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Lecture 13

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Partial Differential Equations

Differential operators: notations

Given: domain $\Omega \subset \mathbb{R}^d$.

- Dot product: for $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, $\mathbf{x} \cdot \mathbf{y} = \sum_{i=1}^{d} x_i y_i$
- Bounded domain $\Omega \subset \mathbb{R}^d$, with piecewise smooth boundary
- Scalar function $u : \Omega \to \mathbb{R}$
- Vector function $\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} : \Omega \to \mathbb{R}^d$
- Write $\partial_i u = \frac{\partial u}{\partial x_i}$
- For a multiindex $\alpha = (\alpha_1 \dots \alpha_d)$, let
  - $|\alpha| = \alpha_1 + \dots + \alpha_d$
  - $\partial^\alpha u = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdot \dots \cdot \partial x_d^{\alpha_d}}$

Basic Differential operators

- Gradient of scalar function $u : \Omega \to \mathbb{R}$
  $$\mathrm{grad} = \nabla = \begin{pmatrix} \partial_1 \\ \vdots \\ \partial_d \end{pmatrix} : \ u \mapsto \nabla u = \begin{pmatrix} \partial_1 u \\ \vdots \\ \partial_d u \end{pmatrix}$$
- Divergence of vector function $\mathbf{v} = \Omega \to \mathbb{R}^d$
  $$\mathrm{div} = \nabla \cdot : \ \mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_d \end{pmatrix} \mapsto \nabla \cdot \mathbf{v} = \partial_1 v_1 + \cdots + \partial_d v_d$$
- Laplace operator of scalar function $u : \Omega \to \mathbb{R}$
  $$\Delta = \mathrm{div} \cdot \mathrm{grad} = \nabla \cdot \nabla : \ u \mapsto \Delta u = \partial_{11} u + \cdots + \partial_{dd} u$$

Lipschitz domains

Definition:

- Let $D \subset \mathbb{R}^n$. A function $f : D \to \mathbb{R}^m$ is called *Lipschitz continuous* if there exists $c > 0$ such that $\|f(x) - f(y)\| \leq c\|x - y\|$
- A hypersurface in $\mathbb{R}^n$ is a *graph* if for some k it can be represented as

  $$x_k = f(x_1, \dots, x_{k-1}, x_{k+1}, \dots, x_n)$$

  defined on some domain $D \subset \mathbb{R}^{n-1}$
- A domain $\Omega \subset \mathbb{R}^n$ is a *Lipschitz domain* if for all $x \in \partial\Omega$, there exists a neigborhood of x on $\partial\Omega$ which can be represented as the graph of a Lipschitz continuous function.

Corollaries

- Boundaries of Lipschitz domains are continuous
- Boundaries of Lipschitz domains have no cusps (e.g. the graph of $y = \sqrt{|x|}$ has a cusp at $x = 0$)
- Polygonal domains are Lipschitz
- Standard PDE calculus happens in Lipschitz domains

Divergence theorem (Gauss' theorem)

Theorem: Let Ω be a bounded Lipschitz domain and $\mathbf{v}: \Omega \to \mathbb{R}^d$ be a continuously differentiable vector function. Let $\mathbf{n}$ be the outward normal to Ω. Then,

$$\int_\Omega \nabla \cdot \mathbf{v} \, d\mathbf{x} = \int_{\partial\Omega} \mathbf{v} \cdot \mathbf{n} \, ds$$

$\square$

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 (REV)* $\omega \subset \Omega$
- 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:

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

- Using Gauss' theorem, rewrite this as

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

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

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

Second order PDEs

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

For solvability we need additional conditions:

- Initial condition in the time dependent case: $u(x,0) = u_0(x)$
- Boundary conditions: behavior of solution on $\partial\Omega$?

