Scientific Computing TU Berlin Winter 2021/22 © Jürgen Fuhrmann
Notebook 22

The finite volume method for the discetization of PDEs

Motivation

Regard stationary second order PDE with Robin boundary conditions as a system of two first order equations in a Lipschitz domain Ω:

$$\begin{aligned} \nabla\cdot\vec{j} &= f & \text{continuity equation in } \Omega\\ \vec{j} &= -\delta\vec\nabla u & \text{flux law in } \Omega\\ -\vec{j}\cdot\vec{n} + \alpha u &= \beta & \text{on } \Gamma \end{aligned}$$

- Derivation of the continuity equation was based on the consideration of species balances of an representative elementary volume (REV)
- Why not just subdivide the computational domain into a finite number of REV's ?
  - Assign a value of u to each REV
  - Approximate $\vec\nabla u$ by finite differece of u values in neigboring REVs
  - ... call REVs *control volumes* or *finite volumes*

Constructing control volumes

Assume $\Omega \subset \mathbb{R}^d$ is a polygonal domain such that $\partial\Omega = \bigcup_{m\in\mathcal{G}} \Gamma_m$, where Γ_m are planar such that $\vec{n}|_{\Gamma_m} = \vec{n}_m$.

Subdivide Ω into into a finite number of *control volumes* $\bar{\Omega} = \bigcup_{k\in\mathcal{N}} \bar{\omega}_k$ such that

- ω_k are open convex domains such that $\omega_k \cap \omega_l = \emptyset$ if $\omega_k \neq \omega_l$
- $\sigma_{kl} = \bar{\omega}_k \cap \bar{\omega}_l$ are either empty, points or straight lines. If $|\sigma_{kl}| > 0$ we say that ω_k, ω_l are neighbours.
- $\vec{n}_{kl} \perp \sigma_{kl}$: normal of $\partial\omega_k$ at σ_{kl}
- $\mathcal{N}_k = \{l \in \mathcal{N} : |\sigma_{kl}| > 0\}$: set of neighbours of ω_k
- $\gamma_{km} = \partial\omega_k \cap \Gamma_m$: boundary part of $\partial\omega_k$
- $\mathcal{G}_k = \{m \in \mathcal{G} : |\gamma_{km}| > 0\}$: set of non-empty boundary parts of $\partial\omega_k$.

$\Rightarrow \partial\omega_k = \left(\cup_{l\in\mathcal{N}_k}\sigma_{kl}\right) \bigcup \left(\cup_{m\in\mathcal{G}_k}\gamma_{km}\right)$

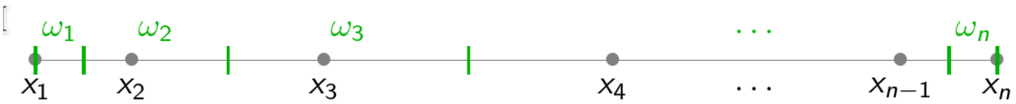
To each control volume ω_k assign a *collocation point*: $\vec{x}_k \in \bar{\omega}_k$ such that\

- *Admissibility condition*:if $l \in \mathcal{N}_k$ then the line $\vec{x}_k\vec{x}_l$ is orthogonal to σ_{kl}
  - For a given function $u : \Omega \to \mathbb{R}$ this will allow to associate its value $u_k = u(\vec{x}_k)$ as the value of an unknown at $\vec{x}_k$.
  - For two neigboring control volumes ω_k, ω_l , this will allow to approximate $\vec{\nabla} u \cdot \vec{n}_{kl} \approx \frac{u_l - u_k}{h_{kl}}$
- *Placement of boundary unknowns at the boundary*: if ω_k is situated at the boundary, i.e. for $|\partial\omega_k \cap \partial\Omega| > 0$, then $\vec{x}_k \in \partial\Omega$
  - This will allow to apply boundary conditions in a direct manner

1D case

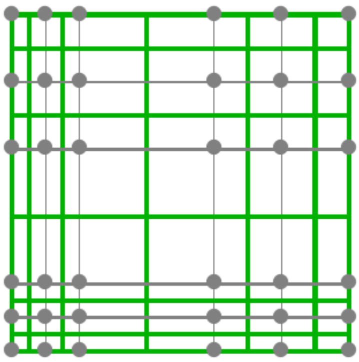
Let $\Omega = (a, b)$ be subdivided into intervals by $x_1 = a < x_2 < x_3 < \dots < x_{n-1} < x_n = b$. Then we set

$$\omega_k = \begin{cases} \left(x_1, \frac{x_1+x_2}{2}\right), & k = 1 \\ \left(\frac{x_{k-1}+x_k}{2}, \frac{x_k+x_{k+1}}{2}\right), & 1 < k < n \\ \left(\frac{x_{n-1}+x_n}{2}, x_n\right), & k = n \end{cases}$$



