# The Crank-Nicolson Hermite Cubic Orthogonal Spline Collocation Method for the Heat Equation with Nonlocal Boundary Conditions

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Dedicated to Professor Graeme Fairweather in honor of his 70<sup>th</sup> Birthday.

**Abstract.** We formulate and analyze the Crank-Nicolson Hermite cubic orthogonal spline collocation method for the solution of the heat equation in one space variable with nonlocal boundary conditions involving integrals of the unknown solution over the spatial interval. Using an extension of the analysis of Douglas and Dupont [23] for Dirichlet boundary conditions, we derive optimal order error estimates in the discrete maximum norm in time and the continuous maximum norm in space. We discuss the solution of the linear system arising at each time level via the capacitance matrix technique and the package COLROW for solving almost block diagonal linear systems. We present numerical examples that confirm the theoretical global error estimates and exhibit superconvergence phenomena.

AMS subject classifications: 65N35, 65N12, 65N15

**Key words**: Heat equation, nonlocal boundary conditions, orthogonal spline collocation, Hermite cubic splines, convergence analysis, superconvergence.

# 1 Introduction

Consider the heat equation

$$u_t - u_{xx} = f(x,t), \quad x \in [0,1], \quad t \in [0,T],$$
(1.1)

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subject to the initial condition

$$u(x,0) = g(x), \quad x \in [0,1],$$
 (1.2)

and the nonlocal boundary conditions

$$u(0,t) = \int_0^1 \alpha(x)u(x,t)dx + g_0(t), \quad u(1,t) = \int_0^1 \beta(x)u(x,t)dx + g_1(t), \quad t \in [0,T], \quad (1.3)$$

where  $\alpha, \beta \in C[0,1]$  and

$$\|\alpha\|_{L^1(0,1)} < 1, \quad \|\beta\|_{L^1(0,1)} < 1.$$
 (1.4)

It is shown in [14] that such problems arise in thermoelasticity. The existence, uniqueness and properties of solutions, even in several space variables, have been studied in [14, 15, 28, 31].

Finite difference methods have been used frequently for the numerical solution of (1.1)-(1.3). One of the first was that of Wang and Lin [48] who formulated a method based on the Crank-Nicolson (CN) method with Simpson's rule to approximate the integrals in (1.3). No analysis was provided. Ekolin [24] considered the forward and backward Euler methods and the CN method, each with the trapezoidal rule for the approximation of the integrals, and derived error estimates for all three methods. Ekolin's analysis of the CN method requires the condition

$$\|\alpha\|_{L^{2}(0,1)} + \|\beta\|_{L^{2}(0,1)} < \frac{\sqrt{3}}{2},$$
(1.5)

in addition to (1.4). Liu [36] considered  $\theta$ -methods with  $\theta \ge 1/2$  and derived error estimates with (1.5) replaced by the weaker condition

$$\|\alpha\|_{L^{2}(0,1)}^{2} + \|\beta\|_{L^{2}(0,1)}^{2} < 2.$$
(1.6)

In [43], Pan provided analyses of the forward and backward Euler methods without constraints on the functions  $\alpha$  and  $\beta$ . Sun [47] derived a method which is fourth-order accurate in space and second-order in time under the condition

$$\|\alpha\|_{L^2(0,1)} + \|\beta\|_{L^2(0,1)} < \sqrt{0.432}.$$
(1.7)

This method is based on the high-order method (HOM) of Douglas [21] (which is not referenced in [47]) together with Simpson's rule for the approximation of the integrals. In [40], the method claimed by Dehghan [17] to be fourth-order in space is shown to be only second-order, and the correct fourth-order method is derived, a method which is similar to that of Sun [47]. In [17, 40], this implicit method is called Crandall's method when in fact it is also based on the HOM of Douglas of which the method of Crandall [13] is the special case in which a specific value of the mesh ratio yields an explicit method. A

new fourth-order explicit method is considered in [38] together with the method of Crandall [13]. To obtain accuracy higher than second-order in time, multi-time level methods are derived in [41]. Richardson extrapolation is used in [7] to improve the accuracy of finite difference approximations based on the  $\theta$ -method. In [27], a method based on Keller's box scheme [32] is formulated in which the problem is rewritten as a first order system in which no integral terms appear. Stability analyses of basic finite difference methods are given in [5, 11, 30, 45].

