Recap: the finite Volume method
Finite volumes: motivation

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

\[ \nabla \cdot \vec{j} = f \quad \text{continuity equation in } \Omega \]
\[ \vec{j} = -\delta \vec{\nabla} u \quad \text{flux law in } \Omega \]
\[ \vec{j} \cdot \vec{n} = \alpha u - g \quad \text{on } \Gamma \]

- 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 difference of $u$ values in neighboring REVs
  - ... call REVs “control volumes” or “finite volumes”
Assume $\Omega \subset \mathbb{R}^d$ is a polygonal domain such that $\partial \Omega = \bigcup_{m \in \mathcal{G}} \Gamma_m$, where $\Gamma_m$ are planar such that $\vec{n}|_{\Gamma_m} = \vec{n}_m$.

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

- $\omega_k$ 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 $\omega_k$, $\omega_l$ are neighbours.
- $\vec{\nu}_{kl} \perp \sigma_{kl}$: normal of $\partial \omega$ at $\sigma_{kl}$
- $\mathcal{N}_k = \{l \in \mathcal{N} : |\sigma_{kl}| > 0\}$: set of neighbours of $\omega_k$
- $\gamma_{km} = \partial \omega_k \cap \Gamma_m$: domain boundary part of $\partial \omega_k$
- $\mathcal{G}_k = \{m \in \mathcal{G} : |\gamma_{km}| > 0\}$: set of non-empty boundary parts of $\omega_k$.

$\Rightarrow \partial \omega_k = \left( \bigcup_{l \in \mathcal{N}_k} \sigma_{kl} \right) \bigcup \left( \bigcup_{m \in \mathcal{G}_k} \gamma_{km} \right)$
To each control volume $\omega_k$ assign a collocation point: $\vec{x}_k \in \bar{\omega}_k$ such that

- **Admissibility condition:**
  if $l \in N_k$ then the line $\vec{x}_k \vec{x}_l$ is orthogonal to $\sigma_{kl}$
  - For a given function $u: \Omega \rightarrow \mathbb{R}$ 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 neighboring control volumes $\omega_k, \omega_l$, this will allow to approximate $\vec{\nabla} u \cdot \vec{v}_{kl} \approx \frac{u_l - u_k}{h}$
- **Placement of boundary unknowns at the boundary:**
  if $\omega_k$ 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
Let $\Omega = (a, b)$ be subdivided into intervals by $x_1 = a < x_2 < x_3 < \cdots < x_{n-1} < x_n = b$. Then we set

$$\omega_k = \begin{cases} 
(x_1, \frac{x_1 + x_2}{2}), & k = 1 \\
\left(\frac{x_{k-1} + x_k}{2}, \frac{x_k + x_{k+1}}{2}\right), & 1 < k < n \\
\left(\frac{x_{n-1} + x_n}{2}, x_n\right), & k = n
\end{cases}$$
Control Volumes for a 2D tensor product mesh

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

- Gray: original grid lines and points.
- Green: boundaries of control volumes.
Control volumes on boundary conforming Delaunay mesh

- Obtain a boundary conforming Delaunay triangulation with vertices $\vec{x}_k$
- Construct restricted Voronoi cells $\omega_k$ with $\vec{x}_k \in \omega_k$
  - Corners of Voronoi cells are either cell circumcenters of 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: connected neighborhood graph of Voronoi cells
- Boundary placement of collocation points of boundary control volumes
Discretization of continuity equation

- Stationary continuity equation: \( \nabla \cdot \vec{j} = f \)
- Integrate over control volume \( \omega_k \):

\[
0 = \int_{\omega_k} \nabla \cdot \vec{j} \, d\omega - \int_{\omega_k} f \, d\omega \\
= \int_{\partial \omega_k} \vec{j} \cdot \vec{n}_\omega \, ds - \int_{\omega_k} f \, d\omega \\
= \sum_{l \in N_k} \int_{\sigma_{kl}} \vec{j} \cdot \vec{n}_{kl} \, ds + \sum_{m \in G_k} \int_{\gamma_{km}} \vec{j} \cdot \vec{n}_m \, ds - \int_{\omega_k} f d\omega
\]
Approximation of flux between control volumes

Utilize flux law: \( \vec{j} = -\delta \vec{\nabla} u \)

- Admissibility condition \( \Rightarrow \vec{\xi}_k \vec{\xi}_l \parallel \nu_{kl} \)
- Let \( u_k = u(\vec{\xi}_k) \), \( u_l = u(\vec{\xi}_l) \)
- \( h_{kl} = |\vec{\xi}_k - \vec{\xi}_l|: \) distance between neighboring collocation points
- Finite difference approximation of normal derivative:
  \[
  \vec{\nabla} u \cdot \vec{v}_{kl} \approx \frac{u_l - u_k}{h_{kl}}
  \]

\( \Rightarrow \) flux between neighboring control volumes:

\[
\int_{\sigma_{kl}} \vec{j} \cdot \vec{v}_{kl} \, ds \approx \frac{|\sigma_{kl}|}{h_{kl}} \delta(u_k - u_l)
\]

\[= \frac{|\sigma_{kl}|}{h_{kl}} g(u_k, u_l)\]

where \( g(\cdot, \cdot) \) is called flux function
Approximation of Robin boundary conditions

