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Lecture 19

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More complicated integrals

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

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

- P^1 stiffness matrix elements

$$a_{ij} = \int_K \kappa(x)\ \nabla\lambda_i\ \nabla\lambda_j\ d\mathbf{x}$$

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

Quadrature rules

- *Quadrature rule*:

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

- 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.

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

- Error estimate:

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

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	$(\frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5-\sqrt{5}}{20}, \frac{5+3\sqrt{5}}{20}) \dots$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}$

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

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

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

$$f_i = \int_K f(x)\lambda_i(x)\; d\mathbf{x} \approx \frac{1}{3}|K|f(a_i)$$

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

$$a_{ij} = \int_K \kappa(x)\, \nabla\lambda_i\, \nabla\lambda_j\; d\mathbf{x} = \frac{1}{3}(\kappa(a_0)+\kappa(a_1)+\kappa(a_2)) \int_K \nabla\lambda_i\, \nabla\lambda_j\; d\mathbf{x}$$

Stiffness matrix for Laplace operator for P1 FEM

- Element-wise calculation:

$$a_{ij} = a(\phi_i, \phi_j) = \int_\Omega \nabla\phi_i \nabla\phi_j \, d\mathbf{x} = \int_\Omega \sum_{K\in\mathcal{T}_h} \nabla\phi_i|_K \nabla\phi_j|_K \, d\mathbf{x}$$

- Standard assembly loop:

for $i, j = 1 \dots N$ **do**
  set $a_{ij} = 0$
end
for $K \in \mathcal{T}_h$ **do**
  for $m,n=0\dots d$ **do**
    $s_{mn} = \int_K \nabla\lambda_m \nabla\lambda_n \, d\mathbf{x}$
    $a_{j_{dof}(K,m),j_{dof}(K,n)} = a_{j_{dof}(K,m),j_{dof}(K,n)} + s_{mn}$
  end
end

- Local stiffness matrix:

$$S_K = (s_{K;m,n}) = \int_K \nabla\lambda_m \nabla\lambda_n \, d\mathbf{x}$$

Local stiffness matrix calculation for P1 FEM

- $a_0 \dots a_d$: vertices of the simplex K, $a \in K$.
- Barycentric coordinates: $\lambda_j(a) = \frac{|K_j(a)|}{|K|}$
- For indexing modulo d+1 we can write

$$|K| = \frac{1}{d!} \det \left(a_{j+1} - a_j, \dots a_{j+d} - a_j \right)$$
$$|K_j(a)| = \frac{1}{d!} \det \left(a_{j+1} - a, \dots a_{j+d} - a \right)$$

- From this information, we can calculate explicitely$\nabla \lambda_j(x)$ (which are constant vectors due to linearity) and the corresponding entries of the local stiffness

$$s_{ij} = \int_K \nabla \lambda_i \nabla \lambda_j \; d\mathbf{x}$$

Local stiffness matrix calculation for P1 FEM in 2D

- $a_0 = (x_0, y_0) \dots a_d = (x_2, y_2)$: vertices of the simplex K, $a = (x, y) \in K$.
- Barycentric coordinates: $\lambda_j(x, y) = \frac{|K_j(x,y)|}{|K|}$
- For indexing modulo d+1 we can write

$$|K| = \frac{1}{2} \det \begin{pmatrix} x_{j+1} - x_j & x_{j+2} - x_j \\ y_{j+1} - y_j & y_{j+2} - y_j \end{pmatrix}$$
$$|K_j(x, y)| = \frac{1}{2} \det \begin{pmatrix} x_{j+1} - x & x_{j+2} - x \\ y_{j+1} - y & y_{j+2} - y \end{pmatrix}$$

- Therefore, we have

$$|K_j(x, y)| = \frac{1}{2}\left((x_{j+1} - x)(y_{j+2} - y) - (x_{j+2} - x)(y_{j+1} - y)\right)$$
$$\partial_x |K_j(x, y)| = \frac{1}{2}\left((y_{j+1} - y) - (y_{j+2} - y)\right) = \frac{1}{2}(y_{j+1} - y_{j+2})$$
$$\partial_y |K_j(x, y)| = \frac{1}{2}\left((x_{j+2} - x) - (x_{j+1} - x)\right) = \frac{1}{2}(x_{j+2} - x_{j+1})$$

