2}, \frac{1}{2})$	$\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$
	3	4	$(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}), (\frac{1}{5}, \frac{1}{5}, \frac{3}{5}), (\frac{1}{5}, \frac{3}{5}, \frac{1}{5}), (\frac{3}{5}, \frac{1}{5}, \frac{1}{5}),$	$-\frac{9}{16}, \frac{25}{48}, \frac{25}{48}, \frac{25}{48}$
3	1	1	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	1
	1	4	$(1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), (0, 0, 0, 1)$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
	2	4	$(\frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5+3\sqrt{5}}{20}) \ldots$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

Matching of approximation order and quadrature order

- "Variational crime": instead of

$$a(u_h, v_h) = f(v_h)\ \forall v_h \in V_h$$

  we solve

$$a_h(u_h, v_h) = f_h(v_h)\ \forall v_h \in V_h$$

  where a_h, f_h are derived from their exact counterparts by quadrature
- For P^1 finite elements, zero order quadrature for volume integrals and first order quadrature for surface intergals is sufficient to keep the convergence order estimates stated before
- The rule of thumb for the volume quadrature is that the highest order terms must be evaluated exactly if the coefficients of the PDE are constant.

Practical realization of integrals

- Integral over barycentric coordinate function

$$\int_K \lambda_i(x)\ d\vec{x} = \frac{1}{3}|K|$$

- Right hand side integrals. Assume $f(x)$ is given as a piecewise linear function with given values in the nodes of the triangulation

$$f_i = \int_K f(x)\lambda_i(x)\ d\vec{x} \approx \frac{1}{3}|K|(f(a_0) + f(a_1) + f(a_2))$$

- Integral over space dependent heat conduction coefficient: Assume $\delta(x)$ is given as a piecewise linear function with given values in the nodes of the triangulation

$$a_{ij} = \int_K \delta(x)\ \vec{\nabla}\lambda_i\ \vec{\nabla}\lambda_j\ d\vec{x} = \frac{1}{3}(\delta(a_0)+\delta(a_1)+\delta(a_2)) \int_K \vec{\nabla}\lambda_i\ \vec{\nabla}\lambda_j\ d\vec{x}$$

P1 FEM stiffness matrix condition number

- Homogeneous dirichlet boundary value problem

$$-\nabla \cdot \delta \vec{\nabla} u = f \quad \text{in } \Omega$$
$$u|_{\partial\Omega} = 0$$

- Lagrange degrees of freedom $a_1 \dots a_N$ corresponding to global basis functions $\phi_1 \dots \phi_N$ such that $\phi_i|_{\partial\Omega} = 0$ aka $\phi_i \in V_h \subset H_0^1(\Omega)$
- Stiffness matrix $A = (a_{ij})$:

$$a_{ij} = a(\phi_i, \phi_j) = \int_\Omega \delta \vec{\nabla} \phi_i \vec{\nabla} \phi_j \, d\vec{x}$$

- bilinear form $a(\cdot, \cdot)$ is self-adjoint, therefore A is symmetric, positive definite
- Condition number estimate for P^1 finite elements on quasi-uniform triangulation:

$$\kappa(A) \leq ch^{-2}$$

P1 FEM Stiffness matrix row sums

Row sums:

$$\begin{aligned}\sum_{j=1}^{N} a_{ij} = \sum_{j=1}^{N} \int_\Omega \vec{\nabla}\phi_i \vec{\nabla}\phi_j \ dx = \int_\Omega \vec{\nabla}\phi_i \vec{\nabla} \left(\sum_{j=1}^{N} \phi_j \right) \ dx \\ = \int_\Omega \vec{\nabla}\phi_i \vec{\nabla}(1) \ dx \\ = 0\end{aligned}$$

P1 FEM stiffness matrix entry signs

Local stiffness matrix S_K

$$s_{ij} = \int_K \vec{\nabla}\lambda_i \vec{\nabla}\lambda_j \; dx = \frac{|K|}{2|K|^2} \left(y_{i+1} - y_{i+2}, x_{i+2} - x_{i+1}\right) \begin{pmatrix} y_{j+1} - y_{j+2} \\ x_{j+2} - x_{j+1} \end{pmatrix}$$

- Main diagonal entries positive
- Local contributions from element stiffness matrices: Scalar products of vectors orthogonal to edges. These are nonpositive if the angle between the edges are $\leq 90^\circ$
- *weakly acute triangulation*: all triangle angles are less than $\leq 90^\circ$
- In fact, for constant coefficients, in *2D*, Delaunay is sufficient, as contributions from opposite angles compensate each other
- All row sums are zero $\Rightarrow$ A is singular
- Matrix becomes irreducibly diagonally dominant if we add at least one positive value to the main diagonal, e.g. from Dirichlet BC

Stationary linear reaction-diffusion

- Assume additional process in each REV which produces or destroys species depending on the amount of species present with given rate r.