With the assumption that

$$\|\alpha\|_{L^2(0,1)} < 1, \quad \|\beta\|_{L^2(0,1)} < 1$$

the CN and extrapolated CN schemes for the quasilinear equation

$$u_t - (a(x)u_x)_x = f(x,t,u), \quad x \in [0,1], \quad t \in [0,T],$$

with a finite element Galerkin discretization in space were formulated and analyzed in [25]. See also [8], where methods based on the  $\theta$ -method instead of the CN method are analyzed in a similar fashion.

Other numerical techniques for the solution of (1.1)-(1.3) include methods based on Laplace transforms [1,3], radial basis functions [18], nodal spline collocation methods in which the approximate solution is expressed in terms of B-splines in both x and t [33], the Adomian decomposition method [4, 16], a spectral collocation method [29], and a reproducing kernel method [42]. Ang [2] adopted a method of lines approach in which the problem is first reformulated as an integro-differential equation by integrating (1.1) with respect to x, which is approximated using a nodal collocation method. The timestepping is then performed using a multi-step method. Yousefi et al. [49] also recast the problem as an integrodifferential equation, which they solve using a nodal collocation method on the space-time domain in which the approximate solution is expressed in terms of Bernstein polynomials in each variable. A brief numerical comparison of some methods is given in [9].

In this paper, we formulate and analyze a new method in which orthogonal spline collocation with Hermite cubic splines is used for the spatial discretization and the time-stepping is performed using the CN method. For the approximation of the integrals in (1.3), the composite two-point Gauss quadrature rule is employed. To describe this method, we assume that  $\{x_i\}_{i=0}^N$  is a uniform partition of [0,1]; that is,

$$x_i = ih$$
,  $i = 0, \dots, N$ ,  $h = 1/N$ .

The space  $V_h$  of piecewise Hermite cubic splines on [0,1] is defined by

$$V_h = \{ v \in C^1[0,1] : v|_{[x_{i-1},x_i]} \in P_3, \ i = 1, \cdots, N \},$$
(1.8)

where  $P_3$  is the set of polynomials of degree  $\leq 3$ . Let  $\mathcal{G} = \{\xi_{i,k}\}_{i=1,k=1}^{N,2}$  be the set of collocation (Gauss) points defined by

$$\xi_{i,1} = x_{i-1} + \xi_1 h, \quad \xi_{i,2} = x_{i-1} + \xi_2 h, \quad i = 1, \cdots, N,$$

where

$$\xi_1 = \frac{3 - \sqrt{3}}{6}, \quad \xi_2 = \frac{3 + \sqrt{3}}{6}.$$
 (1.9)

Assume  $\{t_n\}_{n=0}^M$  is a uniform partition of [0,T] with  $t_n = n\tau$ ,  $n = 0, \dots, M$ , where  $\tau = T/M$ , and let  $t_{n-1/2} = (t_{n-1}+t_n)/2$ ,  $n = 1, \dots, M$ .

In the CN method, we seek  $\{U^n\}_{n=0}^M \subset V_h$  such that

$$\partial_t U^n(\xi) - U^{n-1/2}_{xx}(\xi) = f(\xi, t_{n-1/2}), \quad \xi \in \mathcal{G}, \quad n = 1, \cdots, M,$$
(1.10)

where

$$\partial_t U^n = \frac{U^n - U^{n-1}}{\tau}, \quad U^{n-1/2} = \frac{U^n + U^{n-1}}{2},$$

with  $U^0$  defined by

$$U_{xx}^{0}(\xi) = g''(\xi), \quad \xi \in \mathcal{G},$$
 (1.11)

and the nonlocal boundary conditions

$$U^{n}(0) = \langle \alpha, U^{n} \rangle + g_{0}(t_{n}), \quad U^{n}(1) = \langle \beta, U^{n} \rangle + g_{1}(t_{n}), \quad n = 0, \cdots, M,$$
(1.12)

where

$$\langle w, z \rangle = \frac{h}{2} \sum_{i=1}^{N} \sum_{k=1}^{2} (wz)(\xi_{i,k}).$$
 (1.13)