Local stiffness matrix calculation for P1 FEM in 2D II

- $$s_{ij} = \int_K \nabla\lambda_i \nabla\lambda_j \; d\mathbf{x} = \frac{|K|}{4|K|^2} \left(y_{i+1} - y_{i+2}, x_{i+2} - x_{i+1}\right) \begin{pmatrix} y_{j+1} - y_{j+2} \\ x_{j+2} - x_{j+1} \end{pmatrix}$$
- So, let $V = \begin{pmatrix} x_1 - x_0 & x_2 - x_0 \\ y_1 - y_0 & y_2 - y_0 \end{pmatrix}$
- Then

$$\begin{aligned} x_1 - x_2 &= V_{00} - V_{01} \\ y_1 - y_2 &= V_{10} - V_{11} \end{aligned}$$

and

$$\begin{aligned} 2|K| \; \nabla\lambda_0 &= \begin{pmatrix} y_1 - y_2 \\ x_2 - x_1 \end{pmatrix} = \begin{pmatrix} V_{10} - V_{11} \\ V_{01} - V_{00} \end{pmatrix} \\ 2|K| \; \nabla\lambda_1 &= \begin{pmatrix} y_2 - y_0 \\ x_0 - x_2 \end{pmatrix} = \begin{pmatrix} V_{11} \\ -V_{01} \end{pmatrix} \\ 2|K| \; \nabla\lambda_2 &= \begin{pmatrix} y_0 - y_1 \\ x_1 - x_0 \end{pmatrix} = \begin{pmatrix} -V_{10} \\ V_{00} \end{pmatrix} \end{aligned}$$

Degree of freedom map representation for P1 finite elements

- List of global nodes $a_0 \dots a_N$: two dimensional array of coordinate values with N rows and d columns
- Local-global degree of freedom map: two-dimensional array C of index values with N_{el} rows and $d+1$ columns such that $C(i,m) = j_{dof}(K_i, m)$.
- The mesh generator triangle generates this information directly

Practical realization of boundary conditions

- Robin boundary value problem

$$
\begin{aligned}
-\nabla \cdot \kappa \nabla u &= f \quad \text{in } \Omega \\
\kappa \nabla u + \alpha(u - g) &= 0 \quad \text{on } \partial\Omega
\end{aligned}
$$

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

$$
\int_\Omega \kappa \nabla u \nabla v \, d\mathbf{x} + \int_{\partial\Omega} \alpha uv \; ds = \int_\Omega fv \, d\mathbf{x} + \int_{\partial\Omega} \alpha gv \, ds \; \forall v \in H^1(\Omega)
$$

- 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

The Finite volume method

Species balance over an REV

- Let $u(\mathbf{x},t) : \Omega \times [0,T] \to \mathbb{R}$ be the local amount of some species.
- Assume representative elementary volume $\omega \subset \Omega$
- Subinterval in time $(t_0, t1) \subset (0, T)$
- $-\delta\nabla u \cdot \mathbf{n}$ describes the flux of these species trough $\partial\omega$, where δ is some transfer coefficient
- Let $f(\mathbf{x},t)$ be some local source of species. Then the flux through the boundary is balanced by the change of the amount of species in ω and the source strength.

$$\begin{aligned}0 &= \int_\omega (u(\mathbf{x},t_1) - u(\mathbf{x},t_0))\,d\mathbf{x} - \int_{t_0}^{t_1}\int_{\partial\omega} \delta\nabla u\cdot\mathbf{n}\,ds\,dt - \int_{t_0}^{t_1}\int_\omega f(\mathbf{x},t)\,ds\\ &= \int_{t_0}^{t_1}\int_\omega \partial_t u(\mathbf{x},t)\,d\mathbf{x}\,dt - \int_{t_0}^{t_1}\int_\omega \nabla\cdot(\delta\nabla u)\,d\mathbf{x}\,dt - \int_{t_0}^{t_1}\int_\omega f(\mathbf{x},t)\,ds\end{aligned}$$

