

# FINITE DIFFERENCE METHODS FOR A NONLOCAL BOUNDARY VALUE PROBLEM FOR THE HEAT EQUATION

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## Abstract.

Three different finite difference schemes for solving the heat equation in one space dimension with boundary conditions containing integrals over the interior of the interval are considered. The schemes are based on the forward Euler, the backward Euler and the Crank-Nicolson methods. Error estimates are derived in maximum norm. Results from a numerical experiment are presented.

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## 1. Introduction.

In this paper we introduce three different finite difference methods for solving the heat equation with integral boundary conditions

$$(1.1) \quad \begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= f(x, t), & x \in [0, 1], 0 < t \leq T, \\ u(0, t) &= \int_0^1 k_0(x)u(x, t) dx + g_0(t), & 0 < t \leq T, \\ u(1, t) &= \int_0^1 k_1(x)u(x, t) dx + g_1(t), & 0 < t \leq T, \\ u(x, 0) &= u_0(x), & x \in [0, 1], \end{aligned}$$

and we give error estimates in the maximum norm for each of these methods.

This kind of problem arises in quasi-static thermoelasticity, for example when  $u$  is the entropy of a homogeneous and isotropic slab, see Day [1], [2]. Day shows that the maximum modulus,  $\max_{x \in [0, 1]} |u(x, t)|$ , is a decreasing function in  $t$ . In [3] Friedman extends this result to a general parabolic equation (in  $n$  dimensions) using

a method based on the maximum principle. He also shows existence and uniqueness of the solution to his extended version of the problem. An example of a related problem is found in [5].

For the interior part of the problem, our discrete methods use the forward Euler, the backward Euler and the Crank-Nicolson schemes, respectively. The integrals in the boundary equations for  $x = 0, 1$  are approximated by the trapezoidal rule. We have chosen this approximation since it is simple and of the same, second, order of accuracy in space as the methods used for the interior part of the problem.

By maximum principle arguments we show that, if the mesh ratio  $\lambda = k/h^2 \leq \frac{1}{2}$ , then the error in the forward Euler method is of second order in space, and that the error in the backward Euler method is of first order in time and second order in space without any restriction on  $\lambda$ . Since the maximum principle for the Crank-Nicolson method is valid only if  $\lambda \leq 1$ , and since we want to be able to choose the mesh parameters  $h, k$  independently, we use energy arguments to show that the maximum norm of the error for the Crank-Nicolson method is second order in both space and time.

This note has the following outline: Section 2 is devoted to the forward Euler method while the backward Euler method is treated in Section 3. Section 4 deals with the Crank-Nicolson method. In Section 5 we give some numerical results.

## 2. The forward Euler method.

Our first and simplest numerical approximation of (1.1) is based on the explicit forward Euler scheme. We start by dividing  $[0, 1] \times [0, T]$  into an  $M \times N$  mesh with step sizes  $h = 1/M$  and  $k = 1/N$  in space and time, respectively. The integrals on the right hand side of the expressions for  $u(0, t)$  and  $u(1, t)$  are approximated by the trapezoidal rule, that is

$$\int_0^1 f(x) dx \sim J_h(f) := \frac{h}{2} f(0) + h \sum_{j=1}^{M-1} f(x_j) + \frac{h}{2} f(1),$$

where  $x_j = jh$ . For the quadrature error,

$$\varepsilon_h(f) = J_h(f) - \int_0^1 f(x) dx,$$

we have the bound

$$(2.1) \quad |\varepsilon_h(f)| \leq Ch^2 \|f\|_{W_\infty^{2,0}},$$

where the norm  $\|\cdot\|_{W_\infty^{m,n}}$  is defined by

$$(2.2) \quad \|u\|_{W_\infty^{m,n}} := \sum_{\substack{\alpha_1 + \alpha_2 \leq m \\ \alpha_2 \leq n}} \left\| \frac{\partial^{\alpha_1 + \alpha_2}}{\partial x^{\alpha_1} \partial t^{\alpha_2}} u \right\|_{L^\infty([0,1] \times [0,T])}.$$

To simplify our notation, we introduce a discrete inner product,  $\langle \cdot, \cdot \rangle$ , for vectors  $V = (V_0, V_1, \dots, V_M)$ , by

$$(2.3) \quad \langle V, W \rangle = \frac{h}{2} V_0 W_0 + h \sum_{j=1}^{M-1} V_j W_j + \frac{h}{2} V_M W_M.$$

We may then write

$$J_h(f) = \langle f, 1 \rangle.$$

The forward and backward difference quotients are denoted by

$$\partial_x U_j^n = h^{-1}(U_{j+1}^n - U_j^n),$$

$$\bar{\partial}_x U_j^n = h^{-1}(U_j^n - U_{j-1}^n),$$

and similarly for the difference quotients in time, for instance,

$$\partial_t U_j^n = k^{-1}(U_j^{n+1} - U_j^n).$$

For the mesh point  $(jh, nk)$  we introduce the notation  $(x_j, t_n)$ , and set  $\lambda = k/h^2$ . Our approximate solution is defined by the following system of equations:

$$(2.4) \quad \begin{aligned} \partial_t U_j^n - \partial_x \bar{\partial}_x U_j^n &= F_j^n, & j = 1, \dots, M-1, 0 \leq n \leq N-1, \\ U_0^n &= \langle K_0, U^n \rangle + G_0^n, & 1 \leq n \leq N, \\ U_M^n &= \langle K_M, U^n \rangle + G_M^n, & 1 \leq n \leq N, \\ U_j^0 &= u_0(x_j), & j = 0, \dots, M, \end{aligned}$$

where

$$(2.5) \quad K_{0,j} = k_0(x_j), \quad K_{M,j} = k_1(x_j),$$

$$(2.6) \quad G_0^n = g_0(t_n), \quad G_M^n = g_1(t_n),$$

and

$$(2.7) \quad F_j^n = f(x_j, t_n).$$

On each time level, the solution at interior mesh points is given by explicit equations. The two boundary values are the solution of a  $2 \times 2$  linear system of equations. That is, given  $U^n$  we can use the following scheme to compute  $U^{n+1}$ : First compute the interior part of  $U^{n+1}$  by

$$U_j^{n+1} = \lambda(U_{j-1}^n + U_{j+1}^n) + (1 - 2\lambda)U_j^n + kF_j^n, \quad j = 1, \dots, M-1.$$

