Chapter 3
Finite Difference Methods (FDM)

3.1 Notations, General Properties

The basic idea of finite difference methods (FDMs) consists in approximating the derivatives of a partial differential equation with appropriate finite differences. This approach will be explained in one dimension. Basic FDMs in multiple dimensions are tensor product applications of the one-dimensional approach, compare Numerical Mathematics III.

Let the domain $\Omega = (a, b)$ be decomposed with a mesh consisting of grid points or nodes $\{x_i\}_{i=1}^n$ with $x_i < x_{i-1}$, $i = 1, \ldots, n$, $x_1 = a$, $x_n = b$, and let

$$h_i = x_i - x_{i-1}, \quad i = 2, \ldots, n, \quad h = \max_{i=2,\ldots,n} h_i.$$

Definition 3.1 (Grid function). A vector $\underline{v}_h = (v_1, \ldots, v_n)^T \in \mathbb{R}^n$, which assigns to each node a value, is called grid function. The restriction of a function $v \in C(\overline{\Omega})$ to a grid function is denoted by $R_h v$, i.e., $R_h v := (v(x_1), v(x_2), \ldots, v(x_n))^T$. $\Box$

Definition 3.2 (Finite difference operators). Let $v(x)$ be a sufficiently smooth function and denote $v_i = v(x_i)$, where x_i are the nodes of the grid. Then, following difference quotients (finite differences) are defined:

- forward difference
$$D^+ v(x_i) = \frac{v_{i+1} - v_i}{h_{i+1}},$$
- backward difference
$$D^- v(x_i) = \frac{v_i - v_{i-1}}{h_i},$$
- central difference
$$D^0 v(x_i) = \frac{v_{i+1} - v_{i-1}}{h_i + h_{i+1}},$$
- second order difference: let $\tilde{h}_i := (h_i + h_{i+1})/2$,

$$D^+D^-(v)(x_i) = \frac{1}{\tilde{h}_i}\left(D^+v(x_i) - D^-v(x_i)\right) = \frac{1}{\tilde{h}_i}\left(\frac{v_{i+1}-v_i}{h_{i+1}} - \frac{v_i - v_{i-1}}{h_i}\right). \tag{3.1}$$

On an equidistant grid, the second order difference simplifies to

$$D^+D^-(v)(x_i) = \frac{v_{i+1} - 2v_i + v_{i-1}}{h^2}.$$

□

Definition 3.3 (Consistency of a finite difference operator, discrete maximum norm). Let $\mathcal{A}$ be a differential operator. The finite difference operator $A_h : \mathbb{R}^n \to \mathbb{R}^n$ is said to be consistent with $\mathcal{A}$ of order k if for all sufficiently smooth functions v

$$\max_{1\le i\le n} |(\mathcal{A}v)(x_i) - (A_h R_h v)_i| =: \|\mathcal{A}v - A_h R_h v\|_{\infty,h} = \mathcal{O}\left(h^k\right).$$

Here, $\|\cdot\|_{\infty,h}$ is the discrete maximum norm in the space of grid functions. □

The order of consistency of a finite difference operator is usually determined with a Taylor series expansion. For an equidistant grid, $h = h_i$ for all i, one finds that the finite difference operators $D^+v(x_i), D^-v(x_i), D^0v(x_i)$ are consistent to $\mathcal{A} = \frac{d}{dx}$ of first, first, and second order, respectively. From the Taylor series expansion for the second order difference operator (3.1)

$$v''(x_i) - D^+D^-(v)(x_i) = -\frac{1}{3}(h_{i+1} - h_i)v'''(x_i) + \mathcal{O}\left(\tilde{h}_i^2\right),$$

one concludes that this approximation is of first order for $h_i \neq h_{i+1}$ and of second order for $h_i = h_{i+1}$.

Consider now a linear partial differential equation $\mathcal{A}u = f$ and a linear finite difference approximation of the form

$$A_h \underline{u}_h := R_h(\mathcal{A}u) = R_h(f) = \underline{f}_h \tag{3.2}$$

on an equidistant grid. The boundary conditions should be integrated in this scheme by corresponding rows in A_h.

