

On the Sharpness of Error Bounds for the Numerical Solution of Initial Boundary Value Problems by Finite Difference Schemes

H. Esser, St. J. Goebbels and R. J. Nessel

Abstract. The present paper studies the sharpness of error bounds obtained for approximate solutions of initial boundary value problems by finite difference schemes. Whereas the direct estimates in terms of partial moduli of continuity for partial derivatives of the (exact) solutions follow by standard methods (stability inequality plus Taylor expansion of the truncation error), the sharpness of these bounds is established by an application of a quantitative extension of the uniform boundedness principle. To verify the relevant resonance condition a general procedure is suggested, in contrast to our previous investigations which were based on rather specific properties of the discrete Green's functions associated. Exemplarily, details are worked out in connection with Crank-Nicolson, Du Fort-Frankel and Saul'yev schemes.

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1. Introduction

The initial boundary value problems to be discussed are given via (with $a < b$ for $a, b \in \mathbb{R}$, the real axis)

$$\begin{aligned} Lu(x, t) &= \varphi(x, t) & \text{for } (x, t) \in \Omega &= \{(x, t) : a < x < b, t \geq 0\} \\ u(x, t) &= \psi_0(x, t) & \text{for } (x, t) \in \Gamma_0 &= \{(x, t) : a < x < b, t = 0\} \\ u(x, t) &= \psi_1(x, t) & \text{for } (x, t) \in \Gamma_1 &= \{(x, t) : x \in \{a, b\}, t \geq 0\} \end{aligned} \quad (1.1)$$

where L is a linear (parabolic) differential operator and the data φ , ψ_0 and ψ_1 are real-valued functions defined on Ω , Γ_0 and Γ_1 , respectively. It is important to note that we only discuss those problems (1.1) for which solutions u not only exist but indeed belong to appropriate Banach spaces $C^{(r,s)}(\bar{\Omega})$ of real-valued functions on $\bar{\Omega} = \Omega \cup \Gamma_1$ which possess continuous partial derivatives of order $r \in \mathbb{N}_0$ ($:= \mathbb{N} \cup \{0\}$), with \mathbb{N} the set of

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natural numbers) with regard to x and of order $s \in \mathbb{N}_0$ with regard to t such that the norms

$$\|u\|_{C(\bar{\Omega})} = \sup_{(x,t) \in \bar{\Omega}} |u(x,t)| \quad (u \in C(\bar{\Omega}) = C^{(0,0)}(\bar{\Omega}))$$

$$\|u\|_{C^{(r,s)}(\bar{\Omega})} = \|u\|_{C(\bar{\Omega})} + \sum_{i=1}^r \left\| \frac{\partial^i u}{\partial x^i} \right\|_{C(\bar{\Omega})} + \sum_{j=1}^s \left\| \frac{\partial^j u}{\partial t^j} \right\|_{C(\bar{\Omega})}$$

are finite. Let $h = \frac{b-a}{n}$ for $n \in \mathbb{N}$ and $k = \lambda(h)$ for some positive function λ with $\lim_{h \rightarrow 0+} \lambda(h) = 0$. On the uniform grid ($n_0 \in \mathbb{N}_0$)

$$\Omega_h = \left\{ (x,t) : x = a + ih, t = jk \quad (1 \leq i \leq n-1, j \in \mathbb{N}_0, j \geq n_0) \right\}$$

$$\Gamma_{0,h} = \left\{ (x,t) : x = a + ih, t = jk \quad (1 \leq i \leq n-1, j \in \mathbb{N}_0, 0 \leq j \leq n_0) \right\}$$

$$\Gamma_{1,h} = \left\{ (x,t) : x \in \{a,b\}, t = jk \quad (j \in \mathbb{N}_0) \right\}$$

$$\bar{\Omega}_h = \Omega_h \cup \Gamma_{0,h} \cup \Gamma_{1,h}$$

($n_0 \geq 1$ corresponds to multi-step methods, cf. Section 4) consider a discretization of (1.1) given by

$$\begin{aligned} L_h u_h(x,t) &= J_h \varphi(x,t) && \text{for } (x,t) \in \Omega_h \\ u_h(x,t) &= \psi_0(x,t) && \text{for } (x,t) \in \Gamma_{0,h} \\ u_h(x,t) &= \psi_1(x,t) && \text{for } (x,t) \in \Gamma_{1,h} \end{aligned} \tag{1.2}$$

where J_h is a linear averaging operator and L_h a finite difference operator of type

$$L_h u_h(x,t) = \sum_{\eta \in \bar{\Omega}_h} \gamma_{h,(x,t)}(\eta) u_h(\eta)$$

with real-valued coefficients $\gamma_{h,(x,t)}(\eta)$ such that the set $\{\gamma_{h,(x,t)}(\eta) : \eta \in \bar{\Omega}_h\}$ is finite for every fixed $(x,t) \in \Omega_h$.

In the following we are interested in sharp estimates for the error $\|u_h - u\|_{\bar{\Omega}_{h,T}}$, measured by sup-norms like ($T > 0$)

$$\|v_h\|_{\bar{\Omega}_{h,T}} = \sup \left\{ |v_h(x,t)| : (x,t) \in \bar{\Omega}_{h,T} := \{(x,t) \in \bar{\Omega}_h : 0 \leq t \leq T\} \right\}. \tag{1.3}$$

The error bounds are given in terms of partial moduli of continuity for partial derivatives of solutions of (1.1), thereby confining ourselves to those problems (1.1) for which the solutions actually belong to the appropriate space $C^{(r,s)}(\bar{\Omega})$. It may be mentioned that these error bounds are obtained by standard methods (stability inequality and Taylor expansion of the truncation error) and include those known for smooth solutions. On the basis of a quantitative extension of the uniform boundedness principle it is then shown that these error bounds are sharp in the following sense: There exists a problem (1.1) with suitable data φ, ψ_0 and ψ_1 such that on the one side the solution belongs to the Lipschitz class under consideration, thus admits a certain (large-) O -rate of

approximation which, on the other hand, cannot be improved to the corresponding (small-) σ -rate.

To work out this program, Section 2 does not only recall some basic facts concerning discrete Green's functions but also adapts the quantitative uniform boundedness principle mentioned to the present situation of numerical approximations. Indeed, whereas our previous contributions (cf. [1, 2, 4]) were based upon rather specific properties of the discrete Green's functions in order to verify the relevant resonance condition, the procedure in Section 2 is quite general (see also the concluding remarks in Section 6). The following sections outline the details in connection with a general Crank-Nicolson scheme (Section 3), a Du Fort-Frankel scheme (Section 4) and a Saulyev scheme (Section 5) in order to illustrate the wide applicability of the method.

2. Discrete Green's functions and a quantitative uniform boundedness principle

For the definition of discrete Green's functions and for a useful representation of errors we need some further properties of (1.2).

(H₁) For each $h = \frac{b-a}{n}$ ($n \in \mathbb{N}$) and for all data φ, ψ_0 and ψ_1 there exists a unique solution of problem (1.2) which can be calculated via $(\eta = (x_\eta, t_\eta))$

$$\begin{aligned}
 u_h(x, t) = & \sum_{\eta \in \Omega_h, t_\eta \leq t} \gamma_{(x,t)}^{(1)}(\eta) J_h \varphi(\eta) \\
 & + \sum_{\eta \in \Gamma_{0,h}, t_\eta \leq t} \gamma_{(x,t)}^{(2)}(\eta) \psi_0(\eta) + \sum_{\eta \in \Gamma_{1,h}, t_\eta \leq t} \gamma_{(x,t)}^{(3)}(\eta) \psi_1(\eta)
 \end{aligned} \tag{2.1}$$

with coefficients $\gamma_{(x,t)}^{(j)}(\eta) = \gamma_{h,(x,t)}^{(j)}(\eta)$ ($j = 1, 2, 3$) depending on $h, (x, t)$ and η . Formula (2.1) means that for the computation of $u_h(x, t)$ one only uses informations at the points $\eta = (x_\eta, t_\eta)$ with $t_\eta \leq t$.

(H₂) J_h is a surjection in the sense that for every real-valued function v_h on Ω_h there exists a real-valued φ , defined on Ω , such that $v_h = J_h \varphi$ on Ω_h .

(H₃) For the error (cf. (1.3))

$$R_h u = \|u_h - u\|_{\overline{\Omega}_{h,T}} \tag{2.2}$$

one has $\lim_{h \rightarrow 0+} R_h u = 0$ for all u of the Banach space $C^{(r,s)}(\overline{\Omega})$ under consideration, where u_h is the solution of problem (1.2) corresponding to the given data $\varphi = Lu, \psi_0 = u$ and $\psi_1 = u$. In other words, the discrete solutions u_h should indeed converge to the exact one u .

These requirements have to be verified for each concrete problem: Whereas hypotheses (H₁) and (H₂) are assumed to be known in the examples to be considered, condition (H₃) will in fact be equipped with rates, even establishing (inverse) discrete convergence.

