## Chapter 4 <br> Finite Volume Methods

### 4.1 The Basic Idea

Finite volume methods (FVMs) are a discretization approach for partial differential equations that can be formulated in balance form. For the steadystate convection-diffusion-reaction equation (1.7) with homogeneous Dirichlet boundary conditions, the balance form is given by

$$
\begin{align*}
\nabla \cdot(-\varepsilon \nabla u+u \boldsymbol{b})+\sigma u & =f & & \text { in } \Omega, \\
u & =0 & & \text { on } \partial \Omega . \tag{4.1}
\end{align*}
$$

The derivation of FVMs starts by decomposing $\Omega$ into so-called control volumes $\left\{\omega_{i}\right\}_{i=1}^{n}$ (open sets) such that

$$
\bar{\Omega}=\bigcup_{i=1}^{n} \overline{\omega_{i}}, \quad \omega_{i} \cap \omega_{j}=\emptyset \text { for } i \neq j .
$$

Then, (4.1) is integrated on $\Omega$, integration by parts is applied to the first term on the left-hand side of (4.1) on each control volume. In this way, the balance equation (4.1) is transformed to an equation that involves the boundaries of the control volumes $\left\{\partial \omega_{i}\right\}_{i=1}^{n}$

$$
\begin{equation*}
\sum_{i=1}^{n}\left(\int_{\partial \omega_{i}}(-\varepsilon \nabla u+u \boldsymbol{b}) \cdot \boldsymbol{n}_{\omega_{i}} d \boldsymbol{s}+\int_{\omega_{i}} \sigma u d \boldsymbol{x}\right)=\sum_{i=1}^{n} \int_{\omega_{i}} f d \boldsymbol{x}, \tag{4.2}
\end{equation*}
$$

where $\boldsymbol{n}_{\omega_{i}}$ is the outward pointing unit normal on $\partial \omega_{i}$. The terms in the boundary integrals, the so-called fluxes, couple the balance laws of neighboring control volumes.

Note that (4.2) is satisfied if for each $i=1, \ldots, n$,

$$
\begin{equation*}
\int_{\partial \omega_{i}}(-\varepsilon \nabla u+u \boldsymbol{b}) \cdot \boldsymbol{n}_{\omega_{i}} d \boldsymbol{s}+\int_{\omega_{i}} \sigma u d \boldsymbol{x}=\int_{\omega_{i}} f d \boldsymbol{x} . \tag{4.3}
\end{equation*}
$$

In the case $\sigma=0$ in $\Omega$, (4.3) represents a local conservation property: the flux across $\partial \omega_{i}$ equals the sources in $\omega_{i}$. The main motivation of the construction of FVMs consists in transferring the local conservation property from the continuous problem to the discrete setting, thus constructing a physically consistent discretization in this respect. The corresponding discrete local conservation property is often of major importance in applications and it is the reason why these methods can be found in many software packages. To construct a FVM, one needs to

- define the decomposition of $\Omega$,
- define a discrete version of the fluxes,
- prescribe a quadrature rule for evaluating all integrals in (4.2).


### 4.2 Voronoi Box Finite Volume Methods

This section present one particular finite volume method. For defining this method, it is convenient to consider a triangulation from a special class. Then, the control volumes are constructed with the help of this triangulation.

Definition 4.1 (Delaunay triangulation). A triangulation $\mathcal{T}_{h}$ of $\Omega$ is called a Delaunay triangulation if, for every mesh cell $K \in \mathcal{T}_{h}$, the interior of its circumball does not contain any other vertex of the triangulation. This property is called (global) empty circumball (circumdisk) property.

In this course, only simplicial triangulations will be considered. Then, the Delaunay property is in two dimensions equivalent with the requirement that for each edge, which is not contained on the boundary, the sum of the two opposite angles is smaller than or equal to $\pi$.

Delaunay triangulations possess some optimality properties in $\mathbb{R}^{d}, d \geq 2$, see (Cheng et al., 2013, Section 4.3). For example, it is known, e.g., see Sibson (1978), (Edelsbrunner, 2001, p. 11), (Cheng et al., 2013, Theorem 2.8) that among all triangulations of the convex hull of a given set of points in $\mathbb{R}^{2}$, any Delaunay triangulation maximizes the minimal angle.