Then let

$$\gamma_0 = h \sum_{j=1}^{M-1} K_{0,j} U_j^{n+1} + G_0^{n+1},$$

$$\gamma_M = h \sum_{j=1}^{M-1} K_{M,j} U_j^{n+1} + G_M^{n+1}$$

The boundary values  $U_0^{n+1}$  and  $U_M^{n+1}$  are now computed from the equations

$$U_0^{n+1} = \frac{\gamma_0(1 - hK_{M,M}) + \gamma_M hK_{0,M}}{1 - h(K_{0,0} + K_{M,M}) + h^2(K_{0,M}K_{M,0} - K_{0,0}K_{M,M})},$$

$$U_M^{n+1} = \frac{\gamma_0 hK_{M,0} + \gamma_M(1 - hK_{0,0})}{1 - h(K_{0,0} + K_{M,M}) + h^2(K_{0,M}K_{M,0} - K_{0,0}K_{M,M})}.$$

The results in this section will be expressed in terms of the maximum norm, defined by

$$|V|_{\mathcal{S}} = \max_{s \in \mathcal{S}} |V_s|.$$

The sets  $[0, \dots, M]$  and  $[0, \dots, N]$  will be denoted by  $\mathcal{M}$  and  $\mathcal{N}$ , respectively. We define discrete operators  $\mathcal{L} = \mathcal{L}_{kh}$ ,  $l_0 = l_{0,h}$ ,  $l_M = l_{M,h}$  by

$$(2.9) \quad (\mathcal{L}U)_j^n = \partial_t U_j^n - \partial_x \bar{\delta}_x U_j^n, \quad j = 1, \dots, M-1, \quad 0 \leq n \leq N-1,$$

$$(l_0 U)^n = U_0^n - \langle K_0, U^n \rangle, \quad 0 \leq n \leq N,$$

$$(l_M U)^n = U_M^n - \langle K_M, U^n \rangle, \quad 0 \leq n \leq N.$$

The existence theorem and error estimate for the solution of (2.4) are based on the following a priori estimate.

LEMMA 2.1. Assume that  $0 < \lambda \leq \frac{1}{2}$  and

$$(2.10) \quad \langle |K_0|, 1 \rangle \leq \varrho < 1, \quad \langle |K_m|, 1 \rangle \leq \varrho < 1.$$

Then we have

$$(2.11) \quad |U|_{\mathcal{M} \times \mathcal{N}} \leq \frac{1}{1 - \varrho} (|\mathcal{L}U|_{\mathcal{M} \times \mathcal{N}} + |l_0 U|_{\mathcal{N}} + |l_M U|_{\mathcal{N}} + |U^0|_{\mathcal{M}}).$$

The proof of Lemma 2.1 is based on the wellknown maximum principle for the forward Euler method given in the following lemma.

LEMMA 2.2 If  $0 < \lambda \leq 1/2$  and  $\mathcal{L}V \leq 0$ , then we have

$$\max_{j \in \mathcal{M}, n \in \mathcal{N}} V_j^n \leq \max_{j \in \mathcal{M}, n \in \mathcal{N}} (V_0^n, V_M^n, V_j^0).$$

PROOF. From the definition of  $\mathcal{L}V$  and the difference quotients we have that the condition  $\mathcal{L}V \leq 0$  can be written as

$$V_j^{n+1} \leq (1 - 2\lambda)V_j^n + \lambda(V_{j+1}^n + V_{j-1}^n).$$

Assume that the maximum is attained at the interior mesh point  $(x_j, t_{n+1})$ . Then since the coefficients to the right add up to one and are all non-negative, and since the values of  $V$  present on the right hand side are at most  $V_j^{n+1}$ , they all have to equal this number. Repeated use of this implies that  $V_j^n$  must take its maximum somewhere on the left or right boundary or on the initial line. ■

We are now prepared to prove the a priori estimate of Lemma 2.1.

PROOF. Let  $H_j = -\frac{1}{2}x_j(1 - x_j)$  and set  $\omega_j^n = U_j^n + \kappa H_j$  where  $\kappa = |\mathcal{L}U|_{\mathcal{M} \times \mathcal{N}}$ . Since  $(\mathcal{L}H)_j^n = -1$  we have

$$(2.12) \quad (\mathcal{L}\omega)_j^n = (\mathcal{L}U)_j^n - \kappa \leq 0.$$

By the definition of  $H_j$  we also have that  $H_0 = H_M = 0$ ,  $H_j \leq 0$  for  $j = 0, \dots, M$ , and  $\max_j(-H_j) = 1/8$ . From inequality (2.12) and Lemma 2.2 we have

$$\begin{aligned} \max_{n,j} \omega_j^n &\leq \max_{n,j} (\omega_0^n, \omega_M^n, \omega_j^0) = \max_{n,j} (U_0^n, U_M^n, U_j^0 + \kappa H_j) \\ &\leq \max_{n,j} (U_0^n, U_M^n, U_j^0) \leq \max(|U_0|_{\mathcal{N}}, |U_M|_{\mathcal{N}}) + |U^0|_{\mathcal{M}}, \end{aligned}$$

and hence

$$\begin{aligned} \max_{n,j} U_j^n &\leq \max_{n,j} \omega_j^n + \kappa \max_j (-H_j) \\ &\leq \max(|U_0|_{\mathcal{N}}, |U_M|_{\mathcal{N}}) + |U^0|_{\mathcal{M}} + \frac{\kappa}{8}. \end{aligned}$$

If we replace  $U_j^n$  by  $-U_j^n$  in the definition of  $\omega_j^n$  above, we will get the same bound for  $\max_{n,j}(-U_j^n)$ , so that we may conclude

$$(2.13) \quad |U|_{\mathcal{M} \times \mathcal{N}} \leq \max(|U_0|_{\mathcal{N}}, |U_M|_{\mathcal{N}}) + |U^0|_{\mathcal{M}} + \frac{1}{8} |\mathcal{L}U|_{\mathcal{M} \times \mathcal{N}}.$$