- True for all $\omega \subset \Omega$, $(t_0, t1) \subset (0, T) \Rightarrow$ parabolic second order PDE

$$\partial_t u(x,t) - \nabla\cdot(\delta\nabla u(x,t)) = f(x,t)$$

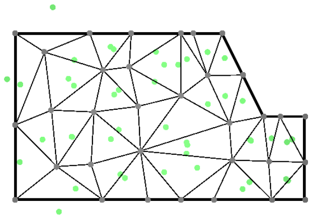
Boundary conforming Delaunay triangulations

Definition: An admissible triangulation of a polygonal Domain $\Omega \subset \mathbb{R}^d$ has the boundary conforming Delaunay property if

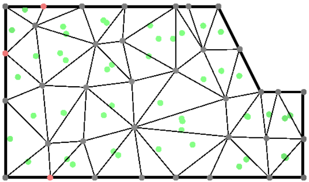
(i) All simplices are Delaunay

(ii) All boundary simplices (edges in 2D, facets in 3d) have the Gabriel property, i.e. their minimal circumdisks are empty

- Equivalent definition in 2D: sum of angles opposite to interior edges $\leq \pi$, angle opposite to boundary edge $\leq \frac{\pi}{2}$
- Creation of boundary conforming Delaunay triangulation description may involve insertion of Steiner points at the boundary



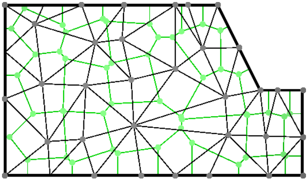
Delaunay grid of Ω



Boundary conforming Delaunay grid of Ω

Domain blendend Voronoi cells

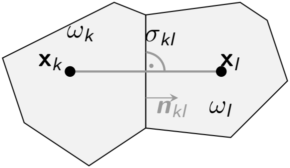
- For Boundary conforming Delaunay triangulations, the intersection of the Voronoi diagram with the domain yields a well defined dual subdivision which can be used for finite volume discretizations



Constructing control volumes I

- Assume Ω is a polygon
- Subdivide the domain Ω into a finite number of **control volumes** : $\bar{\Omega} = \bigcup_{k \in \mathcal{N}} \bar{\omega}_k$ such that
  - ω_k are open (not containing their boundary) convex domains
  - $\omega_k \cap \omega_l = \emptyset$ if $\omega_k \neq \omega_l$
  - $\sigma_{kl} = \bar{\omega}_k \cap \bar{\omega}_l$ are either empty, points or straight lines
  - we will write $|\sigma_{kl}|$ for the length
  - if $|\sigma_{kl}| > 0$ we say that ω_k, ω_l are neigbours
  - neigbours of ω_k: $\mathcal{N}_k = \{l \in \mathcal{N} : |\sigma_{kl}| > 0\}$
- To each control volume ω_k assign a **collocation point**: $\mathbf{x}_k \in \bar{\omega}_k$ such that
  - **admissibility condition**: if $l \in \mathcal{N}_k$ then the line $\mathbf{x}_k\mathbf{x}_l$ is orthogonal to σ_{kl}
  - if ω_k is situated at the boundary, i.e. $\gamma_k = \partial\omega_k \cap \partial\Omega \neq \emptyset$, then $\mathbf{x}_k \in \partial\Omega$

Constructing control volumes II



- We know how to construct this partition:
  - obtain a boundary conforming Delaunay triangulation
  - construct restricted Voronoi cells

Discretization ansatz for Robin boundaray value problem

$$-\nabla \cdot \kappa \nabla u = f \text{ in } \Omega$$
$$\kappa \nabla u \cdot \mathbf{n} + \alpha(u - g) = 0 \text{ on } \partial\Omega$$

- Given control volume ω_k, integrate equation over control volume

$$\begin{aligned}
0 &= \int_{\omega_k} (-\nabla \cdot \kappa \nabla u - f)\, d\omega \\
&= -\int_{\partial\omega_k} \kappa \nabla u \cdot \mathbf{n}_k d\gamma - \int_{\omega_k} f d\omega && \text{(Gauss)} \\
&= -\sum_{L \in \mathcal{N}_k} \int_{\sigma_{kl}} \kappa \nabla u \cdot \mathbf{n}_{kl} d\gamma - \int_{\gamma_k} \kappa \nabla u \cdot \mathbf{n} d\gamma - \int_{\omega_k} f d\omega \\
&\approx \sum_{L \in \mathcal{N}_k} \frac{\sigma_{kl}}{h_{kl}} (u_k - u_l) + |\gamma_k| \alpha (u_k - g_k) - |\omega_k| f_k
\end{aligned}$$