Closely connected to Delaunay triangulations are Voronoi boxes.
Definition 4.2 (Voronoi box, Voronoi region). Given a finite set $S$ of $n$ mutually different points in $\mathbb{R}^{d}, d \in\{2,3\}$. The Voronoi box or Voronoi region of a point $\boldsymbol{p} \in S$ is the set of all $\boldsymbol{x} \in \mathbb{R}^{d}$ that are closer to $\boldsymbol{p}$ than to any other point in $S$

$$
V_{\boldsymbol{p}}=\left\{\boldsymbol{x} \in \mathbb{R}^{d}:\|\boldsymbol{x}-\boldsymbol{p}\|_{2}<\|\boldsymbol{x}-\boldsymbol{q}\|_{2} \forall \boldsymbol{q} \in S \backslash\{\boldsymbol{p}\}\right\} .
$$

Remark 4.3 (Geometric properties of the Voronoi boxes). Consider first the case that $S$ contains two points. Then, the Voronoi box for each point is a
half space. In addition, the line connecting both points is perpendicular to the hyperplane (line in 2d, plane in 3d) between the half spaces. For the general case that $S$ contains $n$ mutually different points, one can deduce from the first property that the Voronoi box of every point $\boldsymbol{p} \in S$, which is given as the intersection of finitely many half spaces, is a convex polyhedron, which is possibly unbounded, with at most $n-1$ faces. If the polyhedron is bounded, then it is the convex hull of its vertices. The connecting line of the points that generate Voronoi boxes whose closure has a common face with a positive ( $d-1$ )-dimensional measure is perpendicular to the common face.

By definition, the intersection of two Voronoi boxes is empty. But each point $\boldsymbol{x} \in \mathbb{R}^{d}$ belongs at least to the closure of one Voronoi box. Thus, the closure of the Voronoi boxes covers the entire space $\mathbb{R}^{d}$. If a point $\boldsymbol{x}$ belongs to the closure of more than one Voronoi box, then it has the same distance to more than one point of $S$.

Given a domain $\Omega$ with polyhedral boundary, finite element methods can be defined on Delaunay triangulations and finite volume methods on a decomposition of $\Omega$ with Voronoi boxes. From the practical point of view, one starts with a Delaunay triangulation of $\Omega$ and constructs the Voronoi boxes. Consider a triangulation $\mathcal{T}_{h}$ of $\Omega$ into simplicial mesh cells and an arbitrary mesh cell $K \in \mathcal{T}_{h}$. If $\mathcal{T}_{h}$ is Delaunay, then the vertices of $K$ are the so-called generators of Voronoi boxes. The midpoint $\boldsymbol{m}_{K}$ of the closed circumball (circumdisk in 2d) $S_{K}$ of $K$ has the same distance from all vertices of $K$ (the notation circumball will be used in the following for all dimensions). Hence, $\boldsymbol{m}_{K}$ belongs to the closure of the Voronoi boxes of all vertices of $K$. There is no other vertex of the triangulation within $S_{K}$, since otherwise $\boldsymbol{m}_{K}$ would be closer to this vertex than to the vertices of $K$ and, consequently, $\boldsymbol{m}_{K}$ would not belong to the closure of the Voronoi boxes of the vertices of $K$.

In two dimensions, the midpoint of the circumball of a triangle is the crosspoint of the perpendicular bisectors. Connecting these crosspoints with the center of the edges, gives for each vertex of the grid a polygonal subdomain that contains the vertex. Equivalently, one can connect the crosspoints across edges. These polygonal subdomains are the Voronoi boxes, see Figure 4.1. With this construction, the edge and the corresponding part of the boundary of the Voronoi box are orthogonal. In three dimensions, the center of the circumball is the intersection of three bisector planes, or, which is equivalent of all bisector planes. A bisector plane contains the midpoint of an edge of the tetrahedron and it is orthogonal to this edge. Then, the Voronoi box around a vertex is a polyhedron whose vertices are the midpoints of the circumballs of the tetrahedra which contain this vertex and each face of the polyhedron is orthogonal to one of the edges where the vertex is an end point.


Fig. 4.1 Local grid with crosspoints of the perpendicular bisectors of the triangles (left), corresponding Voronoi box of the vertex in the center (right).