But by the definition of  $l_0$  and (2.10) we have

$$|U_0^n| \leq \langle |K_0|, 1 \rangle |U^n|_{\mathcal{M}} + |l_0 U^n| \leq \varrho |U|_{\mathcal{M} \times \mathcal{N}} + |l_0 U|_{\mathcal{N}},$$

and hence

$$(2.14) \quad |U_0|_{\mathcal{N}} \leq \varrho |U|_{\mathcal{M} \times \mathcal{N}} + |l_0 U|_{\mathcal{N}},$$

and similarly for  $|U_M|_{\mathcal{N}}$ . We now combine inequality (2.13) with (2.14) and the corresponding estimate for  $|U_M|_{\mathcal{N}}$  to obtain

$$|U|_{\mathcal{M} \times \mathcal{N}} \leq \varrho |U|_{\mathcal{M} \times \mathcal{N}} + |l_0 U|_{\mathcal{N}} + |l_M U|_{\mathcal{N}} + |U^0|_{\mathcal{M}} + \frac{1}{8} |\mathcal{L}U|_{\mathcal{M} \times \mathcal{N}}.$$

Moving the first term on the right hand side over to the left and dividing by  $1 - \varrho \neq 0$  completes the proof. ■

We will now give an existence theorem for the solution of our discrete problem (2.4).

**THEOREM 2.3.** *Assume  $0 < \lambda \leq \frac{1}{2}$  and that (2.10) holds, then our discrete problem (2.4) admits a unique solution.*

PROOF. The discrete system (2.4) is a system of  $(M + 1)$  linear equations in  $(M + 1)$  unknowns at each time step. In order to show existence it suffices to show uniqueness, that is, that the homogeneous problem has only the trivial solution. But if  $U^0 = F_j^n = G_0^n = G_M^n = 0$ , then  $\mathcal{L}U = l_0U = l_MU = 0$ , and hence, by Lemma 2.1,  $U_j^n \equiv 0$ . ■

REMARK. If  $k_0$  and  $k_1$  in the model problem are continuous functions such that

$$(2.15) \quad \int_0^1 |k_0(x)| dx < 1, \quad \int_0^1 |k_1(x)| dx < 1,$$

then there exist  $\varrho$  and  $h_0$  such that, for all  $h$  with  $0 < h \leq h_0$ , assumption (2.10) is valid. Hence for  $h \leq h_0$  our discrete problem defined by (2.4)–(2.7) has a unique solution. The condition in (2.15) is necessary to get a continuous solution of (1.1) such that the maximum modulus  $\max_{x \in [0, 1]} |u(x, t)|$  is a decreasing function in  $t$ ; see [3] or [2].

We will now give an error estimate for our discrete approximation of (1.1).

THEOREM 2.4. Assume that  $k_0, k_1 \in C^2([0, 1])$  are such that

$$\|k_0\|_{L_1([0, 1])} < 1 \quad \text{and} \quad \|k_1\|_{L_1([0, 1])} < 1.$$

Let  $U_j^n$  be the solution of (2.4)–(2.7) and  $u \in C^{4,2}([0, 1] \times [0, T])$  the solution of (1.1). If  $0 < \lambda \leq \frac{1}{2}$ , then there exists an  $h_0$  such that

$$\|U - u\|_{\mathcal{M} \times \mathcal{N}} \leq Ch^2 \|u\|_{W_\infty^{4,2}} \text{ for } h \leq h_0.$$

PROOF. By the above remark there exists  $h_0 > 0$  such that assumption (2.10) is valid for all  $h \leq h_0$ .

Let  $Z_j^n = U_j^n - u(x_j, t_n)$  denote the error at the mesh point  $(x_j, t_n)$ . We will apply Lemma 2.1 to  $Z_j^n$ , and hence we need estimates of the terms on the right hand side of (2.11). We start with  $|\mathcal{L}Z|_{\mathcal{M} \times \mathcal{N}}$ . From the definition of  $\mathcal{L}$  and  $Z_j^n$  and (1.1) and (2.4) we have

$$\begin{aligned} (\mathcal{L}Z)_j^n &= (\mathcal{L}U)_j^n - \mathcal{L}u(x_j, t_n) \\ &= f(x_j, t_n) - \mathcal{L}u(x_j, t_n) = \left( \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} \right) - (\partial_t u - \partial_x \bar{\partial}_x u) = \tau_j^n. \end{aligned}$$

By expanding the local discretization error  $\tau_j^n$  in Taylor series we get

$$(2.16) \quad |\mathcal{L}Z|_{\mathcal{M} \times \mathcal{N}} \leq Ch^2 \|u\|_{W_\infty^{4,2}}.$$

We now consider the term  $|l_0 Z|_{\mathcal{N}}$ . By the definition of  $l_0$  and  $Z_j^n$  and (1.1) and (2.4)

we have

$$\begin{aligned} (l_0 Z)^n &= U_0^n - \langle K_0, U^n \rangle + \langle K_0, u(\cdot, t_n) \rangle - u(0, t_n) \\ &= G_0^n + \langle K_0, u(\cdot, t_n) \rangle - \int_0^1 k_0(x)u(x, t_n) dx - g_0(t_n) \\ &= \langle K_0, u(\cdot, t_n) \rangle - \int_0^1 k_0(x)u(x, t_n) dx = \varepsilon_n(k_0 u), \end{aligned}$$

and hence by (2.1)

$$(2.17) \quad |l_0 Z|_{\mathcal{N}} \leq Ch^2 \|k_0 u\|_{W_\infty^{2,0}} \leq Ch^2 \|u\|_{W_\infty^{2,0}}.$$