An outline of the remainder of this paper is as follows. In the next section, some basic results are presented. The existence and uniqueness of the approximate solution defined by the CN scheme (1.10)-(1.12) are proved in Section 3, followed by convergence analyses in Section 4. The analyses are carried out under the Assumptions (1.4) and (1.6), and that u,  $\alpha$ ,  $\beta$  are sufficiently smooth so that

$$\int_0^1 \alpha(x)u(x,t_n)dx - \langle \alpha, u(\cdot,t_n) \rangle = \mathcal{O}(h^4); \qquad (1.14)$$

see, for example, [12, (7.54b)]. In Section 5, an algorithm for the solution of the linear equations arising at each time step is described, and in Section 6 results of numerical experiments are presented which confirm the theoretical global error estimates and exhibit superconvergence. In the final section, Section 7, the paper is summarized and future research outlined.

### 2 Preliminaries

Throughout the paper, *C* denotes a positive constant which is independent of *h* and  $\tau$ . Let the subspace  $V_h^0$  of  $V_h$  in (1.8) be defined by

$$V_h^0 = \{ v \in V_h : v(0) = v(1) = 0 \}.$$

It follows from [23, Lemmas 3.1, 3.3] that

$$\langle v'', z \rangle = \langle v, z'' \rangle, \quad v, z \in V_h^0,$$
 (2.1)

and

$$\|v'\|_{L^2(0,1)}^2 \le -\langle v'', v \rangle, \quad v \in V_h^0.$$
 (2.2)

Since  $\xi_1$  and  $\xi_2$  of (1.9) satisfy the inequalities

$$0 < \xi_1 < \frac{1}{2}, \quad \frac{1}{2} < \xi_2 < 1,$$

it follows that  $\langle w, z \rangle$  of (1.13) is a Riemann sum of  $wz : [0,1] \to R$  corresponding to the partition  $\{ih/2\}_{i=0}^{2N}$  of [0,1]. Hence, since  $\alpha, \beta \in C[0,1]$ , we have

$$\lim_{h \to 0} \langle |\alpha|, 1 \rangle = \|\alpha\|_{L^{1}(0,1)}, \quad \lim_{h \to 0} \langle |\beta|, 1 \rangle = \|\beta\|_{L^{1}(0,1)},$$
(2.3a)

$$\lim_{h \to 0} \left[ \langle \alpha, \alpha \rangle + \langle \beta, \beta \rangle \right] = \|\alpha\|_{L^2(0,1)}^2 + \|\beta\|_{L^2(0,1)}^2.$$
(2.3b)

It follows from (1.6) and (2.3b) that, for all *h* sufficiently small,

$$\langle \alpha, \alpha \rangle + \langle \beta, \beta \rangle < 2.$$
 (2.4)

We introduce the following averages:

$$\rho_{\alpha} = \frac{\|\alpha\|_{L^{1}(0,1)} + 1}{2}, \quad \rho_{\beta} = \frac{\|\beta\|_{L^{1}(0,1)} + 1}{2}, \quad \rho = \frac{\|\alpha\|_{L^{2}(0,1)}^{2} + \|\beta\|_{L^{2}(0,1)}^{2} + 2}{2}.$$
(2.5)

It follows from (2.5), (1.4), and (1.6) that

$$\|\alpha\|_{L^{1}(0,1)} < \rho_{\alpha} < 1, \quad \|\beta\|_{L^{1}(0,1)} < \rho_{\beta} < 1, \quad \|\alpha\|_{L^{2}(0,1)}^{2} + \|\beta\|_{L^{2}(0,1)}^{2} < \rho < 2.$$
(2.6)