### 4.2.1 Derivation, Concrete Examples, Assumptions

Let $\Omega$ be a bounded domain with polyhedral boundary. Let a Delaunay triangulation $\mathcal{T}_{h}$, see Definition 4.1, of $\Omega$ be given with $n$ vertices $\left\{\boldsymbol{x}_{i}\right\}_{i=1}^{n}$, where the vertices are numbered such that the first $m<n$ vertices are in $\Omega$ or at the Neumann boundary and the last $n-m$ vertices are situated at the Dirichlet boundary. Then, $\Omega$ can be decomposed into Voronoi boxes $\left\{\omega_{i}\right\}_{i=1}^{n}$, which are the control volumes of the considered method. Hence, each control volume is associated to a vertex of the Delaunay triangulation, such that a so-called vertex-centered finite volume method is constructed.

The method is based on the formulation of the convection-diffusionreaction equation on the control volumes, which reads, compare (4.2),

$$
\begin{equation*}
\int_{\partial \omega_{i}}(-\varepsilon \nabla u+u \boldsymbol{b}) \cdot \boldsymbol{n}_{\omega_{i}} d \boldsymbol{s}+\int_{\omega_{i}} \sigma u d \boldsymbol{x}=\int_{\omega_{i}} f d \boldsymbol{x}, \quad i=1, \ldots, n . \tag{4.4}
\end{equation*}
$$

In Voronoi box finite volume methods, the degrees of freedom are the values of the function in the vertices of the Delaunay triangulation denoted by $u_{i}=$ $u_{h}\left(\boldsymbol{x}_{i}\right), i=1, \ldots, n$.

Now, all terms in (4.4) have to be approximated. For the volume integrals, a simple quadrature rule is used:

$$
\begin{gather*}
\int_{\omega_{i}} \sigma u d \boldsymbol{x} \approx \sigma\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right| u_{i}  \tag{4.5}\\
\int_{\omega_{i}} f d \boldsymbol{x} \approx f\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right| \tag{4.6}
\end{gather*}
$$

By construction, $\omega_{i}$ is a bounded polyhedron, see Remark 4.3. Denote the planar face between $\boldsymbol{x}_{i}$ and its neighbor $\boldsymbol{x}_{j}$ by $\partial \omega_{i j}$, see Figure 4.2 for a two-


Fig. 4.2 Notations in the derivation of the Voronoi box finite volume scheme.
dimensional sketch. The outward pointing unit normal with respect to $\omega_{i}$ is denoted by $\boldsymbol{n}_{i j}$. By construction of the Voronoi boxes, the connecting line $\boldsymbol{h}_{i j}=\boldsymbol{x}_{j}-\boldsymbol{x}_{i}$ is perpendicular to $\partial \omega_{i j}$, compare Remark 4.3, such that $\boldsymbol{n}_{i j}=$ $\boldsymbol{h}_{i j} /\left\|\boldsymbol{h}_{i j}\right\|_{2}$. The orthogonality of the planar faces of the control volumes and the connecting lines of the vertices of the mesh is a key property of Voronoi box finite volume methods.

Let $\boldsymbol{x}_{i j}$ be the intersection of $\partial \omega_{i j}$ and $\boldsymbol{h}_{i j}$ and let $\Lambda_{i}$ be the index set of the neighbors of $\boldsymbol{x}_{i}$ in $\mathcal{T}_{h}$. Note that $\boldsymbol{x}_{i j}$ is generally not the barycenter of $\partial \omega_{i j}$. Then, the integral on the boundary of the control volume is approximated also by a simple quadrature rule in the following way

$$
\begin{align*}
\int_{\partial \omega_{i}} & (-\varepsilon \nabla u+u \boldsymbol{b}) \cdot \boldsymbol{n}_{\omega_{i}} d \boldsymbol{s} \\
& =\sum_{j \in \Lambda_{i}}\left(\int_{\partial \omega_{i j}}(-\varepsilon \nabla u+u \boldsymbol{b}) \cdot \boldsymbol{n}_{i j} d \boldsymbol{s}\right) \\
& \approx \sum_{j \in \Lambda_{i}}\left(-\varepsilon \nabla u\left(\boldsymbol{x}_{i j}\right) \cdot \boldsymbol{n}_{i j}\left|\partial \omega_{i j}\right|+u\left(\boldsymbol{x}_{i j}\right) \int_{\partial \omega_{i j}} \boldsymbol{b} \cdot \boldsymbol{n}_{i j} d \boldsymbol{s}\right) \\
& =\sum_{j \in \Lambda_{i}}\left(-\varepsilon \nabla u\left(\boldsymbol{x}_{i j}\right) \cdot \boldsymbol{n}_{i j}+u\left(\boldsymbol{x}_{i j}\right) \beta_{i j}\right)\left|\partial \omega_{i j}\right|, \tag{4.7}
\end{align*}
$$

with

$$
\begin{equation*}
\beta_{i j}=\frac{1}{\left|\partial \omega_{i j}\right|} \int_{\partial \omega_{i j}} \boldsymbol{b} \cdot \boldsymbol{n}_{i j} d \boldsymbol{s}, \tag{4.8}
\end{equation*}
$$