Similarly, for  $|l_M Z|_{\mathcal{N}}$  we have

$$(2.18) \quad |l_M Z|_{\mathcal{N}} \leq Ch^2 \|k_1 u\|_{W_\infty^{2,0}} \leq Ch^2 \|u\|_{W_\infty^{2,0}},$$

and for the initial value  $Z_j^0$  we find

$$(2.19) \quad Z_j^0 = U_j^0 - u(x_j, 0) = U_j^0 - u_0(x_j) = 0.$$

From Lemma 2.1 and (2.16)–(2.19) we now conclude

$$|U - u|_{\mathcal{M} \times \mathcal{N}} \leq Ch^2 \|u\|_{W_\infty^{4,2}},$$

which completes the proof.  $\blacksquare$

### 3. The backward Euler method.

In this section we will study the application of the implicit backward Euler scheme to our model problem. The integrals on the right hand side of the expression for  $u(0, t)$  and  $u(1, t)$  are again approximated by the trapezoidal rule. In this case we obtain the following system of equations:

$$(3.1) \quad \begin{aligned} \bar{\partial}_t U_j^n - \partial_x \bar{\partial}_x U_j^n &= F_j^n, & j = 1, \dots, M-1, \quad 1 \leq n \leq N, \\ U_0^n &= \langle K_0, U^n \rangle + G_0^n, & 1 \leq n \leq N, \\ U_M^n &= \langle K_M, U^n \rangle + G_M^n, & 1 \leq n \leq N, \\ U_j^0 &= u_0(x_j), & j = 0, \dots, M, \end{aligned}$$

where  $K_{0,j}$ ,  $K_{M,j}$ ,  $G_0^n$ ,  $G_M^n$  and  $F_j^n$  are defined by (2.5)–(2.7).

We define the operator  $\bar{\mathcal{L}} = \bar{\mathcal{L}}_{kh}$ , associated with the interior part of our system of equations, by

$$(3.2) \quad (\bar{\mathcal{L}}U)_j^n = \bar{\partial}_t U_j^n - \partial_x \bar{\partial}_x U_j^n, \quad j = 1, \dots, M-1, \quad 1 \leq n \leq N.$$

The results in this section will be based on the well-known maximum principle for the backward Euler method:

LEMMA 3.1. *If  $\mathcal{L}V \leq 0$ , then we have*

$$\max_{j \in \mathcal{M}, n \in \mathcal{N}} V_j^n \leq \max_{j \in \mathcal{M}, n \in \mathcal{N}} (V_0^n, V_M^n, V_j^0).$$

PROOF. The condition  $\mathcal{L}V \leq 0$  is equivalent to

$$(1 + 2\lambda)V_j^n \leq V_j^{n-1} + \lambda(V_{j-1}^n + V_{j+1}^n).$$

The proof is completed in the same way as that of Lemma 2.2. ■

Our next lemma is an a priori estimate, which will be used to show existence, uniqueness, and an error estimate for the solution  $U_j^n$  of our system of equations (3.1), together with (2.5)–(2.7).

LEMMA 3.2. *Assume that*

$$(3.3) \quad \langle |K_0|, 1 \rangle \leq \varrho < 1 \quad \text{and} \quad \langle |K_M|, 1 \rangle \leq \varrho < 1.$$

Then

$$|U|_{\mathcal{M} \times \mathcal{N}} \leq \frac{1}{1 - \varrho} (|\mathcal{L}U|_{\mathcal{M} \times \mathcal{N}} + |U^0|_{\mathcal{M}} + |l_0 U|_{\mathcal{N}} + |l_M U|_{\mathcal{N}}).$$

The proof of this lemma is analogous to that of Lemma 2.1 and will not be presented. Our next theorem gives existence and uniqueness for the solution of our discrete problem (3.1).

THEOREM 3.3. *If assumption (3.3) is satisfied, then (3.1) has a unique solution.*

This theorem is proved in the same way as Theorem 2.3. We will now give an error estimate for the backward Euler method.

THEOREM 3.4. *Assume that  $k_0, k_1 \in C^2([0, 1])$  are such that*

$$(3.4) \quad \|k_0\|_{L_1([0, 1])} < 1 \quad \text{and} \quad \|k_1\|_{L_1([0, 1])} < 1.$$

*Let  $U_j^n$  be the solution of (3.1), (2.5)–(2.7) and  $u \in C^{4,2}([0, 1] \times [0, T])$  be the solution of (1.1). Then there exists  $h_0 > 0$  such that*

$$|U - u|_{\mathcal{M} \times \mathcal{N}} \leq C(h^2 + k) \|u\|_{W_\infty^{4,2}} \quad \text{for} \quad h \leq h_0.$$

PROOF. As in the proof of Theorem 2.4 there exists an  $h_0$  such that for  $h \leq h_0$



assumption (3.3) is valid. With  $Z_j^n = U_j^n - u(x_j, t_n)$  we also have

$$(3.5) \quad |l_0 Z|_{\mathcal{N}} \leq Ch^2 \|u\|_{W_\infty^{2,0}},$$

$$(3.6) \quad |l_M Z|_{\mathcal{N}} \leq Ch^2 \|u\|_{W_\infty^{2,0}},$$

and

$$(3.7) \quad Z_j^0 = 0.$$

For  $(\bar{\mathcal{L}}Z)_j^n$  we have

$$\begin{aligned} (\bar{\mathcal{L}}Z)_j^n &= (\bar{\mathcal{L}}u)_j^n - \bar{\mathcal{L}}u(x_j, t_n) = F_j^n - \bar{\mathcal{L}}u(x_j, t_n) = f(x_j, t_n) - \bar{\mathcal{L}}u(x_j, t_n) \\ &= \left( \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} \right) - (\bar{\partial}_t u - \partial_x \bar{\partial}_x u) = \bar{\tau}_j^n. \end{aligned}$$

The truncation error  $\bar{\tau}_j^n$  is expanded in Taylor series as in the proof of Theorem 2.4 and it follows that

$$(3.8) \quad |\bar{\mathcal{L}}Z|_{\mathcal{M} \times \mathcal{N}} \leq C(h^2 + k) \|u\|_{W_\infty^{4,2}}.$$