For $(\xi, \eta) \in \bar{\Omega}_h \times \Omega_h$ the discrete Green's function $G_h(\xi, \eta)$ is then defined for each fixed $\eta \in \Omega_h$ as the unique solution of

$$(L_h G_h(\cdot, \eta))(\xi) = \begin{cases} 1 & \text{if } \xi = \eta \\ 0 & \text{else} \end{cases} \quad \text{for } \xi \in \Omega_h$$

$$G_h(\xi, \eta) = 0 \quad \text{for } \xi \in \Gamma_{0,h} \cup \Gamma_{1,h}.$$

Note that G_h is well-defined in view of the assumptions (H₁) - (H₂). Moreover, (2.1) implies that

$$G_h(\xi, \eta) = 0 \quad \text{for all } \xi = (x_\xi, t_\xi) \text{ with } t_\xi < t_\eta. \tag{2.3}$$

Lemma 2.1: *Let v_h be a real-valued function on $\bar{\Omega}_h$ with $v_h(x, t) = 0$ for $(x, t) \in \Gamma_{0,h} \cup \Gamma_{1,h}$. Then for every $\xi \in \bar{\Omega}_h$ there holds true the representation*

$$v_h(\xi) = \sum_{\eta \in \Omega_h} G_h(\xi, \eta) L_h v_h(\eta) = \sum_{\eta \in \Omega_h, t_\eta \leq t_\xi} G_h(\xi, \eta) L_h v_h(\eta). \tag{2.4}$$

Proof: First observe that the sum in (2.4) is indeed finite because of (2.3). Denoting the right-hand side of (2.4) by $w_h(\xi)$, one has

$$L_h(w_h - v_h)(\xi) = 0 \quad \text{for } \xi \in \Omega_h \quad \text{and} \quad (w_h - v_h)(\xi) = 0 \quad \text{for } \xi \in \Gamma_{0,h} \cup \Gamma_{1,h}$$

so that (2.4) follows from the unique solvability of (1.2), assumed by hypothesis (H₁) ■

In particular, since for the error $u_h - u$ one has $(u_h - u)(x, t) = 0$ for $(x, t) \in \Gamma_{0,h} \cup \Gamma_{1,h}$ (cf. (1.1) and (1.2)), one can apply Lemma 2.1 to obtain the representation of the error (cf. (2.2))

$$R_h u = \left\| \sum_{\eta \in \Omega_h} G_h(\cdot, \eta) L_h(u_h - u)(\eta) \right\|_{\bar{\Omega}_{h,T}} = \left\| \sum_{\eta \in \Omega_h, T} G_h(\cdot, \eta) \tau_h u(\eta) \right\|_{\bar{\Omega}_{h,T}} \tag{2.5}$$

where the truncation error τ_h is defined by

$$\tau_h u := L_h(u_h - u) = J_h \varphi - L_h u = J_h L u - L_h u \tag{2.6}$$

(cf. (1.1) and (1.2)).

As is well-known, to prove convergence (cf. hypothesis (H₃)), it is sufficient to show consistency and stability (note that for a consistent discretization stability is actually equivalent to (inverse) discrete convergence). Indeed, a stability inequality like

$$\|v_h\|_{\bar{\Omega}_{h,T}} \leq M \|L_h v_h\|_{\Omega_{h,T-k}} \tag{2.7}$$

(with a constant $M < \infty$, independent of h and $k < T$) where v_h is defined on $\bar{\Omega}_h$ satisfying $v_h = 0$ on $\Gamma_{0,h} \cup \Gamma_{1,h}$, immediately leads to the estimate

$$R_h u \leq M \|L_h(u_h - u)\|_{\Omega_{h,T-k}} = M \|\tau_h u\|_{\Omega_{h,T-k}} \tag{2.8}$$

(cf. (2.2) and (2.6)). It therefore remains to treat the truncation error (consistency). For this purpose we introduce the partial moduli of continuity

$$\begin{aligned} \omega_{(1,0)}(\delta, u, \overline{\Omega}_T) &= \sup \left\{ |u(x + \varepsilon, t) - u(x, t)| : (x, t), (x + \varepsilon, t) \in \overline{\Omega}_T, |\varepsilon| \leq \delta \right\} \\ \omega_{(2,0)}(\delta, u, \overline{\Omega}_T) &= \sup \left\{ |u(x + \varepsilon, t) - 2u(x, t) + u(x - \varepsilon, t)| : (x \pm \varepsilon, t) \in \overline{\Omega}_T, |\varepsilon| \leq \delta \right\} \end{aligned}$$

for $\delta \geq 0$, with an analogous definition for the partial moduli $\omega_{(0,j)}(\delta, u, \overline{\Omega}_T)$ ($j = 1, 2$) with respect to the variable t . Here $\overline{\Omega}_T = \{(x, t) \in \overline{\Omega} : t \leq T\}$ (cf. (1.3)). In our applications in Sections 3-5 the approximation error $R_h u$ will be estimated by a (linear) combination of partial moduli. The sharpness of these estimates will then be established in connection with Lipschitz classes, determined by abstract moduli of continuity, i.e. by functions ω (e.g. $\omega(\delta) = \delta^\alpha$ with $0 < \alpha \leq 1$), continuous on $[0, \infty)$ such that, for $0 < \delta, \varepsilon$,

$$0 = \omega(0) < \omega(\delta) \leq \omega(\delta + \varepsilon) \leq \omega(\delta) + \omega(\varepsilon). \tag{2.9}$$

For moduli ω additionally satisfying

$$\lim_{\delta \rightarrow 0+} \frac{\omega(\delta)}{\delta} = \infty \tag{2.10}$$

this will be achieved by an application of the following quantitative extension of the uniform boundedness principle.

For a (real) Banach space X with norm $\|\cdot\|_X$ let X^* be the set of all sublinear, non-negative-valued, bounded functionals F on X , i.e. F maps X into $[0, \infty)$ such that, for all $f, g \in X$ and $\alpha \in \mathbb{R}$,

$$F(f + g) \leq Ff + Fg \quad \text{and} \quad F(\alpha f) = |\alpha|Ff$$

$$\|F\|_{X^*} := \sup\{Ff : \|f\|_X \leq 1\} < \infty.$$

Theorem 2.1: *Suppose that for a sequence of remainders $(F_n)_{n=1}^\infty \subset X^*$ and for a measure of smoothness $\{S_\delta\}_{\delta>0} \subset X^*$ there are test elements $g_n \in X$ such that $(\delta > 0, n \rightarrow \infty)$*

$$\|g_n\|_X = \mathcal{O}(1) \tag{2.11}$$

$$F_n g_n \neq o(1) \tag{2.12}$$

$$S_\delta g_n \leq K \min \left\{ 1, \frac{\sigma(\delta)}{\rho_n} \right\} \tag{2.13}$$

where $\sigma(\delta)$ is a function, strictly positive on $(0, \infty)$, and $(\rho_n)_{n=1}^\infty \subset (0, \infty)$ is a strictly decreasing sequence with $\lim_{n \rightarrow \infty} \rho_n = 0$. Then for each modulus ω satisfying (2.9) and (2.10) there exists a counterexample $f_\omega \in X$ with

$$S_\delta f_\omega = \mathcal{O}(\omega(\sigma(\delta))) \quad (\delta \rightarrow 0+)$$

$$F_n f_\omega \neq o(\omega(\rho_n)) \quad (n \rightarrow \infty).$$

For a proof and further comments see [2, 3] and the literature cited there.

In the context of this paper the Banach space X will always be identified with $C^{(r,s)}(\bar{\Omega})$ for appropriate values of $r, s \in \mathbb{N}_0$, whereas the measure of smoothness $\{S_\delta\}$ will be the combination of partial moduli of continuity of the exact solution mentioned. Clearly, for the remainder functional F_n we choose R_h for $h = \frac{b-a}{n}$ (cf. (2.2)). To prepare a suitable choice of test elements, the following property of discrete Green's functions will be useful in connection with the resonance condition (2.12) for the error. In fact, the next lemma is particularly important for a treatment of the case $\omega(\delta) = \delta$, so far excluded by (2.10).