Fig. 4.3 Degenerated situation with $\left|\partial \omega_{i j}\right|=0$ : two triangles forming a square.
if $\left|\partial \omega_{i j}\right|>0$. If $\partial \omega_{i j}$ is degenerated, see Figure 4.3 for such a situation, then it is set $\beta_{i j}=0$.

The term in parentheses is a flux given on the connecting line of $\boldsymbol{x}_{i}$ and $\boldsymbol{x}_{j}$, which has to be approximated. For this purpose, one can use a stable approximation for one-dimensional problems, namely a fitted upwind finite difference formula, see Definition 3.17. In the finite volume context, it is usual to write the schemes with the help of the signed local mesh Péclet number

$$
\begin{equation*}
\mathrm{Pe}_{i j}^{ \pm}=\frac{\beta_{i j}\left\|\boldsymbol{h}_{i j}\right\|_{2}}{2 \varepsilon} \in \mathbb{R}, \tag{4.9}
\end{equation*}
$$

since $\beta_{i j}$ might be an arbitrary real number. Then, the term in parentheses in the last line of (4.7) is approximated by using in addition a finite difference for the normal derivative and the arithmetic mean for the unknown value of $u$ in $\boldsymbol{x}_{i j}$

$$
\begin{equation*}
-\varepsilon \nabla u\left(\boldsymbol{x}_{i j}\right) \cdot \boldsymbol{n}_{i j}+u\left(\boldsymbol{x}_{i j}\right) \beta_{i j} \approx-\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right) \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\beta_{i j} \frac{u_{i}+u_{j}}{2} \tag{4.10}
\end{equation*}
$$

where $\kappa: \mathbb{R} \rightarrow \mathbb{R}^{+}$is the upwind function.
Example 4.4 (Simple upwind finite volume method). The fitting function for the simple upwind method is given by

$$
\begin{equation*}
\kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)=1+\left|\mathrm{Pe}_{i j}^{ \pm}\right|, \tag{4.11}
\end{equation*}
$$

see (3.13). Consider the case $\beta_{i j}>0$, i.e., the flux is from $\boldsymbol{x}_{i}$ to $\boldsymbol{x}_{j}$, then one gets with (4.10) the numerical flux

$$
\begin{aligned}
& -\varepsilon \kappa\left(\operatorname{Pe}_{i j}^{ \pm}\right) \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\beta_{i j} \frac{u_{i}+u_{j}}{2} \\
& =-\varepsilon \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\beta_{i j}\left(-\varepsilon \frac{\left\|\boldsymbol{h}_{i j}\right\|_{2}}{2 \varepsilon} \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\frac{u_{i}+u_{j}}{2}\right)=-\varepsilon \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\beta_{i j} u_{i} .
\end{aligned}
$$

Analogously, one obtains for $\beta_{i j}<0$

$$
-\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right) \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\beta_{i j} \frac{u_{i}+u_{j}}{2}=-\varepsilon \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\beta_{i j} u_{j} .
$$

In both cases, only the upwind node contributes to the discretization of the convective term.

Example 4.5 (Exponentially fitted finite volume method, Scharfetter-Gummel $F V M$ ). The derivation of the exponentially fitted finite volume method is based on the Iljin-Allen-Southwell scheme from Definition 3.18. Here, the fitting function is

$$
\begin{equation*}
\kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)=\mathrm{Pe}_{i j}^{ \pm} \operatorname{coth}\left(\mathrm{Pe}_{i j}^{ \pm}\right) . \tag{4.12}
\end{equation*}
$$

Note that

$$
\begin{equation*}
\operatorname{coth}(x)=1+\frac{2}{\exp (2 x)-1}, \quad x \operatorname{coth}(x)=(-x) \operatorname{coth}(-x) \quad \forall x \in \mathbb{R} \tag{4.13}
\end{equation*}
$$