The a priori estimate of Lemma 3.2, and (3.5)–(3.8) now give

$$\|U - u\|_{\mathcal{M} \times \mathcal{N}} \leq C(h^2 + k) \|u\|_{W_\infty^{4,2}},$$

which completes the proof of Theorem 3.4.  $\blacksquare$

#### 4. The Crank-Nicolson method.

In the previous section we discussed an implicit  $O(h^2 + k)$  method, based on the implicit backward Euler scheme. We will now present another implicit method, based on the Crank-Nicolson scheme, which is of order  $O(h^2 + k^2)$ . In addition to the mesh points  $(x_j, t_n) = (jh, nk)$  we define  $t_{n+1/2} = (n + 1/2)k$ . The discrete solution is now given by the following system of equations:

$$(4.1) \quad \partial_t U_j^n - \partial_x \bar{\partial}_x \left( \frac{U_j^{n+1} + U_j^{n-1}}{2} \right) = F_j^n, \quad \begin{aligned} j &= 1, \dots, M-1, \\ 0 \leq n &\leq N-1, \end{aligned}$$

$$\begin{aligned} U_0^n &= \langle K_0, U^n \rangle + G_0^n, & 1 \leq n \leq N, \\ U_M^n &= \langle K_M, U^n \rangle + G_M^n, & 1 \leq n \leq N, \\ U_j^0 &= u_0(x_j), & j = 0, \dots, M, \end{aligned}$$

where  $K_0, K_M, G_0^n, G_M^n$  are defined by (2.5), (2.6), and  $F_j^n$  by

$$(4.2) \quad F_j^n = f(x_j, t_{n+1/2}).$$

Since the maximum principle for the Crank-Nicolson method is only valid for the mesh ratio  $\lambda \leq 1$ , we will use the energy method to derive an error estimate in maximum norm. For vectors  $V = (V_0, V_1, \dots, V_M)$  we thus introduce the norm

$$\|V\| = \langle V, V \rangle^{1/2} = \left\{ \frac{h}{2} (V_0^2 + V_M^2) + h \sum_{j=1}^{M-1} V_j^2 \right\}^{1/2}$$

corresponding to the inner product  $\langle \cdot, \cdot \rangle$ , defined in (2.3). We also define discrete analogues of the  $L_2$ -norm on  $[0, T]$  and  $[0, 1] \times [0, T]$  by

$$\|V\|_N = \left( k \sum_{n=0}^N (V^n)^2 \right)^{1/2},$$

and

$$\| \|V\| \|_N = \left( k \sum_{n=0}^N \|V^n\|^2 \right)^{1/2}.$$

In order to be able to give expressions such as  $\langle \partial_x V, W \rangle$  a meaning we extend the vectors  $V$  and  $W$  by  $V_{-1} = V_{M+1} = W_{-1} = W_{M+1} = 0$ . In the case when  $V_0 = V_M = W_0 = W_M = 0$ , we then have by partial summation that

$$\begin{aligned} (4.3) \quad \langle \partial_x V, W \rangle &= h \sum_{j=0}^M \frac{V_{j+1} - V_j}{h} W_j = -h \sum_{j=0}^M V_j \frac{W_j - W_{j-1}}{h} \\ &= -\langle V, \bar{\partial}_x W \rangle. \end{aligned}$$

As in the previous sections we define a discrete operator  $\tilde{\mathcal{L}} = \tilde{\mathcal{L}}_{kh}$ , associated with the left hand side of the first equation in our discrete problem (4.1),

$$(4.4) \quad (\tilde{\mathcal{L}}U)_j^n = \partial_t U_j^n - \partial_x \bar{\partial}_x \left( \frac{U_j^{n+1} + U_j^n}{2} \right), \quad j = 1, \dots, M-1, \quad 0 \leq n \leq N-1.$$

The operators  $l_0$  and  $l_M$  are defined by (2.9).

We are now prepared to state an a priori estimate for (4.1).

LEMMA 4.1. *Assume that there exist  $h_0$  and  $q < 1$  such that for all  $h \leq h_0$*

$$(4.5) \quad \|K_0\| + \|K_M\| \leq q(3/(4 + 2h_0^2))^{1/2}.$$

*Then we have, for  $h \leq h_0$ ,*

$$(4.6) \quad \|U\|_{\mathcal{M} \times \mathcal{N}} \leq C \{ \| \tilde{\mathcal{L}}U \|_N + \|U^0\| + \| \partial_x U^0 \| + \| \partial_t l_0 U \|_N + \| \partial_t l_M U \|_N \}.$$

The proof of this a priori estimate is based on the following two lemmas. The first is an energy estimate.

LEMMA 4.2. Assume that  $W_0^l = W_M^l = 0$ , for  $l \leq n$ . Then

$$(4.7) \quad \|\partial_t W\|_{n-1}^2 + \|\bar{\partial}_x W^n\|^2 \leq \|\bar{\partial}_x W^0\|^2 + \|\tilde{\mathcal{L}}W\|_{n-1}^2.$$

PROOF. By the definition of  $\tilde{\mathcal{L}}W$  we have

$$\partial_t W_j^l - \partial_x \bar{\partial}_x \left( \frac{W_j^{l+1} + W_j^l}{2} \right) = (\tilde{\mathcal{L}}W)_j^l, \quad j = 1, \dots, M-Z, \quad l \geq 0.$$

Multiply this equation by  $h\partial_t W_j^l$  and sum over  $j$ . By use of partial summation as in (4.3) we find, since  $W_j^l$  vanishes for  $j = 0$  and  $M$ , that

$$(4.8) \quad \|\partial_t W^l\|^2 + \left\langle \bar{\partial}_x \frac{W^{l+1} + W^l}{2}, \bar{\partial}_x \partial_t W^l \right\rangle = \langle (\tilde{\mathcal{L}}W)^l, \partial_t W^l \rangle.$$

We now rewrite the second term on the left hand side as follows:

$$\begin{aligned} \left\langle \bar{\partial}_x \frac{W^{l+1} + W^l}{2}, \bar{\partial}_x \partial_t W^l \right\rangle &= \left\langle \partial_x \frac{W^{l+1} + W^l}{2}, \bar{\partial}_x \frac{W^{l+1} - W^l}{k} \right\rangle \\ &= \frac{1}{2k} (\|\bar{\partial}_x W^{l+1}\|^2 - \|\bar{\partial}_x W^l\|^2) \\ &= \frac{1}{2} \partial_t \|\bar{\partial}_x W^l\|^2. \end{aligned}$$