Second order parabolic PDEs

- Heat conduction:
  u: temperature
  $\delta = \lambda$: heat conduction coefficient
  f: heat source
  flux$=-\lambda\nabla u$: "Fourier law"
- Diffusion of molecules in a given medium
  u: concentration
  $\delta = D$
  diffusion coefficient
  f: species source
  flux$=-D\nabla u$: "Fick's law"

Second order elliptic PDEs

Stationary case: $\partial_t u = 0 \Rightarrow$ second order *elliptic* PDE

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

- Stationary heat conduction, stationary diffusion
- Incompressible flow in saturated porous media: u: pressure
  $\delta = k$: permeability, flux$=-k\nabla u$: "Darcy's law"
- Electrical conduction: u: electric potential
  $\delta = \sigma$: electric conductivity
  flux$=-\sigma\nabla u \equiv$ current density: "Ohms's law"
- Poisson equation (electrostatics in a constant magnetic field):
  u: electrostatic potential, ∇u: electric field,
  $\delta = \varepsilon$: dielectric permittivity, f: charge density

Second order PDEs: boundary conditions

- Combine PDE in the interior with boundary conditions on variable u and/or or normal flux $\delta\nabla u \cdot \mathbf{n}$
- Assume $\partial\Omega = \cup_{i=1}^{N_\Gamma}\Gamma_i$ is the union of a finite number of non-intersecting subsets Γ_i which are locally Lipschitz.
- On each Γ_i, specify one of
  - Dirichlet ("first kind"): let $g_i : \Gamma_i \to \mathbb{R}$ (homogeneous for $g_i = 0$)
    $$u(x) = u_{\Gamma_i}(x) \quad \text{for } x \in \Gamma_i$$
  - Neumann ("second kind"): Let $g_i : \Gamma_i \to \mathbb{R}$ (homogeneus for $g_i = 0$)
    $$\delta\nabla u(x) \cdot \mathbf{n} = g_i(x) \quad \text{for } x \in \Gamma_i$$
  - Robin ("third kind"): let $\alpha_i, g_i : \Gamma_i \to \mathbb{R}$
    $$\delta\nabla u(x) \cdot \mathbf{n} + \alpha_i(x)\,(u(x) - g_i(x)) = 0 \quad \text{for } x \in \Gamma_i$$
- Boundary functions may be time dependent.

The Dirichlet penalty method

- We will see later that the implementation of Dirichlet boundary may be connected with certain technical difficulties
- The Dirichlet penalty method provides a simple way to avoid these difficulties: let $\varepsilon > 0$:

$$\delta \nabla u_\varepsilon(x) \cdot \mathbf{n} + \frac{1}{\varepsilon}\left(u_\varepsilon(x) - g_i(x)\right) = 0 \quad \text{for } x \in \Gamma_i$$

- It is conceivable that for $\varepsilon \to 0$, u_ε converges to u with

$$u(x) = g_i(x) \quad \text{for } x \in \Gamma_i$$

- Proper way of handling the parameter leads to exact fulfillment of Dirichlet boundary condition in the floating point precision

PDEs: generalizations

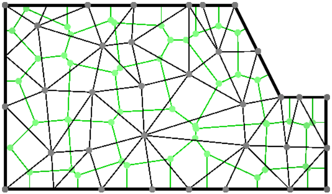
- δ may depend on $\mathbf{x}$, u, $|\nabla u|$ ... $\Rightarrow$ equations become nonlinear
- Coupled second order equations:
  - temperature can influence conductvity
  - source terms can describe chemical reactions between different species
  - chemical reactions can generate/consume heat
  - Electric current generates heat ("Joule heating")
  - ...
- Momentom balance $\rightarrow$ Navier-Stokes equations of fluid flow

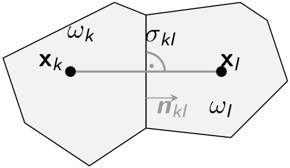
The Finite volume method

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 neighbours
  - neighbours 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}
  - **placement of boundary unknowns**:
    if ω_k is situated at the boundary, i.e. for $|\partial\omega_k \cap \partial\Omega| > 0$, then $\mathbf{x}_k \in \partial\Omega$, and $\partial\omega_k \cap \partial\Omega = \cup_{i=1}^{N_\Gamma}\gamma_{i,k}$ (where $\gamma_{i,k} = \emptyset$ is possible).