Inserting the fitting function in (4.10) and using (4.9) and (4.13) yields

$$
\begin{aligned}
& -\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right) \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\beta_{i j} \frac{u_{i}+u_{j}}{2} \\
& =\varepsilon\left(-\mathrm{Pe}_{i j}^{ \pm} \operatorname{coth}\left(\mathrm{Pe}_{i j}^{ \pm}\right) \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\mathrm{Pe}_{i j}^{ \pm} \frac{u_{j}+u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}\right) \\
& =\frac{\varepsilon}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}\left[\left(\mathrm{Pe}_{i j}^{ \pm}+\mathrm{Pe}_{i j}^{ \pm} \operatorname{coth}\left(\mathrm{Pe}_{i j}^{ \pm}\right)\right) u_{i}-\left(-\mathrm{Pe}_{i j}^{ \pm}+\mathrm{Pe}_{i j}^{ \pm} \operatorname{coth}\left(\mathrm{Pe}_{i j}^{ \pm}\right)\right) u_{j}\right] \\
& =\frac{\varepsilon}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}\left[\left(\mathrm{Pe}_{i j}^{ \pm}-\mathrm{Pe}_{i j}^{ \pm} \operatorname{coth}\left(-\mathrm{Pe}_{i j}^{ \pm}\right)\right) u_{i}-\left(-\mathrm{Pe}_{i j}^{ \pm}+\mathrm{Pe}_{i j}^{ \pm} \operatorname{coth}\left(\mathrm{Pe}_{i j}^{ \pm}\right)\right) u_{j}\right] \\
& =\frac{\varepsilon}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}\left[\frac{-2 \mathrm{Pe}_{i j}^{ \pm}}{\exp \left(-2 \mathrm{Pe}_{i j}^{ \pm}\right)-1} u_{i}-\frac{2 \mathrm{Pe}_{i j}^{ \pm}}{\exp \left(2 \mathrm{Pe}_{i j}^{ \pm}\right)-1} u_{j}\right] .
\end{aligned}
$$

In the literature, this formula is often expressed in terms of the Bernoulli function ${ }^{1}$

$$
B(x)= \begin{cases}\frac{x}{\exp (x)-1}, & x \in \mathbb{R} \backslash\{0\}, \\ 1, & x=0,\end{cases}
$$

[^0]as
$$
-\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right) \frac{u_{j}-u_{i}}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\beta_{i j} \frac{u_{i}+u_{j}}{2}=\frac{\varepsilon}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}\left(B\left(-2 \mathrm{Pe}_{i j}^{ \pm}\right) u_{i}-B\left(2 \mathrm{Pe}_{i j}^{ \pm}\right) u_{j}\right)
$$

Note that $B(x)>0$ for $x \in \mathbb{R}$ and the fitted upwind function can be expressed, using (4.13), as

$$
\kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)=\mathrm{Pe}_{i j}^{ \pm}+B\left(2 \mathrm{Pe}_{i j}^{ \pm}\right) .
$$

Inserting the approximations (4.5), (4.6), and (4.10) in (4.4) gives the Voronoi box finite volume method

$$
\begin{align*}
\sum_{j \in \Lambda_{i}}\left(-\frac{\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}\right. & \left.\left(u_{j}-u_{i}\right)+\frac{\beta_{i j}}{2}\left(u_{i}+u_{j}\right)\right)\left|\partial \omega_{i j}\right|+\sigma\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right| u_{i} \\
& =f\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right|, \quad i=1, \ldots, m  \tag{4.14}\\
u_{i} & =0, \quad i=m+1, \ldots n .
\end{align*}
$$

After having derived the basic scheme (4.14), several assumptions are necessary for performing the numerical analysis. First, an assumptions on $\beta_{i j}$ is formulated.

Remark 4.6 (Assumption with respect to $\beta_{i j}$ ).
A1 Skew symmetry. It holds that

$$
\begin{equation*}
\beta_{i j}+\beta_{j i}=0 \quad \forall i, j . \tag{4.15}
\end{equation*}
$$

In view of definition (4.8) of $\beta_{i j}$, this assumption is natural since $\boldsymbol{n}_{i j}=$ $-\boldsymbol{n}_{j i}$.