2D Rectangular domain

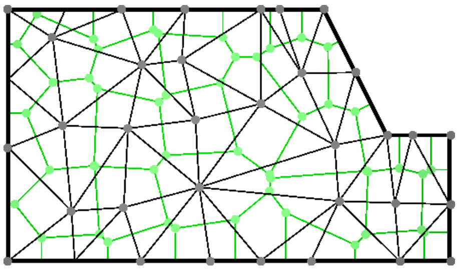
- Let $\Omega = (a, b) \times (c, d) \subset \mathbb{R}^2$.
- Assume subdivisions $x_1 = a < x_2 < x_3 < \dots < x_{n-1} < x_n = b$ and $y_1 = c < y_2 < y_3 < \dots < y_{n-1} < y_n = d$
- $\Rightarrow$ 1D control volumes ω_k^x and ω_k^y
- Set $\vec{x}_{kl} = (x_k, y_l)$ and $\omega_{kl} = \omega_k^x \times \omega_l^y$.

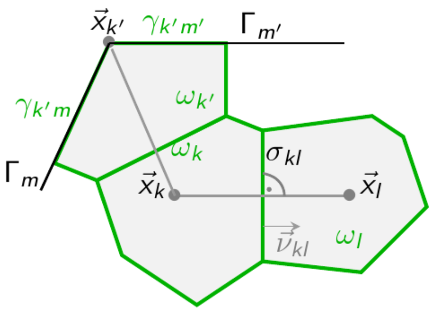


- Green: Control volume boundaries
- Gray: original grid lines and points

2D, polygonal domain

- Obtain a boundary conforming Delaunay triangulation with vertices $\vec{x}_k$
- Construct restricted Voronoi cells ω_k with $\vec{x}_k \in \omega_k$
- Corners of Voronoi cells are either cell circumcenters or midpoints of boundary edges
- Admissibility condition $\vec{x}_k\vec{x}_l \perp \sigma_{kl} = \bar{\omega}_k \cap \bar{\omega}_l$ fulfilled in a natural way
- Triangulation edges $\equiv$ connected neigborhood graph of Voronoi cells
- Triangulation nodes $\equiv$ collocation points
- Boundary placement of collocation points of boundary control volumes





Discretization of second order PDE

Discretization of continuity equation

- Stationary continuity equation: $\nabla \cdot \vec{j} = f$
- Integrate over control volume ω_k:

$$\begin{aligned} 0 &= \int_{\omega_k} \nabla \cdot \vec{j}\, d\omega - \int_{\omega_k} f\, d\omega \\ &= \int_{\partial\omega_k} \vec{j} \cdot \vec{n}_\omega\, ds - \int_{\omega_k} f\, d\omega \\ &= \sum_{l \in \mathcal{N}_k} \int_{\sigma_{kl}} \vec{j} \cdot \vec{n}_{kl}\, ds + \sum_{m \in \mathcal{G}_k} \int_{\gamma_{km}} \vec{j} \cdot \vec{n}_m\, ds - \int_{\omega_k} f d\omega \\ &= \text{flux between CV} + \text{flux in/out of } \Omega - \text{sources} \end{aligned}$$

Approximation of flux between control volumes

- Utilize flux law: $\vec{j} = -\delta\vec{\nabla}u$
- Admissibility condition $\Rightarrow \vec{x}_k\vec{x}_l \parallel \vec{n}_{kl}$
- Let $u_k = u(\vec{x}_k)$, $u_l = u(\vec{x}_l)$
- $h_{kl} = |\vec{x}_k - \vec{x}_l|$: distance between neigboring collocation points
- Finite difference approximation of normal derivative:

$$\vec{\nabla}u \cdot \vec{n}_{kl} \approx \frac{u_l - u_k}{h_{kl}}$$

- $\Rightarrow$ flux between neigboring control volumes:

$$\begin{aligned}\int_{\sigma_{kl}} \vec{j} \cdot \vec{n}_{kl}\, ds &\approx \frac{|\sigma_{kl}|}{h_{kl}}\delta(u_k - u_l)\\ &=: \frac{|\sigma_{kl}|}{h_{kl}}g(u_k, u_l)\end{aligned}$$

where $g(\cdot, \cdot)$ is called *flux function*

Approximation of boundary fluxes

- Utilize boundary condition $\vec{j} \cdot \vec{n} = \alpha u - \beta$
- Assume $\alpha|_{\Gamma_m} = \alpha_m, \beta|_{\Gamma_m} = \beta_m$
- Approximation of $\vec{j} \cdot \vec{n}_m$ at the boundary of ω_k:

$$\vec{j} \cdot \vec{n}_m \approx \alpha_m u_k - \beta_m$$

- Approximation of flux from ω_k through Γ_m:

$$\int_{\gamma_{km}} \vec{j} \cdot \vec{n}_m\, ds \approx |\gamma_{km}|(\alpha_m u_k - \beta_m)$$