Lemma 2.2: *For $T > 0$ let $g \in C^{(r,s)}(\bar{\Omega})$ (such that Lg is well-defined) be a function with $g = 0$ on $\Gamma_0 \cup \Gamma_1$ and, if $n_0 > 0$, additionally with $g = 0$ on $\Gamma_{0,h}$ for each $h \leq \delta_0$ ($\delta_0 > 0$), but $g \neq 0$ on Ω_T . Then there exists $\delta > 0$ such that, for all $h < \delta$,*

$$\left\| \sum_{\eta \in \Omega_{h,T}} G_h(\cdot, \eta) J_h Lg(\eta) \right\|_{\bar{\Omega}_{h,T}} > \frac{1}{2} \|g\|_{C(\bar{\Omega}_T)} > 0. \tag{2.14}$$

Proof: Obviously, g may be considered as a solution of problem (1.1), corresponding to the data $\varphi = Lg, \psi_0 = 0$ and $\psi_1 = 0$. In view of hypotheses (H₁) and (H₃) the solution g_h of the associated discrete problem (1.2) satisfies, for $h \rightarrow 0+$,

$$\left| \|g_h\|_{\Omega_{h,T}} - \|g\|_{\Omega_{h,T}} \right| \leq R_h g = o(1).$$

Since $\lim_{h \rightarrow 0+} \|g\|_{\Omega_{h,T}} = \|g\|_{C(\bar{\Omega}_T)}$, there exists $\delta > 0$ (without loss of generality, let $\delta < \delta_0$ if $n_0 > 0$) such that $\|g_h\|_{\Omega_{h,T}} > \|g\|_{C(\bar{\Omega}_T)}/2$ for all $h < \delta$. Therefore in view of Lemma 2.1 it follows that

$$\frac{1}{2} \|g\|_{C(\bar{\Omega}_T)} < \|g_h\|_{\Omega_{h,T}} = \left\| \sum_{\eta \in \Omega_{h,T}} G_h(\cdot, \eta) L_h g_h(\eta) \right\|_{\bar{\Omega}_{h,T}} \tag{2.15}$$

already establishing (2.14) ■

Choosing the quantities in Theorem 2.1 as mentioned above, we can then give a sufficient condition for (2.12) to be fulfilled, namely to determine test elements g_n such that

$$\tau_h g_n = M J_h Lg \quad \text{on } \Omega_h \tag{2.16}$$

for a constant $M \neq 0$ and a function g according to the conditions of Lemma 2.2. Indeed, because of (2.5) and (2.14) for $\frac{b-a}{h} = n \rightarrow \infty$

$$R_h g_n = \left\| \sum_{\eta \in \Omega_{h,T}} G_h(\cdot, \eta) \tau_h g_n(\eta) \right\|_{\bar{\Omega}_{h,T}} = |M| \left\| \sum_{\eta \in \Omega_{h,T}} G_h(\cdot, \eta) J_h Lg(\eta) \right\|_{\bar{\Omega}_{h,T}} \neq o(1).$$

It is property (2.16) which will be verified for the examples in Sections 3 - 5. It may be mentioned that in [4] the resonance condition (2.12) has been established by means

of a rather specific structure of the difference operators involved. The treatment given here in particular shows that one does not need any additional assumptions upon the discretization (1.2) to ensure (2.16). Moreover, note that if the discrete Green's functions are positive, say, we may continue the argument in (2.15) according to

$$\frac{1}{2} \|g\|_{C(\bar{\Omega}_T)} < \|g_h\|_{\Omega_{h,T}} \leq \|J_h Lg\|_{\Omega_{h,T}} \left\| \sum_{\eta \in \Omega_{h,T}} G_h(\cdot, \eta) \right\|_{\bar{\Omega}_{h,T}}$$

If $\|J_h Lg\|_{\Omega_{h,T}}$ is bounded independently of h , this implies that for $h \rightarrow 0+$

$$\left\| \sum_{\eta \in \Omega_{h,T}} G_h(\cdot, \eta) \right\|_{\bar{\Omega}_{h,T}} \neq o(1). \tag{2.17}$$

In this situation, (2.12) (cf. (2.16)) can be replaced by the postulate (cf. [1]) to determine test elements g_n such that (e.g.)

$$\tau_h g_n(x, t) > C > 0 \quad \text{for all } (x, t) \in \Omega_{h,T}. \tag{2.18}$$

3. Crank-Nicolson scheme

In this section the quantities in connection with problems (1.1) and (1.2) are specified as follows: For $r = 2, s = 1$ (or $s = 2$) we choose

$$Lu(x, t) = \frac{\partial}{\partial t} u(x, t) - \frac{\partial}{\partial x} \left(\alpha(x) \frac{\partial}{\partial x} u(x, t) \right) \tag{3.1}$$

for a coefficient function $\alpha \in C[a, b]$ satisfying $\alpha(x) > \kappa > 0$ for all $x \in [a, b]$. Here $C[a, b]$ is the space of real-valued functions α , continuous on $[a, b]$ with $\|\alpha\| := \max\{|\alpha(x)| : a \leq x \leq b\}$, whereas $C^{(r)}[a, b]$ ($r \in \mathbb{N}$) will denote the subset of all r -times continuously differentiable elements. Concerning the difference scheme let us introduce the notations

$$\begin{aligned} \partial_x u_h(x, t) &= \frac{u_h(x+h, t) - u_h(x, t)}{h}, & \partial_x^0 u_h(x, t) &= \frac{u_h(x+h, t) - u_h(x-h, t)}{2h} \\ \bar{\partial}_x u_h(x, t) &= \frac{u_h(x, t) - u_h(x-h, t)}{h} \\ \partial_t u_h(x, t) &= \frac{u_h(x, t+k) - u_h(x, t)}{k}, & \partial_t^0 u_h(x, t) &= \frac{u_h(x, t+k) - u_h(x, t-k)}{2k} \end{aligned}$$

For a parameter $\vartheta \in [0, 1]$ the operators $L_h = L_h^{(\vartheta)}$ and $J_h = J_h^{(\vartheta)}$ are then defined by ($n_0 = 0$)

$$\begin{aligned} L_h^{(\vartheta)} u_h(x, t) &= \partial_t u_h(x, t) - \partial_x \left(\alpha \left(x - \frac{h}{2} \right) \bar{\partial}_x [\vartheta u_h(x, t+k) + (1-\vartheta) u_h(x, t)] \right) \\ J_h^{(\vartheta)} \varphi(x, t) &= \vartheta \varphi(x, t+k) + (1-\vartheta) \varphi(x, t). \end{aligned} \tag{3.2}$$

Note that for $\vartheta = 0$ this scheme is an explicit Euler scheme, whereas $\vartheta = \frac{1}{2}$ leads to the Crank-Nicolson scheme and $\vartheta = 1$ to an implicit backward Euler scheme (cf. [5: p. 527] and [8: p. 118]).

It is easy to show (cf. [5: pp. 525/528]) that hypotheses (H_1) and (H_2) of Section 2 are satisfied for (3.2). Regarding (H_3) , we need stability and consistency (cf. (2.8)). Concerning stability, let v_h be defined on $\bar{\Omega}_h$ satisfying $v_h = 0$ on $\Gamma_{0,h} \cup \Gamma_{1,h}$. Suppose that either

$$\vartheta \geq \frac{1}{2} \quad \text{or} \quad 2 \left(\frac{k}{h^2} \right) (1 - 2\vartheta) \|\alpha\| < C < 1. \tag{3.3}$$

Then it was shown in [6] (cf. [8: p. 118]) that the stability inequality (2.7) holds true. Concerning consistency, we are in fact interested in the following (quantitative) estimate for the truncation error.

Lemma 3.1: *For $u \in C^{(2,1)}(\bar{\Omega})$, $\alpha \in C^{(3)}[a, b]$ and $T > 0$ one has*

$$\begin{aligned} \left\| \tau_h^{(\vartheta)} u \right\|_{\Omega_{h,T-k}} &:= \left\| J_h^{(\vartheta)} Lu - L_h^{(\vartheta)} u \right\|_{\Omega_{h,T-k}} \\ &\leq \omega_{(0,1)} \left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T \right) + \frac{1}{2} \|\alpha\| \omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) \\ &\quad + \frac{1}{2} h \|\alpha'\| \omega_{(1,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + K_u h^2, \end{aligned} \tag{3.4}$$

the constant K_u being given by

$$K_u = \frac{1}{8} \|\alpha''\| \left\| \frac{\partial^2 u}{\partial x^2} \right\|_{C(\bar{\Omega}_T)} + \frac{1}{24} \|\alpha^{(3)}\| \left\| \frac{\partial u}{\partial x} \right\|_{C(\bar{\Omega}_T)}$$

In the case $\vartheta = \frac{1}{2}$ and $u \in C^{(2,2)}(\bar{\Omega}_T)$ the estimate can be improved to

$$\begin{aligned} \left\| \tau_h^{(1/2)} u \right\|_{\Omega_{h,T-k}} &\leq \frac{k}{4} \omega_{(0,1)} \left(k, \frac{\partial^2 u}{\partial t^2}, \bar{\Omega}_T \right) + \frac{1}{2} \|\alpha\| \omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) \\ &\quad + \frac{1}{2} h \|\alpha'\| \omega_{(1,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + K_u h^2. \end{aligned}$$