With Assumption A1, it follows from (4.9) that

$$
\begin{equation*}
P e_{i j}^{ \pm}=-P e_{j i}^{ \pm} \tag{4.16}
\end{equation*}
$$

Next, assumptions on the fitted upwind function are given.
Remark 4.7 (Assumptions on the fitted upwind function). Let $\kappa: \mathbb{R} \rightarrow \mathbb{R}_{+}$ be the fitted upwind function.
A2 Symmetry. It holds that

$$
\begin{equation*}
\kappa(0)=1, \quad \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)=\kappa\left(P e_{j i}^{ \pm}\right) . \tag{4.17}
\end{equation*}
$$

A3 Bound. It is assumed that

$$
\begin{equation*}
\kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)>\left|P e_{i j}^{ \pm}\right| \tag{4.18}
\end{equation*}
$$

Remark 4.8 (Satisfaction of Assumptions A2 and A3 for the simple upwind and Scharfetter-Gummel FVM).

- Assumption A2. Clearly, (4.17) is satisfied for the simple upwind function (4.11).

The first property of (4.17) follows for the fitted upwind function (4.12) of the Scharfetter-Gummel scheme from

$$
\begin{equation*}
\lim _{x \rightarrow 0+} x \operatorname{coth}(x)=1 \tag{4.19}
\end{equation*}
$$

Using (4.13), one finds that this function also satisfies the second property of (4.17).

- Assumption A3. Again, the satisfaction of (4.18) for the simple upwind function (4.11) is clear.
The satisfaction of (4.18) for the Scharfetter-Gummel scheme follows from

$$
x \operatorname{coth}(x)>x \quad \forall x>0
$$

for $P e_{i j}^{ \pm}>0$, from (4.19) for $P e_{i j}^{ \pm}=0$, and from (4.13) for $P e_{i j}^{ \pm}<0$.
Hence, both the fitted upwind functions of the simple upwind FVM and the Scharfetter-Gummel FVM satisfy Assumptions A2 and A3.

Finally, assumptions on the grid are necessary.
Remark 4.9 (Assumptions on the triangulation).
A4 Delaunay property. The domain $\Omega$ is decomposed by a Delaunay triangulation. A decomposition of this kind is the basis of the derivation of method (4.14).
A5 Connectivity of the inner nodes. Let $\omega_{h}$ denote the set of the inner nodes, then it is assumed that for all $\boldsymbol{x}_{\mathrm{a}}, \boldsymbol{x}_{\mathrm{b}} \in \omega_{h}$ there exist $\boldsymbol{x}_{1}, \ldots, \boldsymbol{x}_{m} \in \omega_{h}$ with $\left|\partial \omega_{a 1}\right|>0,\left|\partial \omega_{12}\right|>0, \ldots,\left|\partial \omega_{m b}\right|>0$.
This assumption implies that there are non-vanishing off-diagonal entries between subsequent nodes in this sequence. It follows the irreducibility of the matrix $A^{\mathrm{i}} \in \mathbb{R}^{m \times m}$, which is the restriction of the full matrix to the inner nodes.

### 4.2.2 Discrete Local Conservation Property, DMP, Existence and Uniqueness of a Solution

Lemma 4.10 (Local discrete conservation property). Let $\sigma=0$ in $\Omega$ and let Assumptions A1, A2, and $\boldsymbol{A} 4$ be satisfied. Denote the discrete flux from $\boldsymbol{x}_{i}$ to $\boldsymbol{x}_{j}$ across $\partial \omega_{i j}$ by

$$
f_{i j}=\left(-\frac{\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}\left(u_{j}-u_{i}\right)+\frac{\beta_{i j}}{2}\left(u_{i}+u_{j}\right)\right)\left|\partial \omega_{i j}\right|
$$

Then, for any connected volume $\omega=\cup_{i=1}^{I} \omega_{i} \subset \Omega$, where $\omega_{i}$ are control volumes, the discrete flux across $\partial \omega$ equals the sum of the sinks and sources in $\omega$.

Proof. The boundary of $\omega$ is the union of certain facets of control volumes $\partial \omega=\cup_{k=1}^{K} \partial \omega_{k *}$ and the discrete flux trough this boundary is given by $\sum_{k=1}^{K} f_{k *}$. By Assumptions A1 and A2, it follows that for all facets of control volumes that do not belong to the boundary of $\omega$, it holds that $f_{i j}=-f_{j i}$. Hence, one obtains with (4.14)

$$
\sum_{k=1}^{K} f_{k *}=\sum_{i=1}^{I} \sum_{j \in \Lambda_{i}} f_{i j}=\sum_{i=1}^{I} f\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right|
$$

which is the statement of the lemma.
Theorem 4.11 (Global DMP for method (4.14)). Let Assumptions A1, $\boldsymbol{A 2}, \boldsymbol{A} 3, \boldsymbol{A} 4$, and $\boldsymbol{A} 5$ be satisfied. Let $\nabla \cdot \boldsymbol{b} \geq 0$ and $\sigma \geq 0$ in $\Omega$. Then, the matrix of method (4.14) is an M-matrix and the finite volume discretization satisfies the global DMP.