Using (2.6), (2.3a), and (2.3b), for all h sufficiently small, we have

$$\langle |\alpha|,1 \rangle \leq \rho_{\alpha}, \quad \langle |\beta|,1 \rangle \leq \rho_{\beta}, \quad \langle \alpha, \alpha \rangle + \langle \beta, \beta \rangle \leq \rho.$$
 (2.7)

Since, by (2.6),  $\rho < 2$ , the last inequality in (2.7) is stronger than the inequality in (2.4). While the inequality in (2.4) is used to prove existence and uniqueness of the approximate solution, the last inequality in (2.7) is used in our convergence analysis.

Consider the functions

$$\phi_0(x) = 1 - x, \quad \phi_1(x) = x.$$
 (2.8)

Since the two-point Gauss quadrature rule is exact for polynomials of degree  $\leq$  3, we have

$$\langle \phi_i, \phi_i \rangle = \|\phi_i^2\|_{L^2(0,1)}^2 = \frac{1}{3}, \quad i = 0, 1, \quad \langle \phi_0, \phi_1 \rangle = \|\phi_0\|_{L^2(0,1)}^2 = \frac{1}{6}.$$
 (2.9)

In the following analysis, frequent use is made of the inequality

$$ab \le \epsilon a^2 + \frac{b^2}{4\epsilon}, \quad a, b \in \mathbb{R}, \quad \epsilon > 0.$$
 (2.10)

In the remainder of this section, we assume that u is a sufficiently smooth function on [0,1] and W and U in  $V_h$  are defined by

$$W(x_i) = u(x_i), \quad W'(x_i) = u'(x_i), \quad i = 0, \cdots, N,$$

the Hermite cubic spline interpolant of *u*, and

$$U''(\xi) = u''(\xi), \quad \xi \in \mathcal{G}, \quad U(0) = u(0), \quad U(1) = u(1),$$
 (2.11)

respectively. Then it follows from the first line of (5.6) in [22] that

$$\langle u'' - W'', \nu \rangle \le Ch^4 \sum_{i=1}^{N} \left( h^{1/2} \| \nu' \|_{L^2(x_{i-1}, x_i)} + h^{1/2} \langle \nu, \nu \rangle_i^{1/2} \right), \quad \nu \in V_h^0,$$
(2.12)

where

$$\langle w, z \rangle_i = \frac{h}{2} \sum_{k=1}^{2} (wz)(\xi_{i,k}), \quad i = 1, \cdots, N.$$

Using (2.12), the Cauchy-Schwarz inequality, (1.13), the inequality [22, (2.6)], namely

$$\langle v, v \rangle^{1/2} \leq C \| v \|_{L^2(0,1)}, \quad v \in V_h^0,$$

and the Poincaré inequality, we have

$$\langle u'' - W'', \nu \rangle \le Ch^4 \left( \|\nu'\|_{L^2(0,1)} + \langle \nu, \nu \rangle^{1/2} \right) \le Ch^4 \|\nu'\|_{L^2(0,1)}, \quad \nu \in V_h^0.$$
(2.13)

It follows from (2.2), (2.11), and (2.13) with v = W - U that

$$||W' - U'||_{L^{2}(0,1)}^{2} \leq -\langle U'' - W'', U - W \rangle = \langle u'' - W'', W - U \rangle \leq Ch^{4} ||W' - U'||_{L^{2}(0,1)},$$

which gives

$$\|W' - U'\|_{L^2(0,1)} \le Ch^4.$$
(2.14)

Then, using Sobolev's inequality

$$\|W - U\|_{L^{\infty}(0,1)} \le \|W' - U'\|_{L^{2}(0,1)}$$

(since (W - U)(0) = 0) and (2.14), we obtain

$$\|W - U\|_{L^{\infty}(0,1)} \le Ch^4.$$
 (2.15)