Proof: Let $(x, t) \in \Omega_{h,T-k}$ be arbitrary, fixed. In view of (1.1), (1.2) and (3.1), (3.2) one has for the truncation error (2.6)

$$\begin{aligned} \tau_h^{(\vartheta)} u(x, t) &= \left[\vartheta \frac{\partial u}{\partial t}(x, t+k) + (1-\vartheta) \frac{\partial u}{\partial t}(x, t) - \partial_t u(x, t) \right] \\ &+ \vartheta \left[-\alpha(x) \frac{\partial^2 u}{\partial x^2}(x, t+k) - \alpha'(x) \frac{\partial u}{\partial x}(x, t+k) + \partial_x \left(\alpha \left(x - \frac{1}{2} h \right) \bar{\partial}_x u(x, t+k) \right) \right] \\ &+ (1-\vartheta) \left[-\alpha(x) \frac{\partial^2 u}{\partial x^2}(x, t) - \alpha'(x) \frac{\partial u}{\partial x}(x, t) + \partial_x \left(\alpha \left(x - \frac{1}{2} h \right) \bar{\partial}_x u(x, t) \right) \right] \\ &=: (\tau_{(1)} + \vartheta \tau_{(2)} + (1-\vartheta) \tau_{(3)}) u(x, t), \end{aligned}$$

say. For $\tau_{(3)}$ it follows that

$$\begin{aligned} |\tau_{(3)}u(x, t)| &\leq \left| \alpha(x) \left(-\frac{\partial^2 u}{\partial x^2}(x, t) + \partial_x \bar{\partial}_x u(x, t) \right) \right| + \left| -\alpha'(x) \frac{\partial u}{\partial x}(x, t) \right. \\ &\quad \left. + \frac{\alpha(x + \frac{1}{2}h) - \alpha(x)}{h} \partial_x u(x, t) + \frac{\alpha(x) - \alpha(x - \frac{1}{2}h)}{h} \bar{\partial}_x u(x, t) \right| \\ &=: S_1 + S_2. \end{aligned}$$

Concerning S_1 one immediately concludes

$$\begin{aligned} S_1 &\leq \|\alpha\| \left| -\frac{\partial^2 u}{\partial x^2}(x, t) + \frac{1}{h^2} \int_0^h (h-s) \frac{\partial^2 u}{\partial x^2}(x+s, t) ds \right. \\ &\quad \left. + \frac{1}{h^2} \int_0^h (h-s) \frac{\partial^2 u}{\partial x^2}(x-s, t) ds \right| \tag{3.5} \\ &\leq \frac{1}{2} \|\alpha\| \omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) \end{aligned}$$

whereas for S_2 a Taylor expansion of α at the point x with suitable ξ_1, ξ_2 leads to

$$\begin{aligned} S_2 &= \left| -\alpha'(x) \frac{\partial u}{\partial x}(x, t) \right. \\ &\quad + \frac{1}{h^2} \left(\left(\frac{h}{2} \alpha'(x) + \frac{h^2}{8} \alpha''(x) + \frac{h^3}{48} \alpha^{(3)}(\xi_1) \right) (u(x+h, t) - u(x, t)) \right. \\ &\quad \left. + \left(\frac{h}{2} \alpha'(x) - \frac{h^2}{8} \alpha''(x) + \frac{h^3}{48} \alpha^{(3)}(\xi_2) \right) (u(x, t) - u(x-h, t)) \right) \left| \right| \\ &\leq S_3 + S_4 \end{aligned}$$

where

$$\begin{aligned} S_3 &= \left| -\alpha'(x) \frac{\partial u}{\partial x}(x, t) + \alpha'(x) \partial_x^0 u(x, t) \right| \\ &\leq \|\alpha'\| \left| \frac{1}{2h} \int_0^h (h-s) \left(\frac{\partial^2 u}{\partial x^2}(x+s, t) - \frac{\partial^2 u}{\partial x^2}(x-s, t) \right) ds \right| \\ &\leq \frac{1}{2} h \|\alpha'\| \omega_{(1,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) \end{aligned}$$

and

$$\begin{aligned} S_4 &= \left| \frac{1}{8} \alpha''(x) h^2 \partial_x \bar{\partial}_x u(x, t) \right| \\ &\quad + \frac{h}{48} \left(\left| \alpha^{(3)}(\xi_1) h \partial_x u(x, t) \right| + \left| \alpha^{(3)}(\xi_2) h \bar{\partial}_x u(x, t) \right| \right) \\ &\leq \frac{1}{8} h^2 \|\alpha''\| \left\| \frac{\partial^2 u}{\partial x^2} \right\|_{C(\bar{\Omega}_T)} + \frac{1}{24} h^2 \|\alpha^{(3)}\| \left\| \frac{\partial u}{\partial x} \right\|_{C(\bar{\Omega}_T)} \\ &=: K_u h^2. \end{aligned}$$

An analogous estimate may also be obtained for $\tau_{(2)}$ so that

$$\begin{aligned} & \vartheta |\tau_{(2)}u(x, t)| + (1 - \vartheta) |\tau_{(3)}u(x, t)| \\ & \leq \frac{1}{2} \|\alpha\| \omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + \frac{1}{2} h \|\alpha'\| \omega_{(1,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + K_u h^2. \end{aligned}$$

It remains to discuss $\tau_{(1)}$. On the one hand side,

$$\begin{aligned} |\tau_{(1)}u(x, t)| & \leq \vartheta \left| \frac{\partial u}{\partial t}(x, t+k) - \partial_t u(x, t) \right| + (1 - \vartheta) \left| \frac{\partial u}{\partial t}(x, t) - \partial_t u(x, t) \right| \\ & = \vartheta \left| \frac{1}{k} \int_0^k \left(\frac{\partial u}{\partial t}(x, t+k) - \frac{\partial u}{\partial t}(x, t+s) \right) ds \right| \\ & \quad + (1 - \vartheta) \left| \frac{1}{k} \int_0^k \left(\frac{\partial u}{\partial t}(x, t) - \frac{\partial u}{\partial t}(x, t+s) \right) ds \right| \\ & \leq \omega_{(0,1)} \left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T \right). \end{aligned}$$

On the other hand, if $\vartheta = \frac{1}{2}$ and $u \in C^{(2,2)}(\bar{\Omega}_T)$, then

$$\begin{aligned} |\tau_{(1)}u(x, t)| & = \left| \frac{1}{2} \left(\frac{\partial u}{\partial t}(x, t+k) + \frac{\partial u}{\partial t}(x, t) \right) \right. \\ & \quad \left. - \frac{1}{2k} \left(k \frac{\partial u}{\partial t}(x, t) + \int_0^k (k-s) \frac{\partial^2 u}{\partial t^2}(x, t+s) ds \right) \right. \\ & \quad \left. + k \frac{\partial u}{\partial t}(x, t+k) - \int_0^k (k-s) \frac{\partial^2 u}{\partial t^2}(x, t+k-s) ds \right| \\ & \leq \frac{k}{4} \omega_{(0,1)} \left(k, \frac{\partial^2 u}{\partial t^2}, \bar{\Omega}_T \right). \end{aligned}$$

Summarizing, the assertions of Lemma 3.1 are completely established ■

With the aid of stability (cf. (2.7)) and consistency (with rates, cf. (2.6) and Lemma 3.1) we obtain the following a-priori estimate for the error (cf. (2.8)).

Theorem 3.1: *Let $\alpha \in C^{(3)}[a, b]$, $T > k$ and $0 \leq \vartheta \leq 1$ be arbitrary, fixed. Given a problem (1.1), (3.1) with solution u satisfying $u \in C^{(2,1)}(\bar{\Omega})$, let u_h be the solution of the associated discrete problem (1.2), (3.2).*

a) *If one of the assumptions (3.3) is satisfied, then for the remainder (2.2) there holds true*

$$\begin{aligned} R_h^{(\vartheta)} u & \leq M \left[\omega_{(0,1)} \left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T \right) + \frac{1}{2} \|\alpha\| \omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) \right. \\ & \quad \left. + \frac{1}{2} h \|\alpha'\| \omega_{(1,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + K_u h^2 \right] \end{aligned} \tag{3.6}$$

with constants M and K_u given via (2.7) and Lemma 3.1, respectively.

b) For $\vartheta = \frac{1}{2}$ and if u additionally satisfies $u \in C^{(2,2)}(\bar{\Omega}_T)$, then

$$R_h^{(1/2)}u \leq M \left[\frac{k}{4} \omega_{(0,1)} \left(k, \frac{\partial^2 u}{\partial t^2}, \bar{\Omega}_T \right) + \frac{1}{2} \|\alpha\| \omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + \frac{1}{2} h \|\alpha'\| \omega_{(1,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + K_u h^2 \right]. \tag{3.7}$$

These direct estimates are sharp in the following sense.