  Search function $u : \Omega \to \mathbb{R}$ such that

$$-\nabla \cdot \delta \vec{\nabla} u + ru = f \quad \text{in}\Omega$$
$$\delta \vec{\nabla} u \cdot \vec{n} + \alpha(u - g) = 0 \quad \text{on}\partial\Omega$$

- Coercivity guaranteed e.g. for $\alpha \geq 0$, $r > 0$ which means species destruction FEM formulation: search $u_h \in V_h = \mathrm{span}\{\phi_1 \dots \phi_N\}$ such that

$$\underbrace{\int_\Omega \delta \vec{\nabla} u_h \vec{\nabla} v_h \, d\vec{x}}_{\text{"stiffness matrix"}} + \underbrace{\int_\Omega r u_h v_h d\vec{x}}_{\text{"mass matrix"}} + \underbrace{\int_{\partial\Omega} \alpha u_h v_h \, ds}_{\text{"boundary mass matrix"}}$$
$$= \int_\Omega f v_h \, d\vec{x} + \int_{\partial\Omega} \alpha g v_h \, ds \; \forall v_h \in V_h$$

- Coercivity + symmetry $\Rightarrow$ positive definiteness

Mass matrix properties

- Mass matrix (for $r = 1$): $M = (m_{ij})$:

$$m_{ij} = \int_\Omega \phi_i \phi_j \; dx$$

- Self-adjoint, coercive bilinear form $\Rightarrow$ M is symmetric, positiv definite
- For a family of quasi-uniform, shape-regular triangulations, for every eigenvalue μ one has the estimate

$$c_1 h^d \leq \mu \leq c_2 h^d$$

T $\Rightarrow$ condition number $\kappa(M)$ bounded by constant independent of h:

$$\kappa(M) \leq c$$

- How to see this ? Let $u_h = \sum_{i=1}^N U_i \phi_i$, and μ an eigenvalue (positive,real!) Then

$$||u_h||_0^2 = (U, MU)_{\mathbb{R}^N} = \mu(U, U)_{\mathbb{R}^N} = \mu||U||^2_{\mathbb{R}^N}$$

From quasi-uniformity we obtain

$$c_1 h^d ||U||^2_{\mathbb{R}^N} \leq ||u_h||_0^2 \leq c_2 h^d ||U||^2_{\mathbb{R}^N}$$

Mass matrix M-Property (P1 FEM) ?

- For P^1-finite elements, all integrals $m_{ij} = \int_\Omega \phi_i \phi_j \, dx$ are zero or positive, so we get positive off diagonal elements.
- No M-Property!

Mass matrix lumping (P1 FEM)

- Local mass matrix for P1 FEM on element K
  (calculated by 2nd order exact edge midpoint quadrature rule):

$$M_K = |K| \begin{pmatrix} \frac{1}{6} & \frac{1}{12} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{6} & \frac{1}{12} \\ \frac{1}{12} & \frac{1}{12} & \frac{1}{6} \end{pmatrix}$$

- Lumping: sum up off diagonal elements to main diagonal, set off diagonal entries to zero

$$\tilde{M}_K = |K| \begin{pmatrix} \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{3} \end{pmatrix}$$

- Interpretation as change of quadrature rule to first order exact vertex based quadrature rule
- Loss of accuracy, gain of stability

Effect of mass matrix lumping

- For P1 FEM on weakly acute or Delaunay triangulations, mass matrix lumping can guarantee M-Property of system matrix
- Adding a mass matrix which is not lumped yields a positive definite matrix (due to coercivity) and thus nonsingularity, but *destroys* M-property unless the absolute values of its off diagonal entries are less than those of A, i.e. for small r.
- Same situation witb Robin boundary conditions and boundary mass matrix
- Introducing the Dirichlet Penalty trick at continuous level without mass lumping would be disastrous.