Together with (4.8) this shows

$$\begin{aligned} \|\partial_t W^l\|^2 + \frac{1}{2} \partial_t \|\bar{\partial}_x W^l\|^2 &\leq \|(\tilde{\mathcal{L}}W)^l\| \|\partial_t W^l\| \\ &\leq \frac{1}{2} \|(\tilde{\mathcal{L}}W)^l\|^2 + \frac{1}{2} \|\partial_t W^l\|^2, \end{aligned}$$

and hence

$$\|\partial_t W^l\|^2 + \partial_t \|\bar{\partial}_x W^l\|^2 \leq \|(\tilde{\mathcal{L}}W)^l\|^2.$$

Multiplication of this equation by  $k$ , and summation over  $l$ , from 0 to  $n-1$  gives the desired result. ■

LEMMA 4.3. Assume that  $W_0^n = W_M^n = 0$ . Then

$$\max_{j \in \mathcal{M}} |W_j^n| \leq \|\bar{\partial}_x W^n\|.$$

PROOF. Since  $W_0^n = 0$  we have that

$$W_j^n = h \sum_{l=1}^j \bar{\partial}_x W_l^n, \quad j = 1, \dots, M$$

Hence, since  $W_0^n = W_M^n = 0$ ,

$$\begin{aligned} \max_{j \in \mathcal{M}} |W_j^n| &= \max_{1 \leq j \leq M-1} \left| h \sum_{l=1}^j \bar{\partial}_x W_l^n \right| \leq h \sum_{l=1}^{M-1} |\bar{\partial}_x W_l^n| \\ &= \langle |\bar{\partial}_x W^n|, 1 \rangle - \frac{h}{2} (|\bar{\partial}_x W_0^n| + |\bar{\partial}_x W_M^n|) \\ &\leq \langle |\bar{\partial}_x W^n|, 1 \rangle \leq \|\bar{\partial}_x W^n\| \|1\| = \|\bar{\partial}_x W^n\|. \quad \blacksquare \end{aligned}$$

We will now prove Lemma 4.1.

PROOF. Set

$$(4.9) \quad W_j^n = U_j^n - (1 - x_j) \{ \langle K_0, U^n \rangle - (l_0 U)^n \} - x_j \{ \langle K_M, U^n \rangle - (l_M U)^n \}.$$

Then we have

$$(4.10) \quad \begin{aligned} (\tilde{\mathcal{L}}W)_j^n &= (\tilde{\mathcal{L}}U)_j^n - (1 - x_j) \{ \langle K_0, \partial_t U^n \rangle - \partial_t (l_0 U)^n \} \\ &\quad - x_j \{ \langle K_M, \partial_t U^n \rangle - \partial_t (l_M U)^n \}. \end{aligned}$$

Since the function  $W_j^n$  vanishes for  $j = 0$  and  $M$  we may apply Lemma 4.2 to get

$$(4.11) \quad \|\partial_t W\|_{n-1}^2 + \|\bar{\partial}_x W^n\|^2 \leq \|\bar{\partial}_x W^0\|^2 + \|\tilde{\mathcal{L}}W\|_{n-1}^2, \quad 1 \leq n \leq N.$$

We will now estimate the right hand side of (4.11). We first note that

$$\|1 - x_j\| = \|x_j\| = \left( \frac{h}{2} (0 + (Mh)^2) + h^3 \sum_{j=1}^{M-1} j^2 \right)^{1/2} = ((2 + h^2)/6)^{1/2} \equiv \gamma h.$$

We also note that

$$|\langle K_i, \partial_t U^n \rangle| \leq \|K_i\| \|\partial_t U^n\|, \quad i = 0, M.$$

Let  $\alpha_h = \gamma h (\|K_0\| + \|K_M\|)$ . From equation (4.10) we thus obtain

$$(4.12) \quad \begin{aligned} \|\tilde{\mathcal{L}}W\|_{n-1} &\leq \|\tilde{\mathcal{L}}U\|_{n-1} + \gamma h \{ (\|K_0\| + \|K_M\|) \|\partial_t U\|_{n-1} \\ &\quad + \|\partial_t l_0 U\|_{n-1} + \|\partial_t l_M U\|_{n-1} \} \\ &\leq \|\tilde{\mathcal{L}}U\|_{n-1} + \alpha_h \|\partial_t U\|_{n-1} \\ &\quad + \gamma h (\|\partial_t l_0 U\|_{n-1} + \|\partial_t l_M U\|_{n-1}). \end{aligned}$$

We now need an estimate of  $\|\partial_t U\|_{n-1}$  in terms of  $\|\partial_t W\|_{n-1}$ . By taking a time difference in (4.9) we have

$$\partial_t W_j^n = \partial_t U_j^n - (1 - x_j) \{ \langle K_0, \partial_t U^n \rangle - \partial_t (l_0 U)^n \} - x_j \{ \langle K_M, \partial_t U^n \rangle - \partial_t (l_M U)^n \},$$

and hence

$$\|\partial_t U\|_{n-1} \leq \|\partial_t W\|_{n-1} + \alpha_h \|\partial_t U\|_{n-1} + \gamma h (\|\partial_t l_0 U\|_{n-1} + \|\partial_t l_M U\|_{n-1}).$$

By assumption we have  $\alpha_h < 1/2$ , and hence

$$\|\partial_t U\|_{n-1} \leq \frac{1}{1 - \alpha_h} \{ \|\partial_t W\|_{n-1} + \gamma_h (\|\partial_t l_0 U\|_{n-1} + \|\partial_t l_M U\|_{n-1}) \}.$$

Using this in (4.12) gives

$$\begin{aligned} \|\tilde{\mathcal{L}}W\|_{n-1} &\leq \frac{\alpha_h}{1 - \alpha_h} \|\partial_t W\|_{n-1} + \|\tilde{\mathcal{L}}U\|_{n-1} \\ &\quad + \frac{\gamma_h}{1 - \alpha_h} (\|\partial_t l_0 U\|_{n-1} + \|\partial_t l_M U\|_{n-1}). \end{aligned}$$