Utilize boundary condition $\vec{j} \cdot \vec{n} = \alpha u - g$

- Assume $\alpha|_{\Gamma_m} = \alpha_m$
- Approximation of $\vec{j} \cdot \vec{n}_m$ at the boundary of $\omega_k$:
  $$\vec{j} \cdot \vec{n}_m \approx \alpha_m u_k - g$$

- Approximation of flux from $\omega_k$ through $\Gamma_m$:
  $$\int_{\gamma_{km}} \vec{j} \cdot \vec{n}_m \: ds \approx |\gamma_{km}|(\alpha_m u_k - g)$$
Discrete system of equations

- Let \( f_k = f(\bar{x}_k) \) (or \( f_k = \frac{1}{|\omega_k|} \int_{\omega_k} f(\bar{x}_k) \, d\omega \)).

- The discrete system of equations then writes for \( k \in \mathbb{N} \):

\[
\sum_{l \in \mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}} \delta(u_k - u_l) + \sum_{m \in \mathcal{G}_k} |\gamma_{km}| \alpha_m u_k = |\omega_k| f_k + \sum_{m \in \mathcal{G}_k} |\gamma_{km}| g
\]

\[
 u_k \left( \delta \sum_{l \in \mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}} + \alpha_m \sum_{m \in \mathcal{G}_k} |\gamma_{km}| \right) - \delta \sum_{l \in \mathcal{N}_k} \frac{|\sigma_{kl}|}{h_{kl}} u_l = |\omega_k| f_k + \sum_{m \in \mathcal{G}_k} |\gamma_{km}| g
\]

\[
a_{kk} u_k + \sum_{l=1 \ldots |\mathcal{N}|, l \neq k} a_{kl} u_l = b_k
\]

with \( b_k = |\omega_k| f_k + \sum_{m \in \mathcal{G}_k} |\gamma_{km}| g \) and

\[
a_{kl} = \begin{cases} 
\sum_{l' \in \mathcal{N}_k} \delta \frac{|\sigma_{kl'}|}{h_{kl'}} + \sum_{m \in \mathcal{G}_k} |\gamma_{km}| \alpha_m, & l = k \\
-\delta \frac{|\sigma_{kl}|}{h_{kl}}, & l \in \mathcal{N}_k \\
0, & \text{else}
\end{cases}
\]
Discretization matrix properties

- $N = |\mathcal{N}|$ equations (one for each control volume $\omega_k$)
- $N = |\mathcal{N}|$ 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
Matrix assembly algorithm

Due to the connection between Voronoi diagram and Delaunay triangulation, one can assemble the discrete system based on the triangulation

Necessary information:

- 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: $\{1, 2, 3\} \rightarrow \{k_{T,1}, k_{T,2}, k_{T,3}\}$
- List of (boundary) segments which for each segment describes indices of points belonging to segment

Assembly in two loops:

- Loop over all triangles, calculate triangle contribution to matrix entries
- Loop over all boundary segments, calculate contribution to matrix entries
Matrix assembly – main part

- Loop over all triangles \( T \in \mathcal{T} \), add up edge contributions
  
  for \( k, l = 1 \ldots N \) do
  | set \( a_{kl} = 0 \)
  end

  for \( T \in \mathcal{T} \) do
    for \( i, j = 1 \ldots 3, i \neq j \) do
      \[ \sigma = \sigma_{kT,j,kT,i} \cap \mathcal{T} \]
      \[ s = \frac{|\sigma|}{h_{kT,j,kT,i}} \]
      \[ a_{kT,j,kT,j}^+ = \delta \sigma_h \]
      \[ a_{kT,j,kT,i}^- = \delta \sigma_h \]
      \[ a_{kT,i,kT,j}^- = \delta \sigma_h \]
      \[ a_{kT,i,kT,n}^+ = \delta \sigma_h \]
    end
  end
Matrix assembly – boundary part

- Keep list of global node numbers per boundary element $\gamma$ mapping local node element to the global node numbers: $\{1, 2\} \rightarrow \{k_{\gamma,1}, k_{\gamma,2}\}$

- Keep list of boundary part numbers $m_\gamma$ per boundary element

- Loop over all boundary elements $\gamma \in \mathcal{G}$ of the discretization, add up contributions

\[
\text{for } \gamma \in \mathcal{G} \text{ do}
\]

\[
\text{for } i = 1, 2 \text{ do}
\]

\[
a_{k_{\gamma,i}, k_{\gamma,i}} = \alpha m_\gamma |\gamma \cap \partial \omega_{k_{\gamma,i}}|
\]

\[
\text{end}
\]

\[
\text{end}
\]
RHS assembly: calculate control volumes

- Denote \( w_k = |\omega_k| \)
- Loop over triangles, add up contributions
  
  \[
  \text{for } k = N \text{ do} \\
  \quad \text{set } w_k = 0 \\
  \text{end} \\
  \text{for } \tau \in \mathcal{T} \text{ do} \\
  \quad \text{for } n = 3 \text{ do} \\
  \quad \quad w_k_+ = |\omega_{k, j} \cap \tau| \\
  \quad \text{end} \\
  \text{end}
  \]
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.
Need to calculate $s_a$, $s_b$, $s_c$