Theorem 3.2: Under the assumptions of Theorem 3.1 let $\alpha \in C^{(5)}[a, b]$ and $T > 0$.

a) If $\vartheta \in [0, 1]$ is arbitrary, fixed and $k = \mu h^2$ for a constant $\mu > 0$ (i.e. $\lambda(h) = \mu h^2$), then for every modulus of continuity ω satisfying (2.9) and (2.10) there exists a counterexample $u_\omega \in C^{(2,1)}(\bar{\Omega})$ such that ($\delta \rightarrow 0+$)

$$\omega_{(0,1)} \left(\delta^2, \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T \right) + \omega_{(2,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) + \delta \omega_{(1,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) = \mathcal{O}(\omega(\delta^2)), \tag{3.8}$$

thus $R_h^{(\vartheta)}u_\omega = \mathcal{O}(\omega(h^2))$ (cf. (3.6) for $k = \mu h^2$), but on the other hand ($h \rightarrow 0+$)

$$R_h^{(\vartheta)}u_\omega \neq o(\omega(h^2)). \tag{3.9}$$

Moreover, the counterexample can in fact be chosen such that additionally either

$$\omega_{(2,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) + \delta \omega_{(1,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) = \mathcal{O}(\delta^2) \tag{3.10}$$

or

$$\omega_{(0,1)} \left(\delta^2, \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T \right) = \mathcal{O}(\delta^2) \tag{3.11}$$

is satisfied, i.e. if (3.10) holds true, then the sharpness is based on the remaining module $\omega_{(0,1)}(\delta^2, \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T)$ (cf. (3.8)), whereas in the situation of (3.11) the sum $\omega_{(2,0)}(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T) + \delta \omega_{(1,0)}(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T)$ becomes relevant.

b) Let $\vartheta = \frac{1}{2}$ and $k = \lambda(h) = h$. Then for every modulus of continuity ω satisfying (2.9) and (2.10) there exists a counterexample $u_\omega \in C^{(2,2)}(\bar{\Omega})$ such that

$$\delta \omega_{(0,1)} \left(\delta, \frac{\delta^2 u_\omega}{\partial t^2}, \bar{\Omega}_T \right) + \omega_{(2,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) + \delta \omega_{(1,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) = \mathcal{O}(\omega(\delta^2)), \tag{3.12}$$

thus $R_h^{(1/2)}u_\omega = \mathcal{O}(\omega(h^2))$ (cf. (3.7) for $k = h$), but on the other hand

$$R_h^{(1/2)}u_\omega \neq o(\omega(h^2)).$$

Proof: The assertions follow as applications of Theorem 2.1 in connection with (2.16). To show statement a) with respect to (3.10), choose

$$\begin{aligned}
 X &= C^{(4,1)}(\bar{\Omega}) \quad \text{and} \quad F_n u = R_h^{(\vartheta)} u \quad \text{with} \quad h = \frac{b-a}{n} \\
 S_\delta u &= \omega_{(0,1)} \left(\delta^2, \frac{\partial u}{\partial t}, \bar{\Omega}_T \right), \quad \sigma(\delta) = \delta^2, \quad \rho_n = n^{-2} \\
 g_n(x, t) &= \frac{1}{n^2} \sin \left(2\pi \frac{t}{k} \right) Lg(x, t) = \frac{1}{n^2} \sin \left(\frac{2\pi n^2 t}{\mu(b-a)^2} \right) Lg(x, t)
 \end{aligned} \tag{3.13}$$

where g is an arbitrary, fixed function such that $g \in C^{(r,s)}(\bar{\Omega})$ for each $r, s \in \mathbb{N}_0$, $g = 0$ on $\Gamma_0 \cup \Gamma_1$, but $g \neq 0$ on Ω_T (cf. Lemma 2.2). Note that $Lg \in C^{(4,2)}(\bar{\Omega})$ since $\alpha \in C^{(5)}[a, b]$. Elementary calculations establish conditions (2.11) and (2.13) since

$$S_\delta g_n \leq \begin{cases} 2 \left\| \frac{\partial g_n}{\partial t} \right\|_{C(\bar{\Omega}_T)} = \mathcal{O}(1) \\ \delta^2 \left\| \frac{\partial^2 g_n}{\partial t^2} \right\|_{C(\bar{\Omega}_T)} = \mathcal{O}(\delta^2 n^2) = \mathcal{O} \left(\frac{\sigma(\delta)}{\rho_n} \right) \end{cases} \quad (\delta \rightarrow 0+, n \rightarrow \infty).$$

Concerning (2.12) we proceed via (2.16): On the one hand side, $L_h^{(\vartheta)} g_n = 0$ on Ω_h since $g_n(x, t) = 0$ on $\bar{\Omega}_h$. On the other hand, for every $(x, t) \in \Omega_h$

$$\begin{aligned}
 Lg_n(x, t) &= \frac{2\pi}{\mu(b-a)^2} \cos \left(2\pi \frac{t}{k} \right) Lg(x, t) \\
 &\quad + \frac{1}{n^2} \sin \left(2\pi \frac{t}{k} \right) \left[\frac{\partial Lg}{\partial t}(x, t) - \alpha'(x) \frac{\partial Lg}{\partial x}(x, t) - \alpha(x) \frac{\partial^2 Lg}{\partial x^2}(x, t) \right] \\
 &= \frac{2\pi}{\mu(b-a)^2} Lg(x, t).
 \end{aligned}$$

Therefore it follows for the truncation error (cf. (2.6)) that

$$\tau_h^{(\vartheta)} g_n(x, t) = J_h^{(\vartheta)} Lg_n(x, t) - L_h^{(\vartheta)} g_n(x, t) = \frac{2\pi}{\mu(b-a)^2} J_h^{(\vartheta)} Lg(x, t)$$

which establishes (2.16). Having verified all the conditions of Theorem 2.1 we obtain a counterexample $u_\omega \in C^{(4,1)}(\bar{\Omega})$ ($\subset C^{(2,1)}(\bar{\Omega})$) satisfying (3.9) and $S_\delta u_\omega = \mathcal{O}(\omega(\delta^2))$. Note that because of the additional smoothness of u_ω with regard to the variable x we further have

$$\omega_{(2,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) + \delta \omega_{(1,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) = \mathcal{O}(\delta^2) \quad \left[= \mathcal{O}(\omega(\delta^2)) \right]$$

establishing (3.8) and (3.10).

To construct a counterexample in connection with (3.11) we proceed in the same manner. Again we use the quantities F_n , σ and ρ_n of (3.13), but now in connection with $X = C^{(2,2)}(\bar{\Omega})$ and

$$S_\delta u = \omega_{(2,0)} \left(\delta, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + \delta \omega_{(1,0)} \left(\delta, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right)$$

$$g_n(x, t) = \frac{1}{n^2} \left(1 - \cos \left(2\pi n \frac{x-a}{b-a} \right) \right) \frac{Lg(x, t)}{\alpha(x)}.$$

Note that because of $\alpha(x) > \kappa > 0$ and $\alpha \in C^{(5)}[a, b]$ the test elements g_n even belong to the class $C^{(4,2)}(\bar{\Omega})$. Therefore conditions (2.11) and (2.13) immediately follow. Again the resonance elements g_n have been constructed such that $g_n(x, t) = 0$ for each $(x, t) \in \bar{\Omega}_h$. Together with

$$Lg_n(x, t) = -\alpha(x) \left(\frac{2\pi}{b-a} \right)^2 \frac{Lg(x, t)}{\alpha(x)} = - \left(\frac{2\pi}{b-a} \right)^2 Lg(x, t) \quad ((x, t) \in \Omega_h)$$

this establishes (2.16) (cf. (2.6)). Therefore by Theorem 2.1 there exists a counterexample $u_\omega \in C^{(2,2)}(\bar{\Omega})$ ($\subset C^{(2,1)}(\bar{\Omega})$) which satisfies (3.9) and (3.8) as well as (3.11).

Part b) is a further consequence of Theorem 2.1. Recalling that $k = h = \frac{b-a}{n}$ we use (3.13), but replace the space X , the measure of smoothness S_δ and the test elements g_n by $X = C^{(4,2)}(\bar{\Omega})$,

$$S_\delta u = \delta \omega_{(0,1)} \left(\delta, \frac{\partial^2 u}{\partial t^2}, \bar{\Omega}_T \right) \quad \text{and} \quad g_n(x, t) = \frac{1}{n^2} \sin \left(\frac{2\pi nt}{b-a} \right) Lg(x, t),$$

respectively. Thus the theorem is completely established ■

For the Crank-Nicolson scheme ($\vartheta = \frac{1}{2}$) with constant coefficient function $\alpha(x) \equiv 1$ the sharpness in the remaining case $\omega(\delta) = \delta$ has been shown in [4] using a rather concrete telescope argument applicable to the discrete Green's functions under consideration. Note that the discrete Green's functions for $\vartheta = \frac{1}{2}$ do not have any positivity properties (cf. (2.17)). Here let us continue with another approach, namely to construct a counterexample for $\omega(\delta) = \delta$ using Lemma 2.2.