For the second term on the right hand side of (4.11) we now have

$$(4.13) \quad \begin{aligned} \|\tilde{\mathcal{L}}W\|_{n-1}^2 &\leq (1 + \delta) \left( \frac{\alpha_h}{1 - \alpha_h} \right)^2 \|\partial_t W\|_{n-1}^2 \\ &\quad + C(\delta) \{ \|\tilde{\mathcal{L}}U\|_{n-1}^2 + \|\partial_t l_0 U\|_{n-1}^2 + \|\partial_t l_M U\|_{n-1}^2 \}, \end{aligned}$$

where  $\delta > 0$  is an arbitrary number. For  $h \leq h_0$  we have  $\alpha_h \leq \varrho/2 < 1/2$  and hence  $\frac{\alpha_h}{1 - \alpha_h} \leq \beta < 1$ . This makes it possible to choose  $\delta$ , uniformly in  $h$ , such that

$$(1 + \delta) \left( \frac{\alpha_h}{1 - \alpha_h} \right)^2 \leq \tilde{\beta} < 1.$$

Combining (4.11) with (4.13) yields

$$\|\bar{\partial}_x W^n\|^2 \leq \|\bar{\partial}_x W^0\|^2 + C(\|\tilde{\mathcal{L}}U\|_{n-1}^2 + \|\partial_t l_0 U\|_{n-1}^2 + \|\partial_t l_M U\|_{n-1}^2),$$

and hence

$$(4.14) \quad \|\bar{\partial}_x W^n\| \leq \|\bar{\partial}_x W^0\| + C(\|\tilde{\mathcal{L}}U\|_N + \|\partial_t l_0 U\|_N + \|\partial_t l_M U\|_N), \quad n \leq N.$$

From (4.9) we have

$$\|\bar{\partial}_x W^0\| \leq \|\bar{\partial}_x U^0\| + \alpha_h \|U^0\| + |(l_0 U)^0| + |(l_M U)^0|,$$

which gives

$$\begin{aligned} \|\bar{\partial}_x W^n\| &\leq C(\|\tilde{\mathcal{L}}U\|_N + \|U^0\| + \|\bar{\partial}_x U^0\| + \|\partial_t l_0 U\|_N \\ &\quad + \|\partial_t l_M U\|_N + |(l_0 U)^0| + |(l_M U)^0|), \quad n \leq N. \end{aligned}$$

By Lemma 4.3, we thus have

$$\begin{aligned} |W|_{\mathcal{M} \times \mathcal{N}} &\leq C(\|\tilde{\mathcal{L}}U\|_N + \|U^0\| + \|\bar{\partial}_x U^0\| + \|\partial_t l_0 U\|_N \\ &\quad + |(l_0 U)^0| + \|\partial_t l_M U\|_N + |(l_M U)^0|). \end{aligned}$$

Finally, we have to replace  $W$  in the inequality above by  $U$ . From the definition of  $W_j^n$ , (4.9), we have

$$|U|_{\mathcal{M} \times \mathcal{N}} \leq |W|_{\mathcal{M} \times \mathcal{N}} + (\|K_0\| + \|K_M\|)|U|_{\mathcal{M} \times \mathcal{N}} + |l_0 U|_{\mathcal{N}} + |l_M U|_{\mathcal{N}},$$

and, since by assumption  $\|K_0\| + \|K_M\| \leq \sqrt{3}/2 < 1$ , we get

$$\begin{aligned} |U|_{\mathcal{M} \times \mathcal{N}} &\leq C(\|\tilde{\mathcal{L}}U\|_N + \|U^0\| + \|\bar{\partial}_x U^0\| \\ &\quad + |l_0 U|_{\mathcal{N}} + \|\partial_t l_0 U\|_N + |l_M U|_{\mathcal{N}} + \|\partial_t l_M U\|_N). \end{aligned}$$

The terms  $|l_0 N|_{\mathcal{N}}$ ,  $|l_M U|_{\mathcal{N}}$  above can be estimated in terms of  $\|U^0\|$ ,  $\|\bar{\partial}_x U^0\|$  and  $\|\partial_t l_0 U\|_N$ ,  $\|\partial_t l_M U\|_N$ . To prove this, use the definition of  $l_0$ ,  $l_M$  and estimates analogous to Lemma 4.3. This concludes the proof of Lemma 4.1.  $\blacksquare$

The existence and uniqueness of the solution to equations (4.1) now follows from Lemma 4.1.

**THEOREM 4.4.** *If there exist  $h_0$  and  $\varrho < 1$  such that,*

$$\|K_0\| + \|K_M\| \leq \varrho(3/(4 + 2h_0^2))^{1/2}, \quad \text{for } h \leq h_0,$$

*then our discrete problem (4.1) admits a unique solution.*

The proof of Theorem 4.4 is analogous to that of Theorem 2.3.

We are now prepared to give an error estimate.

**THEOREM 4.5.** *Assume that  $k_0, k_1 \in C^2([0, 1])$  are such that*

$$(4.15) \quad \|k_0\|_{L_2((0, 1))} + \|k_1\|_{L_2((0, 1))} < \sqrt{3}/2.$$

*Let  $u \in C^{4,3}([0, 1] \times [0, T])$  be the solution of (1.1) and  $U_j^n$  that of (4.1). Then there exists  $h_0 > 0$  such that*

$$(4.16) \quad |U - u|_{\mathcal{M} \times \mathcal{N}} \leq C(h^2 + k^2) \|u\|_{W_{\infty}^{4,3}}, \quad \text{for } h \leq h_0.$$

**PROOF.** The proof is an application of Lemma 4.1 to the error  $Z_j^n = U_j^n - u(x_j, t_n)$ . We first note that from (4.15) it follows that there exist  $h_0 > 0$  and  $\varrho < 1$  such that for  $h \leq h_0$  assumption (4.5) is true. We have

$$(\tilde{\mathcal{L}}Z)_j^n = (\tilde{\mathcal{L}}U)_j^n - \tilde{\mathcal{L}}u(x_j, t_n) = \tilde{\tau}_j^n.$$

The local truncation error,  $\tilde{\tau}_j^n$ , is rewritten as in the proof of Theorem 2.4 and expanded in Taylor series around  $(x_n, t_{n+1/2})$ . This shows

$$(4.17) \quad \|\tilde{\tau}\|_N = \|\tilde{\mathcal{L}}Z\|_N \leq C(h^2 + k^2) \|u\|_{W_{\infty}^{4,3}}.$$