Constructing control volumes II





We know how to construct such a partitioning:

- obtain a boundary conforming Delaunay triangulation with vertices x_k
- construct restricted Voronoi cells ω_k with $x_k \in \omega_k$
- Delaunay triangulation gives connected neigborhood graph of Voronoi cells
- Admissibility condition fulfilled in a natural way
- Boundary placement of triangle nodes

Discretization ansatz for Robin boundary value problem

Given constants $\kappa > 0$, $\alpha_i \geq 0$ $(i = 1 \dots N_\Gamma)$

$$-\nabla \cdot \kappa \nabla u = f \text{ in } \Omega$$
$$\kappa \nabla u \cdot \mathbf{n} + \alpha_i (u - g_i) = 0 \text{ on } \Gamma_i \; (i = 1 \dots N_\Gamma) \qquad (*)$$

- Given control volume ω_k, $k \in \mathcal{N}$, integrate

$$\begin{aligned}
0 &= \int_{\omega_k} (-\nabla \cdot \kappa \nabla u - f)\, d\omega \\
&= -\int_{\partial\omega_k} \kappa \nabla u \cdot \mathbf{n}_k d\gamma - \int_{\omega_k} f d\omega \qquad \text{(Gauss)} \\
&= -\sum_{l \in \mathcal{N}_k} \int_{\sigma_{kl}} \kappa \nabla u \cdot \mathbf{n}_{kl} d\gamma - \sum_{i=1}^{N_\Gamma} \int_{\gamma_{ik}} \kappa \nabla u \cdot \mathbf{n} d\gamma - \int_{\omega_k} f d\omega \\
&\approx \sum_{L \in \mathcal{N}_k} \underbrace{\kappa \frac{|\sigma_{kl}|}{h_{kl}} (u_k - u_l)}_{\nabla u \cdot \mathbf{n} \approx \frac{u_l - u_k}{h_{kl}}} + \sum_{i=1}^{N_\Gamma} \underbrace{|\gamma_{i,k}| \alpha_i (u_k - g_{i,k})}_{\text{bound. cond. } (*)} - \underbrace{|\omega_k| f_k}_{\text{quadrature}}
\end{aligned}$$

- Here, $u_k = u(\mathbf{x}_k)$, $g_{i,k} = g_i(\mathbf{x}_k)$, $f_k = f(\mathbf{x}_k)$

Properties of discretization matrix

- $N = |\mathcal{N}|$ equations (one for each control volume ω_k)
- $N = |\mathcal{N}|$ unknowns (one for each collocation point $x_k \in \omega_k$)
- weighted connected edge graph of triangulation $\equiv N \times N$ irreducible sparse discretization matrix $A = (a_{kl})$:

$$a_{kl} = \begin{cases} \sum_{l' \in \mathcal{N}_k} \kappa \frac{|\sigma_{kl'}|}{h_{kl'}} + \sum_{i=1}^{N_\Gamma} |\gamma_{i,k}| \alpha_i, & l = k \\ -\kappa \frac{\sigma_{kl}}{h_{kl}}, & l \in \mathcal{N}_k \\ 0, & else \end{cases}$$

- A is irreducibly diagonally dominant if at least for one i, $|\gamma_{i,k}|\alpha_i > 0$
- Main diagonal entries are positive, off diagonal entries are non-positive
- $\Rightarrow A$ has the M-property.
- A is symmetric $\Rightarrow A$ is positive definite