- Here,
  - $u_k = u(\mathbf{x}_k)$
  - $g_k = g(\mathbf{x}_k)$
  - $f_k = f(\mathbf{x}_k)$

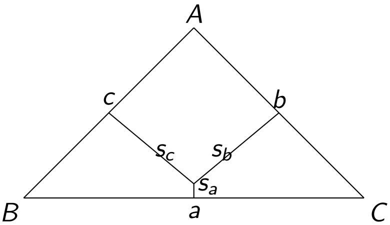
Solvability of discrete problem

- $N = |\mathcal{N}|$ equations (one for each control volume)
- $N = |\mathcal{N}|$ unknowns (one in each collocation point $\equiv$ control volume)
- Graph of discretzation matrix $\equiv$ edge graph of triangulation $\Rightarrow$ matrix is irreducible
- Matrix is irreducibly diagonally dominant
- Main diagonal entries are positive, off diagonal entries are non-positive

$\Rightarrow$ the discretization matrix has the M-property.

In addition, it is symmetric.

Finite volume local stiffness matrix calculation I



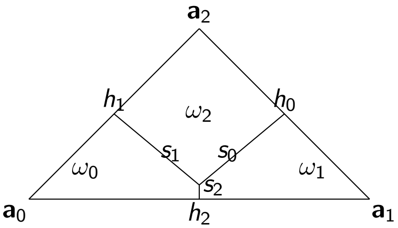
- Triangle edge lengths: a, b, c
- Semiperimeter: $s = \frac{a}{2} + \frac{b}{2} + \frac{c}{2}$
- Square area (from Heron's formula):
  $16A^2 = 16s(s-a)(s-b)(s-c) =$
  $(-a+b+c)(a-b+c)(a+b-c)(a+b+c)$
- Square circumradius: $R^2 = \frac{a^2b^2c^2}{(-a+b+c)(a-b+c)(a+b-c)(a+b+c)} = \frac{a^2b^2c^2}{16A^2}$

Finite volume local stiffness matrix calculation II

- Square of the Voronoi surface contribution via Pythagoras:
  $s_a^2 = R^2 - \left(\frac{1}{2}a\right)^2 = -\frac{a^2\left(a^2-b^2-c^2\right)^2}{4(a-b-c)(a-b+c)(a+b-c)(a+b+c)}$
- Square of edge contribution in the finite volume method:
  $e_a^2 = \frac{s_a^2}{a^2} = -\frac{\left(a^2-b^2-c^2\right)^2}{4(a-b-c)(a-b+c)(a+b-c)(a+b+c)} = \frac{(b^2+c^2-a^2)^2}{64A^2}$
- Edge contribution. $e_a = \frac{s_a}{a} = \frac{b^2+c^2-a^2}{8A}$
- The sign chosen implies a positive value if the angle $\alpha < \frac{\pi}{2}$, and a negative value if it is obtuse. In the latter case, this corresponds to the negative length of the line between edge midpoint and circumcenter, which is exactly the value which needs to be added to the corresponding amount from the opposite triangle in order to obtain the measure of the Voronoi face.

Finite volume local stiffness matrix calculation

$a_0 = (x_0, y_0) \dots a_d = (x_2, y_2)$: vertices of the simplex K Calculate the contribution from triangle to $\frac{\sigma_{kl}}{h_{kl}}$ in the finite volume discretization



Let $h_i = ||a_{i+1} - a_{i+2}||$ (i counting modulo 2) be the lengths of the discretization edges. Let A be the area of the triangle. Then for the contribution from the triangle to the form factor one has

$$\frac{|s_i|}{h_i} = \frac{1}{8A}(h_{i+1}^2 + h_{i+2}^2 - h_i^2)$$

$$|\omega_i| = (|s_{i+1}|h_{i+1} + |s_{i+2}|h_{i+2})/4$$

Assembly loop similar to that from finite elements.