To this end, let $\alpha(x) \equiv 1$ and let $\vartheta \in [0, 1]$ be arbitrary, fixed. Using the abbreviation $d = \frac{\pi}{b-a}$, consider the function

$$g(x, t) = [1 - \exp(-d^2 t)] \sin(d(x - a))$$

in connection with Lemma 2.2. Obviously,

$$Lg(x, t) = d^2 \exp(-d^2 t) \sin(d(x - a)) + d^2 [1 - \exp(-d^2 t)] \sin(d(x - a))$$

$$= d^2 \sin(d(x - a))$$

and therefore

$$J_h^{(\vartheta)} Lg(x, t) = Lg(x, t) = d^2 \sin(d(x - a)). \tag{3.14}$$

To discuss the case $\omega(\delta) = \delta$; one may then use

$$u_\omega(x, t) = \sin(d(x - a)) \tag{3.15}$$

as a counterexample. Indeed, $Lu_\omega(x, t) = d^2u_\omega(x, t)$ and

$$\begin{aligned} L_h^{(\vartheta)}u_\omega(x, t) &= -\frac{1}{h^2} \left[\sin(d(x + h - a)) - 2\sin(d(x - a)) + \sin(d(x - h - a)) \right] \\ &= -\frac{2}{h^2} \left[\sin(d(x - a)) \cos(dh) - \sin(d(x - a)) \right] \end{aligned}$$

so that for the truncation error (cf. (2.6))

$$\begin{aligned} \tau_h^{(\vartheta)}u_\omega(x, t) &= J_h^{(\vartheta)}Lu_\omega(x, t) - L_h^{(\vartheta)}u_\omega(x, t) \\ &= \sin(d(x - a)) \left[d^2 + \frac{2}{h^2} (\cos(dh) - 1) \right] \\ &= \sin(d(x - a)) \left[\frac{d^4}{12} + 2d^4 \sum_{j=3}^\infty \frac{(-1)^j (dh)^{2j-4}}{(2j)!} \right] h^2. \end{aligned}$$

In view of (2.5), (2.14) and (3.14) we finally obtain

$$\begin{aligned} R_h^{(\vartheta)}u_\omega &= \left\| \sum_{\eta \in \Omega_{h,T}} G_h(\cdot, \eta) \tau_h^{(\vartheta)}u_\omega(\eta) \right\|_{\overline{\Omega}_{h,T}} \\ &= \left| \frac{d^2}{12} + 2d^2 \sum_{j=3}^\infty \frac{(-1)^j (dh)^{2j-4}}{(2j)!} \right| h^2 \left\| \sum_{\eta \in \Omega_{h,T}} G_h(\cdot, \eta) J_h^{(\vartheta)}Lg(\eta) \right\|_{\overline{\Omega}_{h,T}} \\ &\neq o(h^2) \end{aligned}$$

but obviously u_ω satisfies (3.10) - (3.12) for $\omega(\delta) = \delta$.

4. Du Fort-Frankel scheme

For this and the next section let $r = 2, s = 1$ and (cf. (1.1))

$$Lu(x, t) = \left(\frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2} \right) u(x, t). \tag{4.1}$$

The Du Fort-Frankel scheme (cf. [8: p. 41]) is given by (cf. (1.2))

$$\begin{aligned} L_h u_h(x, t) &= \partial_t^0 u_h(x, t) \\ &\quad - \frac{1}{h^2} \left[u_h(x + h, t) - u_h(x, t + k) - u_h(x, t - k) + u_h(x - h, t) \right] \\ J_h \varphi &= \varphi. \end{aligned} \tag{4.2}$$

Because of the three time levels involved, this multi-step procedure requires initial data for $t = k$, too, so that we have to choose $n_0 = 1$. Let $\mu(h) := \frac{k}{h^2}$ throughout. Since properties (H₁) and (H₂) of Section 2 are obvious (cf. proof of Lemma 4.1 below), to discuss the convergence property (H₃), let us start with the following stability inequality, a proof of which is included for the sake of completeness.

Lemma 4.1: *If $T > k$ and $\mu(h) \leq \frac{1}{2}$, then*

$$\|v_h\|_{\bar{\Omega}_{h,T}} \leq 2T \|L_h v_h\|_{\Omega_{h,T-k}} \tag{4.3}$$

for every function v_h defined on $\bar{\Omega}_h$ with $v_h(x, t) = 0$ for each $(x, t) \in \Gamma_{0,h} \cup \Gamma_{1,h}$.

Proof: One may interpret v_h as the solution of (1.2), (4.2) corresponding to the data $\psi_0 \equiv 0, \psi_1 \equiv 0$ and $J_h \varphi = L_h v_h$. Then

$$\begin{aligned} v_h(x, t+k) &= \frac{2\mu(h)}{1+2\mu(h)} \left(v_h(x+h, t) + v_h(x-h, t) \right) \\ &\quad + \frac{1-2\mu(h)}{1+2\mu(h)} v_h(x, t-k) + \frac{2k}{1+2\mu(h)} L_h v_h(x, t). \end{aligned} \tag{4.4}$$

Using the matrix

$$A = 2\mu(h)(a_{i,j})_{i,j=1}^{n-1} \in \mathbb{R}^{n-1} \times \mathbb{R}^{n-1}$$

with

$$a_{i,j} = \begin{cases} 1 & \text{for } i = j+1 \text{ or } j = i+1 \\ 0 & \text{else} \end{cases}$$

and the vectors

$$V_j = (v_h(a+h, jk), v_h(a+2h, jk), \dots, v_h(a+(n-1)h, jk))$$

$$Q_j = (L_h v_h(a+h, jk), L_h v_h(a+2h, jk), \dots, L_h v_h(a+(n-1)h, jk))$$

one may write (4.4) as ($j \geq 1$)

$$V_{j+1}^{tr} = \frac{1}{1+2\mu(h)} A V_j^{tr} + \frac{1-2\mu(h)}{1+2\mu(h)} V_{j-1}^{tr} + \frac{2k}{1+2\mu(h)} Q_j^{tr},$$

V^{tr} denoting the transposed of V . Note that the shape of the matrix A already reflects the (homogeneous) boundary condition $\psi_1 = 0$, whereas the initial condition is considered via $V_0 = V_1 = 0$. In terms of the sup-norms

$$\|V\|_\infty = \|(v_1, \dots, v_{n-1})\|_\infty = \sup_{1 \leq i \leq n-1} |v_i|$$

$$\|A\|_\infty = \sup_{0 \neq V \in \mathbb{R}^{n-1}} \frac{\|A V^{tr}\|_\infty}{\|V\|_\infty}$$

one has $\|A\|_\infty \leq 4\mu(h)$. Moreover,

$$0 < \mu(h) \leq \frac{1}{2} \implies \frac{1-2\mu(h)}{1+2\mu(h)} \geq 0$$

so that, for $j \geq 1$,

$$\begin{aligned} \|V_{j+1}\|_\infty &\leq \frac{1}{1+2\mu(h)} \|A\|_\infty \|V_j\|_\infty + \frac{1-2\mu(h)}{1+2\mu(h)} \|V_{j-1}\|_\infty + \frac{2k}{1+2\mu(h)} \|Q_j\|_\infty \\ &\leq \max\{\|V_j\|_\infty, \|V_{j-1}\|_\infty\} + 2k \|Q_j\|_\infty. \end{aligned}$$

Iteration yields

$$\begin{aligned} \|V_j\|_\infty &\leq \max\{\|V_0\|_\infty, \|V_1\|_\infty\} + 2(j-1)k \max_{1 \leq i \leq j-1} \|Q_i\|_\infty \\ &= 2(j-1)k \max_{1 \leq i \leq j-1} \|Q_i\|_\infty \end{aligned}$$

already establishing (4.3) ■

Lemma 4.2: *There exists a constant $\delta > 0$ such that for every $h = \frac{b-a}{n} < \delta$ and $u \in C^{(2,1)}(\bar{\Omega})$ (with $T > k = \mu(h)h^2$)*

$$\begin{aligned} \|\tau_h u\|_{\Omega_{h,T-k}} &\leq \frac{1}{2}\omega_{(0,2)}\left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T\right) \\ &\quad + \mu(h)\omega_{(0,1)}\left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T\right) + \frac{1}{2}\omega_{(2,0)}\left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T\right). \end{aligned}$$

Proof: For arbitrary, fixed $(x, t) \in \Omega_{h,T-k}$ one has

$$\begin{aligned} \tau_h u(x, t) &= \left(\frac{\partial u}{\partial t}(x, t) - \partial_t^0 u(x, t)\right) - \left(\frac{\partial^2 u}{\partial x^2}(x, t) - \partial_x \bar{\partial}_x u(x, t)\right) \\ &\quad - \frac{1}{h^2}\left(u(x, t+k) - 2u(x, t) + u(x, t-k)\right) \\ &=: \left(\tau_{(1)} + \tau_{(2)} + \tau_{(3)}\right)u(x, t), \end{aligned}$$

say. Taylor expansion yields (cf. (3.5))

$$\begin{aligned} \|\tau_{(1)}u\|_{\Omega_{h,T-k}} &= \left\| \frac{1}{2k} \int_0^k \left(\frac{\partial u}{\partial t}(x, t+s) - 2\frac{\partial u}{\partial t}(x, t) + \frac{\partial u}{\partial t}(x, t-s)\right) ds \right\|_{\Omega_{h,T-k}} \\ &\leq \frac{1}{2}\omega_{(0,2)}\left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T\right), \\ \|\tau_{(2)}u\|_{\Omega_{h,T-k}} &\leq \frac{1}{2}\omega_{(2,0)}\left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T\right), \\ \|\tau_{(3)}u\|_{\Omega_{h,T-k}} &= \frac{1}{h^2} \left\| \int_0^k \left(\frac{\partial u}{\partial t}(x, t+s) - \frac{\partial u}{\partial t}(x, t-k+s)\right) ds \right\|_{\Omega_{h,T-k}} \\ &\leq \mu(h)\omega_{(0,1)}\left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T\right) \end{aligned}$$

so that the assertion follows ■

As in the previous section, Lemma 4.1 and 4.2 fit together to the following a-priori estimate for the error (2.2).