Approximation of right hand side

- Let $f_k = \frac{1}{|\omega_k|}\int_{\omega_k} f(\vec{x})\, d\omega$ or $f_k = f(\vec{x}_k)$
- Approximate $\int_{\omega_k} f\, d\omega \approx |\omega_k| f_k$

Discretized system of equations

- The discrete system of equations then writes for $k \in \mathcal{N}$:

$$
\begin{aligned}
\sum_{l\in\mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}}\delta(u_k - u_l) + \sum_{m\in\mathcal{G}_k} |\gamma_{km}|\alpha_m u_k = |\omega_k| f_k + \sum_{m\in\mathcal{G}_k} |\gamma_{km}|\beta_m \\
u_k\left(\delta \sum_{l\in\mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}} + \alpha_m \sum_{m\in\mathcal{G}_k} |\gamma_{km}|\right) - \delta \sum_{l\in\mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}} u_l = |\omega_k| f_k + \sum_{m\in\mathcal{G}_k} |\gamma_{km}|\beta_m
\end{aligned}
$$

- This can be rewritten as

$$
\begin{aligned}
Au = b \\
a_{kk}u_k + \sum_{l=1\dots|\mathcal{N}|, l\neq k} a_{kl}u_l = b_k \qquad \text{for } k = 1\dots|\mathcal{N}|
\end{aligned}
$$

with coefficients

$$
\begin{aligned}
a_{kl} &= \begin{cases} \sum_{l'\in\mathcal{N}_k} \delta\frac{|\sigma_{kl'}|}{h_{kl'}} + \sum_{m\in\mathcal{G}_k} |\gamma_{km}|\alpha_m, & l = k \\ -\delta\frac{\sigma_{kl}}{h_{kl}}, & l \in \mathcal{N}_k \\ 0, & \text{else} \end{cases} \\
b_k &= |\omega_k| f_k + \sum_{m\in\mathcal{G}_k} |\gamma_{km}|\beta_m
\end{aligned}
$$

Matrix properties

- $N = |\mathcal{N}|$ equations (one for each control volume ω_k)
- $N = |\mathcal{N}|$ unknowns (one for each collocation point $x_k \in \omega_k$)
- Matrix is sparse: nonzero entries only for neighboring control volumes
- Matrix graph is connected: nonzero entries correspond to edges in Delaunay triangulation $\Rightarrow$ irreducible
- 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

Assembly algorithm

- Due to the connection between Voronoi diagram and Delaunay triangulation, one can assemble the discrete system based on the triangulation
- Assembly in two loops:
  - Loop over all triangles, calculate triangle contribution to matrix entries
  - Loop over all boundary segments, calculate contribution to matrix entries

1. Loop over all triangles $T \in \mathcal{T}$, add up edge contributions:

Given:

- List of point coordinates $\vec{x}_K$
- List of triangles which for each triangle describes indices of points belonging to triangle
    - This induces a mapping of local node numbers of a triangle T to the global ones: $\{1,2,3\} \to \{k_{T,1}, k_{T,2}, k_{T,3}\}$

for $k,l = 1 \dots N$ set $a_{kl} = 0$

for $k = 1 \dots N$ set $b_k = 0$

for $T \in \mathcal{T}$

for $i \dots 3$

$$b_{k_{T,i}} += |\omega_{k_{T,i}} \cap T| f_{k_{T,i}}$$

for $i,j = 1 \dots 3, i \neq j$

$$\begin{aligned}
\sigma &= \sigma_{k_{T,j},k_{T,i}} \cap T \\
s &= \frac{|\sigma|}{h_{k_{T,j},k_{T,i}}} \\
a_{k_{T,j},k_{T,j}} &+= \delta s \\
a_{k_{T,j},k_{T,i}} &-= \delta s \\
a_{k_{T,i},k_{T,j}} &-= \delta s \\
a_{k_{T,i},k_{T,n}} &+= \delta s
\end{aligned}$$

2. Loop over all boundary segments

- Keep list of global node numbers per boundary element γ mapping local node element to the global node numbers: $\{1,2\} \to \{k_{\gamma,1}, k_{\gamma,2}\}$
- Keep list of boundary part numbers m_γ per boundary element
- Loop over all boundary elements $\gamma \in \mathcal{G}$ of the discretization, add up contributions

for $\gamma \in \mathcal{G}$

for $i = 1,2$

$$a_{k_{\gamma_i},k_{\gamma_i}} += \alpha_{m_\gamma} |\gamma \cap \partial\omega_{k_{\gamma_i}}|$$

$$b_{k_{\gamma_i}} += \beta_{m_\gamma} |\gamma \cap \partial\omega_{k_{\gamma_i}}|$$

- 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