Definition 3.4 (Consistency of a difference scheme and order of consistency). The scheme (3.2) is called consistent of order k in the discrete maximum norm, if

$$\|A_h R_h v - R_h(\mathcal{A}v)\|_{\infty,h} = \mathcal{O}\left(h^k\right)$$

for all sufficiently smooth functions v, where the non-negative constant k is independent of h. □

The consistency measures the difference of applying first the grid function operator and then the finite difference operator to applying first the differential operator and then the grid function operator.

Definition 3.5 (Stability of a difference scheme or finite difference operator). A finite difference scheme or finite difference operator is called stable in the discrete maximum norm, if there is a stability constant C_{S}, which is independent of h, such that

$$\|\underline{v}_h\|_{\infty,h} \le C_{\mathrm{S}} \|A_h \underline{v}_h\|_{\infty,h} \tag{3.3}$$

for all grid functions $\underline{v}_h$. □

Definition 3.6 (Convergence of a difference scheme and order of convergence). The finite difference scheme (3.2) is convergent of order k in the discrete maximum norm, if there are is a positive constant k, which is independent of h, such that

$$\|\underline{u}_h - R_h u\|_{\infty,h} = \mathcal{O}\left(h^k\right).$$

□

Theorem 3.7 (Consistency + stability $\Longrightarrow$ convergence). *A consistent and stable finite difference scheme is convergent. The orders of consistency and convergence are the same.*

Proof. It is

$$\begin{aligned}
\|\underline{u}_h - R_h u\|_{\infty,h} &\overset{\text{stab.}}{\le} C_{\mathrm{S}} \|A_h(\underline{u}_h - R_h u)\|_{\infty,h} \overset{\text{lin.}}{=} C_{\mathrm{S}} \|A_h\underline{u}_h - A_h R_h u\|_{\infty,h} \\
&= C_{\mathrm{S}} \left\|\underline{f}_h - A_h R_h u\right\|_{\infty,h} = C_{\mathrm{S}} \|R_h f - A_h R_h u\|_{\infty,h} \\
&= C_{\mathrm{S}} \|R_h(\mathcal{A}u) - A_h R_h u\|_{\infty,h} \overset{\text{cons.}}{\le} Ch^k,
\end{aligned}$$

where the constant C is the product of the constants from the stability and consistency condition. ■

In practice, one often has very small diffusion. Therefore it is important to construct numerical methods that provide accurate results in this case.

Definition 3.8 (Uniform or robust convergence). A finite difference scheme for the solution of (1.7) is called uniformly or robustly convergent of order p with respect to the diffusion coefficient ε in the discrete maximum norm if an estimate of the form

$$\|R_h u - u_h\|_{\infty,h} \le Ch^p, \quad p > 0, \tag{3.4}$$

holds with a constant C that does not depend on ε, where u_h is the solution of the finite difference scheme. □

Uniform convergence is a desirable but very strong concept.

Lemma 3.9 (FDM leading to an M-matrix is stable). *Let $A \in \mathbb{R}^{n\times n}$ be the matrix that is obtained from a finite difference discretization of* (1.7). *If A is an M-matrix, then the discretization is stable in the sense of Definition 3.5.*

Proof. Take an arbitrary grid function v_h, then it holds that

$$\|v_h\|_{\infty,h} = \left\|A^{-1}Av_h\right\|_{\infty,h} \le \left\|A^{-1}\right\|_{\infty} \|Av_h\|_{\infty,h}.$$

Since A is an M-matrix, there is a majorizing element w_h, see Remark 5.24 below, and estimate (5.29) holds. Consequently, one obtains a bound for the stability constant

$$C_{\mathrm{S}} \le \frac{\|w_h\|_{\infty,h}}{\min_{j=1,\ldots,n}\left(Aw_h\right)_j}.$$

■

3.2 The One-Dimensional Case

Let, without loss of generality, $\Omega = (0,1)$. Then, the model problem of a one-dimensional convection-diffusion-reaction equation that will be considered is the two-point boundary value problem

$$\mathcal{A}u := -\varepsilon u'' + b(x)u' + \sigma(x)u = f(x), \quad x \in (0,1), \quad u(0) = u(1) = 0, \tag{3.5}$$

with $\varepsilon > 0$. It will be assumed that the coefficient functions b, σ, f are sufficiently smooth and that $\sigma(x) \ge 0$ for all $x \in [0,1]$. With respect to the convection, it is assumed that it has the same sign in the whole interval, i.e., concretely that $|b(x)| \ge \beta > 0$ for all $x \in [0,1]$. The presentation will be mostly for the case that $b(x) > 0$ in $[0,1]$.

