

Scientific Computing WS 2020/2021

Slide lecture 6

Jürgen Fuhrmann

[juergen.fuhrmann@wias-berlin.de](mailto:juergen.fuhrmann@wias-berlin.de)

## 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 REV's
  - ... call REV's "control volumes" or "finite volumes"

# Constructing control volumes I

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 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  $\partial\omega_k$  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  $\omega_k$ .

$$\Rightarrow \partial\omega_k = (\bigcup_{l \in \mathcal{N}_k} \sigma_{kl}) \cup (\bigcup_{m \in \mathcal{G}_k} \gamma_{km})$$

# Constructing control volumes II

To each control volume  $\omega_k$  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  $\sigma_{kl}$

- 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  $\vec{\nabla} u \cdot \vec{\nu}_{kl} \approx \frac{u_l - u_k}{h}$

- **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

# Constructing Control Volumes in 1D

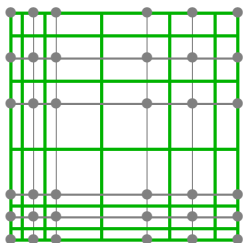
Let  $\Omega = (a, b)$  be subdivided into intervals by  $x_1 = a < x_2 < x_3 < \dots < x_{n-1} < x_n = b$ . Then we set

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



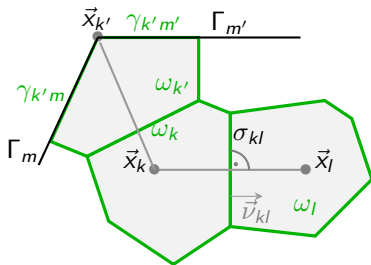
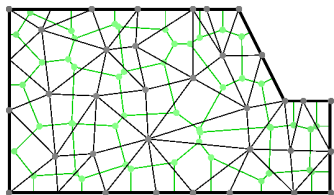
# Control Volumes for a 2D tensor product mesh

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



- 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 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: connected neighborhood graph of Voronoi cells
- Triangulation nodes  $\equiv$  collocation points
- 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  $\omega_k$ :

$$\begin{aligned} 0 &= \int_{\omega_k} \nabla \cdot \vec{j} \, d\omega - \int_{\omega_k} f \, d\omega \\ &= \int_{\partial\omega_k} \vec{j} \cdot \vec{n}_\omega \, ds - \int_{\omega_k} f \, d\omega \\ &= \sum_{l \in \mathcal{N}_k} \int_{\sigma_{kl}} \vec{j} \cdot \vec{\nu}_{kl} \, ds + \sum_{m \in \mathcal{G}_k} \int_{\gamma_{km}} \vec{j} \cdot \vec{n}_m \, ds - \int_{\omega_k} f \, d\omega \end{aligned}$$

# Approximation of flux between control volumes

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

- Admissibility condition  $\Rightarrow \vec{x}_k \vec{x}_l \parallel \nu_{kl}$
- Let  $u_k = u(\vec{x}_k)$ ,  $u_l = u(\vec{x}_l)$
- $h_{kl} = |\vec{x}_k - \vec{x}_l|$ : distance between neighboring collocation points
- Finite difference approximation of normal derivative:

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

$\Rightarrow$  flux between neighboring control volumes:

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

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

# Approximation of 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  $\Gamma_m$ :

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

## Approximation of right hand side

- $f_k = \frac{1}{|\omega_k|} \int_{\omega_k} f(\vec{x}) d\omega$
- Simple quadrature:  $f_k = f(\vec{x}_k)$

# Discrete system of equations

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

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

- Rewrite this as

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

with  $b_k = |\omega_k| f_k + \sum_{m \in \mathcal{G}_k} |\gamma_{km}| g$ ,

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

# 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**  $k, l = 1 \dots N$  **do**

  | set  $a_{kl} = 0$

**end**

**for**  $T \in \mathcal{T}$  **do**

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

$$\sigma = \sigma_{k_{T,j}, k_{T,i}} \cap T$$

$$s = \frac{|\sigma|}{h_{k_{T,j}, k_{T,i}}}$$

$$a_{k_{T,j}, k_{T,j}} + = \delta \sigma_h$$

$$a_{k_{T,j}, k_{T,i}} - = \delta \sigma_h$$

$$a_{k_{T,i}, k_{T,j}} - = \delta \sigma_h$$

$$a_{k_{T,i}, k_{T,i}} + = \delta \sigma_h$$

**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

```
for  $\gamma \in \mathcal{G}$  do  
  | for  $i = 1, 2$  do  
  | |  $a_{k_{\gamma_i}, k_{\gamma_i}} + = \alpha_{m_\gamma} |\gamma \cap \partial\omega_{k_{\gamma_i}}|$   
  | 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  
    |  $w_k + = |\omega_{k,\tau,j} \cap \tau|$   
    end  
  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

# Interpretation of results

- One solution value per control volume  $\omega_k$  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