Also, we have the well-known property of the Hermite cubic spline interpolant (cf. [12, (6.78)]) that

$$\|u - W\|_{L^{\infty}(0,1)} \le Ch^4.$$
 (2.16)

Using the triangle inequality, (2.15) and (2.16), we have

$$\|u - U\|_{L^{\infty}(0,1)} \le \|u - W\|_{L^{\infty}(0,1)} + \|W - U\|_{L^{\infty}(0,1)} \le Ch^{4}.$$
(2.17)

(The bound  $||u-U||_{L^{\infty}(0,1)} \leq Ch^4$  is derived in [6] using a different approach.) Using (2.13), (2.10) and (2.2), we also obtain

$$\langle u'' - W'', \nu \rangle \le \epsilon \|\nu'\|_{L^2(0,1)}^2 + Ch^8 \le \epsilon \langle -\nu'', \nu \rangle + Ch^8, \quad \nu \in V_h^0, \quad \epsilon > 0.$$
(2.18)

# 3 Existence and uniqueness of approximate solution

To show uniqueness, and hence existence, of the approximate solution  $U^n$ ,  $n = 1, \dots, M$ , satisfying (1.10) and (1.12), we consider  $U \in V_h$  such that

$$2U(\xi) - \tau U''(\xi) = 0, \quad \xi \in \mathcal{G}, \quad U(0) = \langle \alpha, U \rangle, \quad U(1) = \langle \beta, U \rangle; \tag{3.1}$$

cf. (1.10) and (1.12) with  $U^{n-1} = f = g_0 = g_1 = 0$ , and U replacing  $U^n$ . Introduce

$$\overline{U} = U - [U(0)\phi_0 + U(1)\phi_1], \qquad (3.2)$$

where  $\phi_0$ ,  $\phi_1$  are defined in (2.8). Since  $U'' = \overline{U}''$  and  $\overline{U} \in V_h^0$ , we have from (3.1) and (2.2) that

$$0 = 2\langle U, \overline{U} \rangle - \tau \langle \overline{U}'', \overline{U} \rangle \ge 2\langle U, \overline{U} \rangle = \langle \overline{U}, \overline{U} \rangle + \langle U, U \rangle - \langle U - \overline{U}, U - \overline{U} \rangle.$$
(3.3)

Using (3.2), (2.9), (2.10), (3.1), the Cauchy-Schwarz inequality, and (2.4), for all h sufficiently small, we have

$$\langle U - \overline{U}, U - \overline{U} \rangle = U^{2}(0) \langle \phi_{0}, \phi_{0} \rangle + U^{2}(1) \langle \phi_{1}, \phi_{1} \rangle + 2U(0)U(1) \langle \phi_{0}, \phi_{1} \rangle$$

$$= \frac{1}{3} [U^{2}(0) + U^{2}(1) + U(0)U(1)] \leq \frac{1}{2} [U^{2}(0) + U^{2}(1)]$$

$$= \frac{1}{2} [\langle \alpha, U \rangle^{2} + \langle \beta, U \rangle^{2}] \leq \frac{1}{2} [\langle \alpha, \alpha \rangle + \langle \beta, \beta \rangle] \langle U, U \rangle$$

$$\leq \langle U, U \rangle.$$

$$(3.4)$$

Combining (3.3) and (3.4), we obtain  $\langle \overline{U}, \overline{U} \rangle \leq 0$  which, by [23, Lemma 2.3] (since  $\overline{U} \in V_h^0$ ), implies  $\overline{U} = 0$ . Hence by (3.2) and (2.8),

$$|U||_{L^{\infty}(0,1)} = ||U(0)\phi_0 + U(1)\phi_1||_{L^{\infty}(0,1)} = \max\{|U(0)|, |U(1)|\}.$$
(3.5)