Theorem 4.1: *Let $\mu(h) \leq \frac{1}{2}$ and $T > k$. Given a problem (1.1), (4.1) with solution u satisfying $u \in C^{(2,1)}(\bar{\Omega})$, let u_h be the solution of the associated discrete problem (1.2), (4.2), using exact starting values $u_h(x, t) = u(x, t)$ on $\Gamma_{0,h}$. Then*

$$\begin{aligned} R_h u &\leq T \left[\omega_{(0,2)}\left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T\right) \right. \\ &\quad \left. + 2\mu(h)\omega_{(0,1)}\left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T\right) + \omega_{(2,0)}\left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T\right) \right]. \end{aligned} \tag{4.5}$$

The sharpness of this estimate is again a consequence of Theorem 2.1.

Theorem 4.2: Let $\mu(h) \leq \frac{1}{2}$ and $T > 0$. For every modulus of continuity ω satisfying (2.9) and (2.10) there exists a counterexample $u_\omega \in C^{(2,1)}(\bar{\Omega})$ such that ($k = \lambda(\delta) = \mu(\delta)\delta^2 \leq \frac{\delta^2}{2}$)

$$\begin{aligned} \omega_{(0,2)} \left(\lambda(\delta), \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T \right) + \mu(\delta)\omega_{(0,1)} \left(\lambda(\delta), \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T \right) \\ + \omega_{(2,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) = \mathcal{O}(\omega(\delta^2)), \end{aligned}$$

thus $R_h u_\omega = \mathcal{O}(\omega(h^2))$ (cf. (4.5)), but on the other hand ($h \rightarrow 0+$)

$$R_h u_\omega \neq o(\omega(h^2)).$$

Proof: Applying Theorem 2.1 we choose (cf. proof of Theorem 3.2)

$$\begin{aligned} X &= C^{(2,3)}(\bar{\Omega}), \quad F_n u = R_h u \quad \text{with } h = \frac{b-a}{n} \\ S_\delta u &= \omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right), \quad \sigma(\delta) = \delta^2, \quad \rho_n = n^{-2} \\ g_n(x, t) &= \frac{1}{n^2} \left(1 - \cos \left(2\pi \frac{x-a}{h} \right) \right) Lg(x, t) \\ &= \frac{1}{n^2} \left(1 - \cos \left(2\pi n \frac{x-a}{b-a} \right) \right) Lg(x, t) \end{aligned}$$

where g is an arbitrarily often differentiable function as described in Lemma 2.2. Conditions (2.11) and (2.13) are satisfied. To examine (2.16) we compute the truncation error (cf. (2.6), $(x, t) \in \Omega_h$):

$$\tau_h g_n(x, t) = Lg_n(x, t) = - \left(\frac{2\pi}{b-a} \right)^2 Lg(x, t) = - \left(\frac{2\pi}{b-a} \right)^2 J_h Lg(x, t).$$

Hence Theorem 2.1 provides a counterexample u_ω as specified, in fact $u_\omega \in C^{(2,3)}(\bar{\Omega})$ so that, additionally,

$$\omega_{(0,2)} \left(\lambda(\delta), \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T \right) + \mu(\delta)\omega_{(0,1)} \left(\lambda(\delta), \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T \right) = \mathcal{O}(\delta^2) = \mathcal{O}(\omega(\delta^2)).$$

Therefore the assertions are completely established ■

Let us mention that for $\mu(h) \leq \frac{1}{2}$ the discrete Green's functions associated with (4.2) are in fact positive so that it is sufficient to examine (2.18) instead of (2.16). In the case that the abstract modulus of continuity is given via $\omega(\delta) = \delta$, the function $u_\omega(x, t) = x^4$ may be used as a counterexample ($(x, t) \in \Omega_h$). Indeed,

$$\begin{aligned} Lu_\omega(x, t) &= -12x^2 \\ L_h u_\omega(x, t) &= -\frac{1}{h^2} \left((x+h)^4 - 2x^4 + (x-h)^4 \right) = -12x^2 - 2h^2 \\ \tau_h u_\omega(x, t) &= (L - L_h)u_\omega(x, t) = 2h^2. \end{aligned}$$

Therefore in view of (2.5) and (2.17) we have shown that $R_h u_\omega \neq o(h^2)$, taking advantage of the positivity of the discrete Green's functions associated.

5. Saul'yev scheme

Another discretization of (1.1), (4.1) in connection with solutions $u \in C^{(2,1)}(\bar{\Omega})$ is given by the Saul'yev scheme

$$\begin{aligned}
 L_h^{(\vartheta)} u_h(x, t) &= \partial_t u_h(x, t) \\
 &\quad - \frac{\vartheta}{h^2} \left[u_h(x - h, t + k) - u_h(x, t + k) - u_h(x, t) + u_h(x + h, t) \right] \\
 &\quad - (1 - \vartheta) \partial_x \bar{\partial}_x u_h(x, t)
 \end{aligned} \tag{5.1}$$

$$J_h^{(\vartheta)} \varphi(x, t) = \vartheta \varphi(x, t + k) + (1 - \vartheta) \varphi(x, t)$$

where $\vartheta \in [0, 1]$ and $n_0 = 0$. For every φ, ψ_0, ψ_1 there exists a unique solution of (1.2), (5.1) (cf. [7: p. 31]), and there holds true the following convergence theorem which in particular implies that hypotheses (H₁) - (H₃) of Section 2 are satisfied.

Theorem 5.1: *Let $\vartheta \in [0, 1]$, $T > k$ be arbitrary, fixed and suppose that $k = \mu h^2$ with $\mu^{-1} \geq \max\{\frac{3}{2} - \vartheta, 1 - \vartheta + \sqrt{1 - \vartheta}\}$. Given a problem (1.1), (4.1) with solution $u \in C^{(2,1)}(\bar{\Omega})$, let u_h be the solution of the associated discrete problem (1.2), (5.1). Then for the remainder (2.2) there holds true*

$$\begin{aligned}
 R_h^{(\vartheta)} u &\leq T \left(\omega_{(0,1)} \left(k, \frac{\partial u}{\partial t}, \bar{\Omega}_T \right) \right. \\
 &\quad \left. + \omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + \vartheta \mu \omega_{(1,0)} \left(h, \frac{\partial u}{\partial t}, \bar{\Omega}_T \right) \right).
 \end{aligned} \tag{5.2}$$

For a proof one may refer to [4] and the literature cited there, in particular to [7: p. 35]. It may be mentioned that for $\vartheta = 0$ the scheme passes into the explicit Euler scheme already considered in Section 3.

