Scientific Computing WS 2017/2018

Lecture 20

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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

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

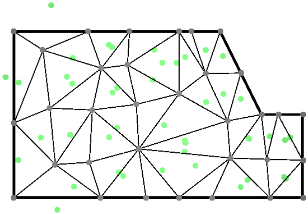
Boundary conforming Delaunay triangulations

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

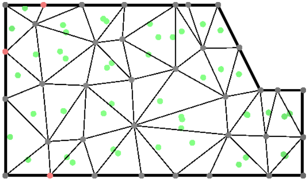
(i) All simplices are Delaunay

(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



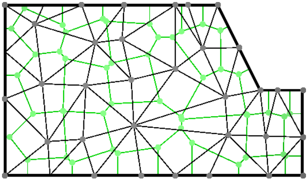
Delaunay grid of Ω



Boundary conforming Delaunay grid of Ω

Domain blendend Voronoi cells

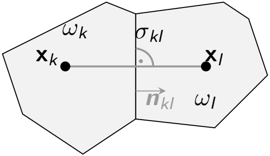
- For Boundary conforming Delaunay triangulations, the intersection of the Voronoi diagram with the domain yields a well defined dual subdivision which can be used for finite volume discretizations



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

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

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

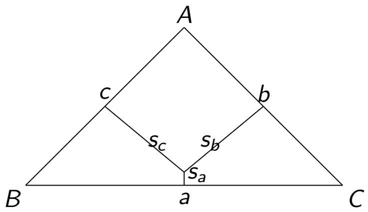
Solvability of discrete problem

- $N = |\mathcal{N}|$ 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



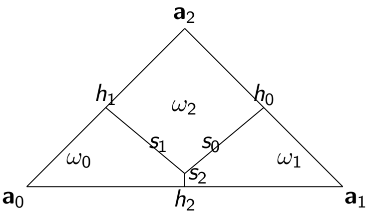
- Triangle edge lengths: a, b, c
- Semiperimeter: $s = \frac{a}{2} + \frac{b}{2} + \frac{c}{2}$
- Square area (from Heron's formula):
  $16A^2 = 16s(s-a)(s-b)(s-c) =$
  $(-a+b+c)(a-b+c)(a+b-c)(a+b+c)$
- Square circumradius: $R^2 = \frac{a^2b^2c^2}{(-a+b+c)(a-b+c)(a+b-c)(a+b+c)} = \frac{a^2b^2c^2}{16A^2}$

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.