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: $R^2 = \frac{a^2 b^2 c^2}{(-a+b+c)(a-b+c)(a+b-c)(a+b+c)} = \frac{a^2 b^2 c^2}{16A^2}$
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:
  \[ e_a^2 = s_a^2 = \frac{\left( a^2 - b^2 - c^2 \right)^2}{4(a-b-c)(a-b+c)(a+b-c)(a+b+c)} = \frac{(b^2+c^2-a^2)^2}{64A^2} \]

- 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

\[ a_0 = (x_0, y_0), \ldots a_d = (x_2, y_2) \]: 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

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

\[
|\omega_i| = \left( |s_{i+1}| h_{i+1} + |s_{i+2}| h_{i+2} \right)/4
\]
Variations of the discretization ansatz

- 3D: tetrahedron based
- $\delta = \delta(x) \Rightarrow \delta(x) \nabla u \approx \delta_{kl} \frac{u_l - u_k}{h_{kl}}$
- Non-constant $\alpha_i, g$
- Nonlinear dependencies ...
Interpretation of results

- One solution value per control volume $w_k$ 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
The problem with Dirichlet boundary conditions

- Eliminate Dirichlet BC algebraically after building of the matrix, i.e. fix “known unknowns” at the Dirichlet boundary ⇒ highly technical
- Modify matrix such that equations at boundary exactly result in Dirichlet values ⇒ loss of symmetry of the matrix
- Penalty method
Dirichlet BC: Algebraic manipulation

- Assume 1D situation with BC $u_1 = g$
- From handling of control volumes without regard of boundary values:

$$AU = \begin{pmatrix} \frac{1}{h} & -\frac{1}{h} & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\ & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \\ & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix}$$

- Fix $u_1$ and eliminate:

$$A'U = \begin{pmatrix} \frac{2}{h} & -\frac{1}{h} & & \\ -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\ & -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \\ & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} u_2 \\ u_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} f_2 + \frac{1}{h}g \\ f_3 \\ \vdots \end{pmatrix}$$

- $A'$ becomes idd and stays symmetric
- operation is quite technical
Dirichlet BC: Modify boundary equations

- From handling of control volumes without regard of boundary values:

\[
AU = \begin{pmatrix}
\frac{1}{h} & -\frac{1}{h} & & & \\
-\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\
& -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\
& & & \ddots & \ddots \\
& & & & \ddots
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
u_3 \\
\vdots
\end{pmatrix}
= \begin{pmatrix}f_1 \\
f_2 \\
f_3 \\
\vdots
\end{pmatrix}
\]

- Modify equation at boundary to exactly represent Dirichlet values

\[
A'U = \begin{pmatrix}
\frac{1}{h} & 0 & & & \\
-\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & & \\
& -\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} & \\
& & & \ddots & \ddots \\
& & & & \ddots
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
u_3 \\
\vdots
\end{pmatrix}
= \begin{pmatrix}\frac{1}{h}g \\
f_2 \\
f_3 \\
\vdots
\end{pmatrix}
\]

- \(A'\) becomes idd
- loses symmetry \(\Rightarrow\) problem e.g. with CG method
Dirichlet BC: Discrete penalty trick

- From handling of control volumes without regard of boundary values:

\[
AU = \begin{pmatrix}
\frac{1}{h} & -\frac{1}{h} & -\frac{1}{h} \\
-\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \\
-\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \\
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
u_3 \\
\end{pmatrix}
= \begin{pmatrix}f_1 \\
f_2 \\
f_3 \\
\end{pmatrix}
\]

- Add penalty terms

\[
A'U = \begin{pmatrix}
\frac{1}{\varepsilon} + \frac{1}{h} & -\frac{1}{h} & -\frac{1}{h} \\
-\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \\
-\frac{1}{h} & \frac{2}{h} & -\frac{1}{h} \\
\end{pmatrix}
\begin{pmatrix}
u_1 \\
u_2 \\
u_3 \\
\end{pmatrix}
= \begin{pmatrix}f_1 + \frac{1}{\varepsilon}g \\
f_2 \\
f_3 \\
\end{pmatrix}
\]

- \(A'\) becomes idd, keeps symmetry, and the realization is technically easy.
- If \(\varepsilon\) is small enough, \(u_1 = g\) will be satisfied exactly within floating point accuracy.
- Iterative methods should be initialized with Dirichlet values.
- Works for nonlinear problems, finite volume methods.
Dirichlet boundary value problem:

\[-\nabla \cdot \delta \nabla u = f \quad \text{in } \Omega\]
\[u|_{\Gamma_m} = g_m\]

Approximate Dirichlet boundary condition by:

\[\delta \nabla u \cdot \vec{n}_m + \frac{1}{\epsilon} u|_{\Gamma_m} = \frac{1}{\epsilon} g_m\]