Using (3.1), (1.13), and the triangle inequality, we have

$$|U(0)| = |\langle \alpha, U \rangle| \le \langle |\alpha|, 1 \rangle ||U||_{L^{\infty}(0,1)}, \quad |U(1)| = |\langle \beta, U \rangle| \le \langle |\beta|, 1 \rangle ||U||_{L^{\infty}(0,1)}.$$
(3.6)

It follows from (3.5), (3.6), and (2.7) that, for all h sufficiently small, we have

$$\|U\|_{L^{\infty}(0,1)} \le \max\{\rho_{\alpha}, \rho_{\beta}\} \|U\|_{L^{\infty}(0,1)}.$$
(3.7)

But, by (2.6),  $\max\{\rho_{\alpha}, \rho_{\beta}\} < 1$ . Hence  $||U||_{L^{\infty}(0,1)} = 0$  and U = 0. This completes the proof of the existence and uniqueness of the approximate solution  $U^n$ ,  $n = 1, \dots, M$ , for all h sufficiently small.

To show uniqueness, and hence existence, of  $U^0 \in V_h$  satisfying (1.11) and (1.12) with n = 0, consider  $U \in V_h$  such that

$$U''(\xi) = 0, \quad \xi \in \mathcal{G}, \quad U(0) = \langle \alpha, U \rangle, \quad U(1) = \langle \beta, U \rangle; \tag{3.8}$$

cf. (1.11) and (1.12) with n = 0,  $g'' = g_0 = g_1 = 0$ , and U replacing  $U^0$ . With  $\overline{U}$  defined in (3.2), using (3.8),  $U'' = \overline{U}''$ ,  $\overline{U} \in V_h^0$ , and (2.2), we have

$$0 = \langle -\overline{U}'', \overline{U} \rangle \geq \|\overline{U}'\|_{L^2(0,1)}^2,$$

which, by a Poincaré inequality, implies  $\overline{U}=0$ . Hence, by the arguments in (3.5)-(3.7), we have U=0. This completes the proof of the existence and uniqueness of the approximate solution  $U^0$  for all h sufficiently small.

We summarize the preceding in the following theorem.

**Theorem 3.1.** Assume that  $\alpha, \beta \in C[0,1]$ ,  $g \in C^2[0,1]$ , and that (1.4) and (1.6) hold. Then, for all *h* sufficiently small, the CN scheme (1.10)-(1.12) has a unique solution.

#### 4 Convergence analysis

To bound the error between the exact solution u of (1.1)-(1.3) and the approximate solution  $\{U^n\}_{n=0}^N$  of (1.10)-(1.12), we introduce

$$v^n = W^n - U^n, \quad \eta^n = u^n - W^n, \quad n = 0, \cdots, M,$$
(4.1)

where  $u^n(\cdot) = u(\cdot, t_n)$ , and  $W^n(\cdot) = W(\cdot, t_n)$ , with  $W(\cdot, t) \in V_h$ ,  $t \in [0, T]$ , defined by

$$W_{xx}(\xi,t) = u_{xx}(\xi,t), \quad \xi \in \mathcal{G}, \quad W(0,t) = u(0,t), \quad W(1,t) = u(1,t), \quad t \in [0,T].$$
(4.2)

It follows from (4.2) and (2.17) and then from replacing u and W with  $u_t$  and  $W_t$ , respectively, that

$$\|u(\cdot,t) - W(\cdot,t)\|_{L^{\infty}(0,1)} \le Ch^{4}, \quad \|(u - W)_{t}(\cdot,t)\|_{L^{\infty}(0,1)} \le Ch^{4}, \quad t \in [0,T].$$
(4.3)

The inequalities in (4.3) and the identity

$$\partial_t \eta^n(\cdot) = \tau^{-1} \int_{t_{n-1}}^{t_n} (u - W)_t(\cdot, s) ds$$

give

$$\|\eta^n\|_{L^{\infty}(0,1)} \le Ch^4, \quad n = 0, \cdots, M, \quad \|\partial_t \eta^n\|_{L^{\infty}(0,1)} \le Ch^4, \quad n = 1, \cdots, M.$$
 (4.4)