Example 3.10 (Standard 1d model problem). The boundary value problem

$$-\varepsilon u'' + u' = 1 \quad \text{in } (0,1), \quad u(0) = u(1) = 0,$$

will serve as a model problem. It has the solution

$$u(x) = x - \frac{\exp\left(-\frac{1-x}{\varepsilon}\right) - \exp\left(-\frac{1}{\varepsilon}\right)}{1 - \exp\left(-\frac{1}{\varepsilon}\right)}. \tag{3.6}$$

The smaller the coefficient ε, the steeper becomes the solution at the right boundary layer, see Figure 3.1. □

If not mentioned otherwise, a decomposition of Ω with an equidistant grid ω_h with $n-1$ intervals, mesh width $h = 1/(n-1)$ and nodes $x_i = (i-1)h$, $i = 1, \ldots, n$, will be considered. Function values in the node x_i will be denoted with the subscript i, e.g., $b(x_i) = b_i$.

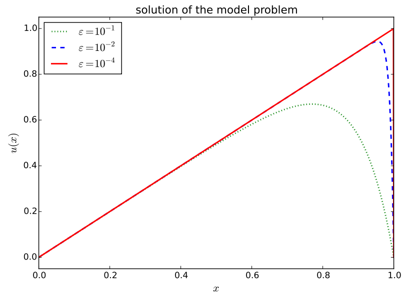

Fig. 3.1 Solution of Example 3.10 for different values of ε.

Definition 3.11 (Local mesh Péclet number). The measure that connects the ratio of convection and diffusion with the mesh size is called local mesh Péclet number

$$\mathrm{Pe}(x) = \frac{|b(x)|\, h}{2\varepsilon}. \tag{3.7}$$

Also the local mesh Péclet numbers will be denoted in the same way as the other functions, i.e., $\mathrm{Pe}(x_i) = \mathrm{Pe}_i$. □

Definition 3.12 (Central finite difference scheme). The central finite difference scheme for (3.5) has the form

$$\begin{aligned} (A_h u_h)_i := -\varepsilon D^+ D^- u_i + b_i D^0 u_i + \sigma_i u_i &= f_i, \quad \text{for } i = 2, \ldots, n-1, \\ u_1 = u_n &= 0, \end{aligned} \tag{3.8}$$

with $u_h = (u_1, u_2, \ldots, u_n)^T$. □

The central difference scheme leads to a tridiagonal system of linear equations

$$a_{i,i-1} u_{i-1} + a_{ii} u_i + a_{i,i+1} u_{i+1} = f_i, \quad i = 2, \ldots, n-1, \quad u_1 = u_n = 0, \tag{3.9}$$

with, for $b(x) > 0$,

$$\begin{aligned} a_{i,i-1} &= -\frac{\varepsilon}{h^2} - \frac{b_i}{2h} = \frac{\varepsilon}{h^2}\left(-1 - Pe_i\right), \quad a_{ii} = \sigma_i + \frac{2\varepsilon}{h^2}, \\ a_{i,i+1} &= -\frac{\varepsilon}{h^2} + \frac{b_i}{2h} = \frac{\varepsilon}{h^2}\left(-1 + Pe_i\right). \end{aligned} \tag{3.10}$$

Remark 3.13 (Failure of the central finite difference scheme in the convection-dominated case). It was found in an exercise problem, that for a special situation, the linear systems of the central finite difference scheme and the Galerkin finite element method coincide. In general, the arising system are not identical, but the behavior of both discretizations is still quite similar. In particular, in the convection-dominated case and on coarse grids, numerical solutions are in general globally polluted with spurious oscillations. □