For the initial value  $Z_j^0$  we find

$$Z_j^0 = U_j^0 - u(x_j, 0) = U_j^0 - u_0(x_j) = 0, \quad j = 0, \dots, M,$$

and hence

$$(4.18) \quad \|Z^0\| = \|\bar{\partial}_x Z^0\| = 0.$$

We shall now estimate the term in (4.6) associated with the boundary  $x = 0$ . From (2.17) we have

$$(l_0 Z)^n = \varepsilon_h(k_0 u(\cdot, t_n))$$

and hence

$$\partial_t(l_0 Z)^n = \varepsilon_h(k_0 \partial_t u(\cdot, t_n)),$$

where  $\varepsilon_h$  is the quadrature error. By (2.1) we have

$$|\partial_t(l_0 Z)^n| \leq Ch^2 \|k_0 \partial_t u(\cdot, t_n)\|_{W_\infty^{2,0}} \leq Ch^2 \|\partial_t u(\cdot, t_n)\|_{W_\infty^{2,0}}.$$

But

$$|\partial_t u(x, t_n)| = k^{-1} \left| \int_{t_n}^{t_{n+1}} \frac{\partial u}{\partial t}(x, \tau) d\tau \right| \leq \left\| \frac{\partial u}{\partial t}(x, \cdot) \right\|_{L_\infty([0, T])}$$

and hence

$$(4.19) \quad \|\partial_t l_0 Z\|_N \leq Ch^2 \|u\|_{W_\infty^{2,1}}.$$

The estimate of  $\|\partial_t l_M U\|_N$  is analogous. Theorem 4.5 now follows from Lemma 4.1 and (4.17), (4.18), (4.19). ■

## 5. A numerical example.

In this section, we will present numerical experiments where we apply our three discrete methods to a specific problem, namely

$$(5.1) \quad \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = e^{-t} \left\{ x(x-1) + \frac{\delta^2}{6(1+\delta^2)} + 2 \right\}, \quad x \in [0, 1], \quad t > 0,$$

$$u(0, t) = -\delta^2 \int_0^1 u(x, t) dx, \quad t > 0,$$

$$u(1, t) = -\delta^2 \int_0^1 u(x, t) dx, \quad t > 0,$$

$$u(x, 0) = x(x-1) + \frac{\delta^2}{6(1+\delta^2)}, \quad x \in [0, 1],$$

where  $\delta = 0.12$ . The boundary kernels,  $k_0 = k_1 = -\delta^2$ , are taken from an example

in Day [1]. The exact solution of (5.1) is given by

$$u(x, t) = e^{-t} \left\{ x(x-1) + \frac{\delta^2}{6(1+\delta^2)} \right\}.$$

The forward Euler system is solved as described in Section 2. The backward Euler system (3.1) and the Crank-Nicolson system (4.1) are treated as general linear systems of equations, with full matrices, and solved by the NAG-library routines F03AFF, for triangular decomposition, and F04AHF, for calculating the solution.

Below are three tables, representing sample calculations using each of the discrete methods. The first column in each table lists the mesh parameter  $M$ , the second shows the error, measured in maximum norm on the  $M \times N$  mesh, covering  $[0, 1] \times [0, T]$ . In the third column the number of time steps required to compute the solution to time  $T = 1.0$  are listed, and the last column shows the amount of CPU-time used, in seconds, for the computation on an IBM 3090 computer. Since the implementation of the backward Euler and Crank-Nicolson methods do not take advantage of the structure of the matrices involved (tridiagonal with full top

Table 1. *Forward Euler method,  $k = 0.4h^2$ .*

| $M$ | Error<br>$ U - u _{M \times N}$ | Number of<br>time steps | CPU-time<br>(seconds) |
|-----|---------------------------------|-------------------------|-----------------------|
| 2   | $1.1 \cdot 10^{-3}$             | 11                      | 0.07                  |
| 4   | $1.5 \cdot 10^{-4}$             | 41                      | 0.04                  |
| 8   | $3.7 \cdot 10^{-5}$             | 161                     | 0.03                  |
| 16  | $9.4 \cdot 10^{-6}$             | 641                     | 0.22                  |
| 32  | $2.3 \cdot 10^{-6}$             | 2561                    | 1.62                  |
| 65  | $5.7 \cdot 10^{-7}$             | 10563                   | 13.15                 |
| 130 | $1.5 \cdot 10^{-7}$             | 42251                   | 103.75                |

Table 2. *Backward Euler method,  $k = \sqrt{h}$*

| $M$ | Error<br>$ U - u _{M \times N}$ | Number of<br>time steps | CPU-time<br>(seconds) |
|-----|---------------------------------|-------------------------|-----------------------|
| 2   | $3.5 \cdot 10^{-3}$             | 3                       | 0.08                  |
| 4   | $1.3 \cdot 10^{-3}$             | 8                       | 0.08                  |
| 8   | $4.4 \cdot 10^{-4}$             | 23                      | 0.09                  |
| 16  | $1.6 \cdot 10^{-4}$             | 64                      | 0.18                  |
| 32  | $5.6 \cdot 10^{-5}$             | 182                     | 0.92                  |
| 65  | $1.9 \cdot 10^{-5}$             | 525                     | 8.34                  |
| 130 | $6.7 \cdot 10^{-6}$             | 1483                    | 81.90                 |



Table 3. *Crank-Nicolson method,  $h = k$ .*

| $M$ | Error<br>$ U - u _{M \times N}$ | Number of<br>time steps | CPU-time<br>(seconds) |
|-----|---------------------------------|-------------------------|-----------------------|
| 2   | $7.5 \cdot 10^{-3}$             | 2                       | 0.07                  |
| 4   | $1.7 \cdot 10^{-3}$             | 4                       | 0.07                  |
| 8   | $3.6 \cdot 10^{-4}$             | 8                       | 0.08                  |
| 16  | $8.4 \cdot 10^{-5}$             | 16                      | 0.10                  |
| 32  | $2.1 \cdot 10^{-5}$             | 32                      | 0.22                  |
| 65  | $5.0 \cdot 10^{-6}$             | 66                      | 1.13                  |
| 130 | $1.3 \cdot 10^{-6}$             | 131                     | 7.51                  |

and bottom rows), the CPU-time used by these two methods is not fully comparable to that of the the forward Euler method.

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