Proof. The diagonal entries of the matrix that are obtained with scheme (4.14) are

$$
a_{i i}=\sum_{j \in \Lambda_{i}}\left(\frac{\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\frac{\beta_{i j}}{2}\right)\left|\partial \omega_{i j}\right|+\sigma\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right|, \quad i=1, \ldots, m .
$$

By assumption, the second term on the right-hand side is non-negative. A sufficient condition for the positivity of the first term is that for all $j \in \Lambda_{i}$

$$
\frac{\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\frac{\beta_{i j}}{2}>0 \Longleftrightarrow \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)>-\frac{\beta_{i j}\left\|\boldsymbol{h}_{i j}\right\|_{2}}{2 \varepsilon}=-\mathrm{Pe}_{i j}^{ \pm}
$$

where the definition (4.9) of the signed Péclet number was used. With Assumption A3, the inequality on the right-hand side is satisfied.

The off-diagonal entries, which belong to the sparsity pattern of the matrix, because $\boldsymbol{x}_{i}$ and $\boldsymbol{x}_{j}$ are neighboring nodes, have the form

$$
a_{i j}=\left(-\frac{\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)}{\left\|\boldsymbol{h}_{i j}\right\|_{2}}+\frac{\beta_{i j}}{2}\right)\left|\partial \omega_{i j}\right| .
$$

They are negative, if $\left|\partial \omega_{i j}\right|>0$ and

$$
\frac{\beta_{i j}}{2}<\frac{\varepsilon \kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)}{\left\|\boldsymbol{h}_{i j}\right\|_{2}} \Longleftrightarrow \mathrm{Pe}_{i j}^{ \pm}=\frac{\beta_{i j}\left\|\boldsymbol{h}_{i j}\right\|_{2}}{2 \varepsilon}<\kappa\left(\mathrm{Pe}_{i j}^{ \pm}\right)
$$

which follows again from Assumption A3.
For the row sums of the inner nodes, with respect to the whole system matrix, one obtains with definition (4.8) of $\beta_{i j}$ and integration by parts

$$
\begin{aligned}
r_{i} & =a_{i i}+\sum_{j \in \Lambda_{i}} a_{i j}=\sum_{j \in \Lambda_{i}} \beta_{i j}\left|\partial \omega_{i j}\right|+\sigma\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right| \\
& =\int_{\partial \omega_{i}} \boldsymbol{b} \cdot \boldsymbol{n}_{\omega_{i}} d \boldsymbol{s}+\sigma\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right|=\int_{\omega_{i}} \nabla \cdot \boldsymbol{b} d \boldsymbol{x}+\sigma\left(\boldsymbol{x}_{i}\right)\left|\omega_{i}\right|, \quad i=1, \ldots, m .
\end{aligned}
$$

By the assumption of the theorem, the row sums are non-negative. Restricting the columns to the inner nodes, such that the matrix $A^{i} \in \mathbb{R}^{m} \times \mathbb{R}^{m}$ of the inner nodes is considered, there will be even at least one positive row sum, since the off-diagonal entries that connect the boundary nodes and the inner nodes are negative by a previous part of the proof. Because of the assumed connectivity of the inner nodes via non-degenerated parts of boundaries of the control volumes, the matrix of the inner nodes is irreducible and therefore, see Remark 5.22 below, it is an M-matrix. From Corollary 5.18, it follows that the full matrix is an M-matrix, too, and Theorem 5.14 gives finally the satisfaction of the DMP.

Corollary 4.12 (Existence and uniqueness of a solution for method (4.14)). Let the assumptions of Theorem 4.11 be satisfied, then method (4.14) possesses a unique solution.

Proof. Method (4.14) leads to an M-matrix, which is non-singular, and thus the linear system of equations has a unique solution.


[^0]:    ${ }^{1}$ The Bernoulli numbers appear in the series expansion of this function.