A possible way to think about the improvement of the central difference scheme consists in modifying this scheme such that the sign condition on the off-diagonal entries in Definition 5.18 of an M-matrix is satisfied, i.e., that $a_{i,i+1} \le 0$ for $b_i > 0$ independently of ε. From (3.10), it can be seen that the positive part of $a_{i,i+1}$ comes only from the discretization of the convective term. Hence, $a_{i,i+1} \le 0$ is achieved by utilizing a discretization of this term that does not use a contribution from the node x_{i+1}.

Definition 3.14 (Simple upwind scheme). The simple upwind scheme for the two-point boundary value problem (3.5) has the form

$$\begin{aligned} -\varepsilon D^+D^-u_i + b_i D^{\mathcal{N}} u_i + \sigma_i u_i &= f_i, \quad \text{for } i = 2, \ldots, n-1, \\ u_1 = u_n &= 0, \end{aligned} \tag{3.11}$$

with

$$D^{\mathcal{N}} := \begin{cases} D^+ & \text{for } b_i < 0, \\ D^- & \text{for } b_i > 0. \end{cases}$$

□

In the upwind scheme, the finite difference approximation of the convective term is computed with values from the upwind direction. For convection-dominated problems, the transport of information occurs in the direction of convection. Hence, the upwind direction is the direction from which information is coming.

In the simple upwind scheme, the second order approximation D^0 is replaced by the first order approximation D^+ or D^-. This reduced order can be observed in the accuracy of the numerical results.

Let A be the matrix of the simple upwind scheme after having eliminated the boundary values u_1 and u_n. This matrix is tridiagonal with the entries

$$\begin{aligned} a_{i,i-1} &= -\frac{\varepsilon}{h^2} - \frac{1}{h}\max\{0, b_i\}, \quad a_{ii} = \sigma_i + \frac{2\varepsilon}{h^2} + \frac{1}{h}\left|b_i\right|, \\ a_{i,i+1} &= -\frac{\varepsilon}{h^2} + \frac{1}{h}\min\{0, b_i\}. \end{aligned} \tag{3.12}$$

One can see that all diagonal entries are positive and all non-diagonal entries non-negative, independently of the size of ε and h. Hence, this matrix satisfies the requirement on the off-diagonal entries from Definition 5.18.

Remark 3.15 (Properties of the simple upwind scheme). One can prove that the matrix of the simple upwind scheme is in fact an M-matrix and therefore it is stable, compare Lemma 3.9. It converges of first order outside layers. Inside layers, there is no convergence as long as $h \ge \varepsilon$. This behavior is not desirable. □

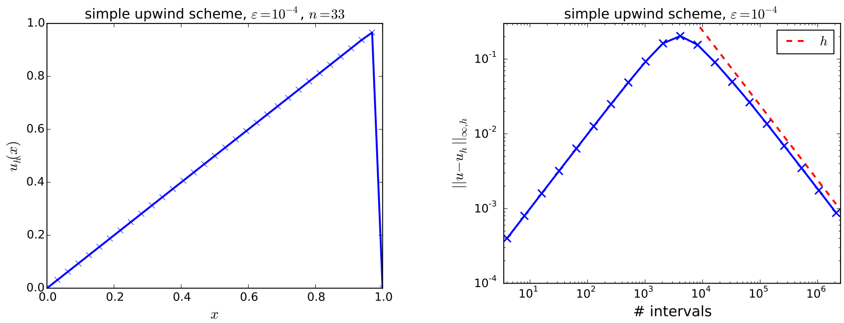

Fig. 3.2 Example 3.16. Numerical results for the simple upwind scheme.

Example 3.16 (Simple upwind scheme). The behavior of the simple upwind scheme is illustrated with results that are obtained for the numerical solution of Example 3.10, see Figure 3.2. On the one hand, one can see that reasonable results are computed on coarse grids. On the other hand, the error in the discrete maximum norm increases until the grid becomes sufficiently fine, as it is mentioned above. For sufficiently fine grids, one can observe first order convergence. □

The difficulties in the numerical solution of convection-dominated problems originate from the different magnitudes of diffusion and convection, and caused by this issue, of the appearance of sharp (thin) layers. From this observation, it follows that the numerical solution becomes the simpler, the larger the diffusion becomes, compared with the convection.