Theorem 5.2: *Let $\vartheta \in (0, 1]$, $T > 0$ and $\mu^{-1} \geq \max\{\frac{3}{2} - \vartheta, 1 - \vartheta + \sqrt{1 - \vartheta}\}$. For every modulus of continuity ω satisfying (2.9), (2.10) there exists a counterexample $u_\omega \in C^{(2,1)}(\bar{\Omega})$ such that*

$$\begin{aligned}
 \omega_{(0,1)} \left(\delta^2, \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T \right) &+ \omega_{(2,0)} \left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}_T \right) \\
 &+ \vartheta \omega_{(1,0)} \left(\delta, \frac{\partial u_\omega}{\partial t}, \bar{\Omega}_T \right) = \mathcal{O}(\omega(\delta)),
 \end{aligned}$$

thus $R_h^{(\vartheta)} u_\omega = \mathcal{O}(\omega(h))$ (cf. (5.2) for $k = \mu h^2$), but on the other hand ($h \rightarrow 0+$)

$$R_h^{(\vartheta)} u_\omega \neq o(\omega(h)).$$

Proof: We specify the quantities in Theorem 2.1 according to

$$\begin{aligned}
 X &= C^{(2,1)}(\bar{\Omega}), \quad F_n u = R_h^{(\vartheta)} u \text{ with } h = \frac{b-a}{n}, \quad \sigma(\delta) = \delta, \quad \rho_n = n^{-1} \\
 S_\delta u &= \omega_{(0,1)} \left(\delta^2, \frac{\partial u}{\partial t}, \bar{\Omega}_T \right) + \omega_{(2,0)} \left(\delta, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T \right) + \omega_{(1,0)} \left(\delta, \frac{\partial u}{\partial t}, \bar{\Omega}_T \right) \\
 g_n(x, t) &= \frac{1}{n^2} \left(1 - \cos \left(2\pi \frac{x-a}{h} \right) \right) Lg(x, t) \\
 &= \frac{1}{n^2} \left(1 - \cos \left(2\pi n \frac{x-a}{b-a} \right) \right) Lg(x, t)
 \end{aligned}$$

where g_n are the same resonance elements as used in the proof of Theorem 4.2. Then (2.11) is satisfied, whereas (2.13) is a consequence of $(\delta \rightarrow 0+, n \rightarrow \infty)$

$$S_\delta g_n \leq \begin{cases} 2 \left\| \frac{\partial g_n}{\partial t} \right\|_{C(\bar{\Omega})} + 4 \left\| \frac{\partial^2 g_n}{\partial x^2} \right\|_{C(\bar{\Omega})} + 2 \left\| \frac{\partial g_n}{\partial t} \right\|_{C(\bar{\Omega})} = \mathcal{O}(1) \\ \delta^2 \left\| \frac{\partial^2 g_n}{\partial t^2} \right\|_{C(\bar{\Omega})} + \delta \left\| \frac{\partial^3 g_n}{\partial x^3} \right\|_{C(\bar{\Omega})} + \delta \left\| \frac{\partial^2 g_n}{\partial x \partial t} \right\|_{C(\bar{\Omega})} = \mathcal{O}(\delta n). \end{cases}$$

Since we have for the truncation error

$$\tau_h g_n = - \left(\frac{2\pi}{b-a} \right)^2 Lg(x, t)$$

condition (2.16) is fulfilled, and Theorem 2.1 provides the desired counterexample ■

In the case $\omega(\delta) = \delta, \vartheta \in (0, 1]$ the function $u_\omega(x, t) = xt$ satisfies $R_h^{(\vartheta)} u_\omega = \mathcal{O}(\delta)$, but on the other hand $R_h^{(\vartheta)} u_\omega \neq \mathcal{O}(h)$ (cf. [4]).

6. Concluding remarks

So far the resonance elements have been constructed on the basis of condition (2.16). But note that the test elements g_n , actually considered in the examples of the previous sections, additionally satisfy the conditions $(M \neq 0)$

$$Lg_n = MLg \quad \text{on } \Omega_h \tag{6.1}$$

$$g_n = 0 \quad \text{on } \bar{\Omega}_h \tag{6.2}$$

where g is an arbitrarily often differentiable function as described in Lemma 2.2. Obviously, (6.2) implies $L_h g_n = 0$, and therefore (2.16) is valid since (cf. (2.6))

$$\tau_h g_n = J_h Lg_n - L_h g_n = MJ_h Lg.$$

It may be mentioned that the two conditions (6.1) and (6.2) allow a further interpretation of the resonance condition (cf. (2.12)): Because the functions $\frac{g_n}{M}$ and g induce

the same data for the discrete problem, namely $\varphi = \frac{Lg_n}{M} = Lg$ on Ω_h and $g_n = g = 0$ on $\Gamma_{0,h} \cup \Gamma_{1,h}$, their discrete counterparts (via (1.2)) are equal: $(\frac{g_n}{M})_h = g_h$. The fact that $\lim_{h \rightarrow 0+} \|g_h\|_{\bar{\Omega}_{h,T}} = \|g\|_{C(\bar{\Omega}_T)}$ then implies that $R_h g_n$ is bounded away from zero ($h = \frac{b-a}{n}$):

$$R_h \left(\frac{g_n}{M}\right) = \left\| \left(\frac{g_n}{M}\right)_h - \frac{g_n}{M} \right\|_{\Omega_{h,T}} = \left\| \left(\frac{g_n}{M}\right)_h \right\|_{\Omega_{h,T}} = \|g_h\|_{\Omega_{h,T}} \tag{6.3}$$

$$\lim_{n \rightarrow \infty} R_h g_n = |M| \|g\|_{C(\bar{\Omega}_T)} > 0.$$

In other words, we have established condition (2.12) of Theorem 2.1 without using discrete Green’s functions explicitly. Nevertheless the representation of the error via (2.5) is still used to derive a lower bound in connection with the abstract modulus of continuity $\omega(\delta) = \delta$ (cf. (3.15)).

The methods employed in this paper are not restricted to initial boundary value problems. In [1] we were concerned with the sharpness of an error bound obtained for the five point discretization of the Dirichlet problem

$$Lu(x, t) = \varphi(x, t) \quad \text{for all } (x, t) \in \Omega = (0, 1)^2 \tag{6.4}$$

$$u(x, t) = \psi(x, t) \quad \text{for all } (x, t) \in \Gamma$$

where $L = \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial t^2}$ is the Laplace operator and Γ the boundary of Ω . Thus the discretization is given by the formula

$$L_h u_h(x, t) = \varphi(x, t) \quad \text{for all } (x, t) \in \Omega_h \tag{6.5}$$

$$u_h(x, t) = \psi(x, t) \quad \text{for all } (x, t) \in \Gamma_h$$

where for $h = \frac{1}{n}$ (uniform grid)

$$\bar{\Omega}_h = \left\{ (x, t) \in \bar{\Omega} : x = ih \text{ and } t = jh \ (i, j \in \mathbb{N}_0) \right\}$$

$$\Omega_h = \bar{\Omega}_h \cap \Omega, \quad \Gamma_h = \bar{\Omega}_h \cap \Gamma$$

$$L_h u_h(x, t) = \partial_x \bar{\partial}_x u_h(x, t) + \partial_t \bar{\partial}_t u_h(x, t).$$

Theorem 6.1: *For a solution $u \in C^{(2,2)}(\bar{\Omega})$ of (6.4) and its discrete counterpart u_h of (6.5) there holds true*

$$R_h u = \|u_h - u\|_{\Omega_h} \leq \frac{1}{4} \left[\omega_{(2,0)} \left(h, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega} \right) + \omega_{(0,2)} \left(h, \frac{\partial^2 u}{\partial t^2}, \bar{\Omega} \right) \right]. \tag{6.6}$$

For a proof of this well-known estimate see also [1] where, above all, it was shown that (6.6) is indeed sharp. It may be mentioned that the relevant argument in [1] was based upon the fact that the discrete Green’s functions associated are non-positive-valued (maximum principle). Using the method of this paper, however, one may immediately proceed as follows.

Theorem 6.2: For every modulus of continuity ω satisfying (2.9) and (2.10) there exists a counterexample $u_\omega \in C^{(2,2)}(\bar{\Omega})$ such that

$$\omega_{(2,0)}\left(\delta, \frac{\partial^2 u_\omega}{\partial x^2}, \bar{\Omega}\right) + \omega_{(0,2)}\left(\delta, \frac{\partial^2 u_\omega}{\partial t^2}, \bar{\Omega}\right) = \mathcal{O}(\omega(\delta^2)),$$

thus $R_h u_\omega = \mathcal{O}(\omega(h^2))$ (cf. (6.6)), but on the other hand ($h \rightarrow 0+$)

$$R_h u_\omega \neq o(\omega(h^2)).$$

Proof: Using Theorem 2.1 we choose

$$X = C^{(2,2)}(\bar{\Omega}), \quad F_n u = R_h u \quad \text{with } h = \frac{1}{n}$$

$$S_\delta u = \omega_{(2,0)}\left(\delta, \frac{\partial^2 u}{\partial x^2}, \bar{\Omega}_T\right) + \omega_{(0,2)}\left(\delta, \frac{\partial^2 u}{\partial t^2}, \bar{\Omega}_T\right), \quad \sigma(\delta) = \delta^2, \quad \rho_n = n^{-2}$$

$$g_n(x, t) = \frac{1}{n^2}(1 - \cos(2\pi n x))Lg(x, t)$$

where $g \neq 0$ is a function arbitrarily often differentiable on $\bar{\Omega}$ such that $g(x, t) = 0$ for $(x, t) \in \Gamma$. Again conditions (2.11) and (2.13) follow by simple calculations, whereas (2.12) is a consequence of the considerations at the beginning of this section (cf. (6.3) with $M = 4\pi^2$), replacing $\bar{\Omega}_T$ and $\Gamma_0 \cup \Gamma_1$ by $\bar{\Omega}$ and Γ , respectively ■

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