Matrix assembly – main part

- Keep list of global node numbers per triangle τ mapping local node numbers of the triangle to the global node numbers: $\{0, 1, 2\} \to \{k_{\tau,0}, k_{\tau,1}, k_{\tau,2}\}$
- Loop over all triangles $\tau \in \mathcal{T}$ of the discretization, add up contributions

for $k, l = 1 \ldots N$ **do**
  set $a_{kl} = 0$
end
for $\tau \in \mathcal{T}$ **do**
  for $n, m = 0 \ldots 2, n \neq m$ **do**

$$\sigma = \sigma_{k_{\tau,m},k_{\tau,n}} \cap \tau$$

$$\sigma_h = \kappa \frac{|\sigma|}{h_{k_{\tau,m},k_{\tau,n}}}$$

$$a_{k_{\tau,m},k_{\tau,m}} += \sigma_h$$

$$a_{k_{\tau,m},k_{\tau,n}} -= \sigma_h$$

$$a_{k_{\tau,n},k_{\tau,m}} -= \sigma_h$$

$$a_{k_{\tau,n},k_{\tau,n}} += \sigma_h$$

  end
end

Matrix assembly – boundary part

- Keep list of global node numbers per boundary element γ mapping local node element to the global node numbers: $\{0,1\} \to \{k_{\gamma,0}, k_{\gamma,1}\}$
- Keep list of boundary part numbers per boundary element i_γ
- Loop over all boundary elements $\gamma \in \mathcal{G}$ of the discretization, add up contributions

for $\gamma \in \mathcal{G}$ **do**
  for $n = 0, 1$ **do**
    $a_{k_{\gamma n},k_{\gamma n}} += \alpha_{i_\gamma} |\gamma \cap \omega_{k_{\gamma n}}|$
  end
end

RHS assembly: calculate control volumes

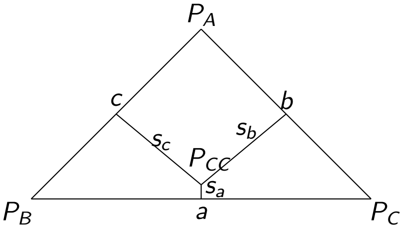
- Denote $w_k = |\omega_k|$
- Loop over triangles, add up contributions

  for $k \dots N$ **do**
  | set $w_k = 0$
  end
  for $\tau \in \mathcal{T}$ **do**
  | **for** $n = \dots 3$ **do**
  | | $w_k {+}{=} |\omega_{k_{\tau,m}} \cap \tau|$
  | **end**
  end

Matrix assembly: summary

- Sufficient to keep list of triangles, boundary segments – they typically come out of the mesh generator
- Be able to calculate triangular contributions to form factors: $|\omega_k \cap \tau|$, $|\sigma_{kl} \cap \tau|$ – we need only the numbers, and not the construction of the geometrical objects
- $O(N)$ operation, one loop over triangles, one loop over boundary elements

Finite volume local stiffness matrix calculation I



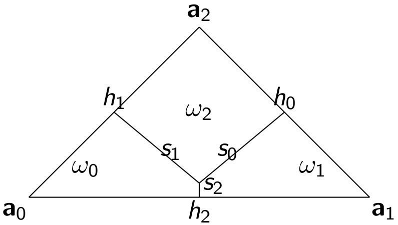
- Triangle edge lengths: a, b, c
- Semiperimeter: $s = \frac{a}{2} + \frac{b}{2} + \frac{c}{2}$
- Square area (from Heron's formula):
  $16A^2 = 16s(s-a)(s-b)(s-c) =$
  $(-a+b+c)\,(a-b+c)\,(a+b-c)\,(a+b+c)$
- Square circumradius: $R^2 = \frac{a^2b^2c^2}{(-a+b+c)(a-b+c)(a+b-c)(a+b+c)} = \frac{a^2b^2c^2}{16A^2}$

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 III

$a_0 = (x_0, y_0) \dots a_d = (x_2, y_2)$: 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

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

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

Variations of the discretization ansatz

- 3D: tetrahedron based
- $\kappa = \kappa(x) \Rightarrow \kappa(x)\nabla u \approx \kappa_{kl}\frac{u_l - u_k}{h_{kl}}$
- Non-constant α_i, g
- Nonlinear dependencies ...

Interpretation of results

- One solution value per control volume ω_k allocated to the collocation point $x_k \Rightarrow$ piecewise constant function on collection of control volumes
- But: x_k are at the same time nodes of the corresponding Delaunay mesh $\Rightarrow$ representation as piecewise linear function on triangles