Consider $b > 0$, then it is

$$\begin{aligned} b_i D^{\mathcal{N}} u_i &= b_i D^- u_i = b_i \frac{u_i - u_{i-1}}{h} = b_i \frac{u_{i+1} - u_{i-1}}{2h} + b_i \frac{-u_{i+1} + 2u_i - u_{i-1}}{2h} \\ &= b_i D^0 u_i - \frac{b_i h}{2} D^+ D^- u_i. \end{aligned}$$

Hence, the simple upwind scheme (3.11) can be written in the form

$$\begin{aligned} -\left(\varepsilon + \frac{b_i h}{2}\right) D^+ D^- u_i + b_i D^0 u_i + \sigma_i u_i = f_i, \quad \text{for } i = 2, \ldots, n-1, \\ u_1 = u_n = 0. \end{aligned} \tag{3.13}$$

One can see that the diffusion coefficient is artificially increased and it has the magnitude $\mathcal{O}(h)$. Consequently, the simple upwind scheme is nothing else than a central difference scheme applied to a problem with sufficiently large, $\mathcal{O}(h)$, diffusion.

One can define methods with artificial diffusion, so-called fitted upwind schemes, also directly.

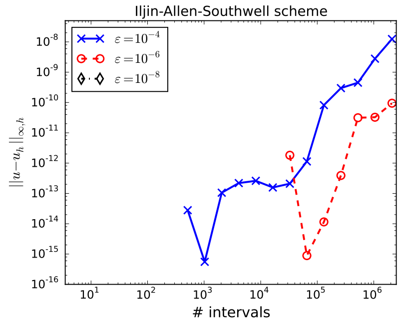

Fig. 3.3 Example 3.19. Numerical results for the Iljin–Allen-Southwell finite difference scheme; missing markers indicate that the error is zero.

Definition 3.17 (Fitted upwind scheme). A fitted upwind finite difference scheme is defined by

$$-\varepsilon\kappa\left(\mathrm{Pe}_i\right)D^+D^-u_i + b_iD^0u_i + \sigma_iu_i = f_i, \quad \text{for } i = 2,\ldots,n-1,$$
$$u_1 = u_n = 0, \tag{3.14}$$

where Pe_i is the local mesh Péclet number defined in (3.7) and $\kappa : \mathbb{R}_0^+ \to \mathbb{R}^+$ is an appropriate function, called upwind function. □

The simple upwind scheme (3.11) is obtained for $\kappa(\mathrm{Pe}_i) = 1 + \mathrm{Pe}_i$, see (3.13). More sophisticated considerations show that the following scheme is in a certain sense an optimal fitted upwind scheme.

Definition 3.18 (Iljin scheme, Iljin–Allen–Southwell scheme). Consider the case $b(x) \geq \beta > 0$. The finite difference scheme

$$-\varepsilon\mathrm{Pe}_i\coth\left(\mathrm{Pe}_i\right)D^+D^-u_i + b_iD^0u_i + \sigma_iu_i = f_i, \quad \text{for } i = 2,\ldots,n-1,$$
$$u_1 = u_n = 0, \tag{3.15}$$

is called Iljin scheme or Iljin–Allen–Southwell (Il'in (1969); Allen & Southwell (1955)) scheme. In some applications it is called also Scharfetter–Gummel scheme (Scharfetter & Gummel (1969)). □

For this scheme, uniform convergence of first order can be proved.

Example 3.19 (Iljin–Allen–Southwell scheme). Results obtained with the Iljin–Allen–Southwell scheme for the numerical solution of Example 3.10 are displayed in Figure 3.3. It can be seen that the error vanishes pointwise if the grid is sufficiently coarse in comparison with the diffusion. If the grids become finer, an increase of the error can be observed, but the errors are still very small. □