Using (4.1), (1.10), (4.2), (1.1), (4.4), and Taylor's theorem, we have

$$\begin{aligned} \partial_t v^n(\xi) - v_{xx}^{n-1/2}(\xi) &= \partial_t W^n(\xi) - W_{xx}^{n-1/2}(\xi) - f(\xi, t_{n-1/2}) \\ &= -\partial_t \eta^n(\xi) + \partial_t u^n(\xi) - u_t(\xi, t_{n-1/2}) + u_{xx}(\xi, t_{n-1/2}) - u_{xx}^{n-1/2}(\xi) \\ &= \mathcal{O}(h^4 + \tau^2), \quad \xi \in \mathcal{G}, \quad n = 1, \cdots, M. \end{aligned}$$

$$(4.5)$$

Let

$$\overline{\nu}^n = \nu^n - [\nu^n(0)\phi_0 + \nu^n(1)\phi_1], \quad n = 0, \cdots, M,$$
(4.6)

where  $\phi_0$  and  $\phi_1$  are defined in (2.8). Then on using (4.5) and  $v_{xx}^{n-1/2} = \overline{v}_{xx}^{n-1/2}$ , we have

$$2\langle \partial_t \nu^n, \partial_t \overline{\nu}^n \rangle - 2\langle \overline{\nu}_{xx}^{n-1/2}, \partial_t \overline{\nu}^n \rangle = \langle \mathcal{O}(h^4 + \tau^2), \partial_t \overline{\nu}^n \rangle, \quad n = 1, \cdots, M.$$
(4.7)

It is easy to verify that

$$2\langle\partial_t \nu^n, \partial_t \overline{\nu}^n\rangle = \langle\partial_t \overline{\nu}^n, \partial_t \overline{\nu}^n\rangle + \langle\partial_t \nu^n, \partial_t \nu^n\rangle - \langle\partial_t (\nu^n - \overline{\nu}^n), \partial_t (\nu^n - \overline{\nu}^n)\rangle, \quad n = 1, \cdots, M.$$
(4.8)

Using (4.6), we have

$$\partial_t(\nu^n-\overline{\nu}^n)=\partial_t\nu^n(0)\phi_0+\partial_t\nu^n(1)\phi_1,$$

and following derivations in (3.4), we obtain

$$\langle \partial_t (\nu^n - \overline{\nu}^n), \partial_t (\nu^n - \overline{\nu}^n) \rangle \leq \frac{1}{2} \left( \left[ \partial_t \nu^n (0) \right]^2 + \left[ \partial_t \nu^n (1) \right]^2 \right), \quad n = 1, \cdots, M.$$
(4.9)

It follows from (4.1), (4.2), (1.3), (1.12), (1.14), (1.13), the boundedness of  $\alpha$ , and (4.4) that

$$\nu^{n}(0) = u^{n}(0) - U^{n}(0) = \int_{0}^{1} \alpha(x)u^{n}(x)dx - \langle \alpha, U^{n} \rangle$$
  
$$= \int_{0}^{1} \alpha(x)u^{n}(x)dx - \langle \alpha, u^{n} \rangle + \langle \alpha, \eta^{n} \rangle + \langle \alpha, \nu^{n} \rangle$$
  
$$= \mathcal{O}(h^{4}) + \langle \alpha, \nu^{n} \rangle, \quad n = 0, \cdots, M.$$
(4.10)

In a similar way and using also Taylor's theorem, we obtain

$$\begin{aligned} \partial_{t}\nu^{n}(0) &= \int_{0}^{1} \alpha(x)\partial_{t}u^{n}(x)dx - \langle \alpha, \partial_{t}u^{n} \rangle + \langle \alpha, \partial_{t}\eta^{n} \rangle + \langle \alpha, \partial_{t}\nu^{n} \rangle \\ &= \int_{0}^{1} \alpha(x) \left[ \partial_{t}u^{n}(x) - u_{t}(x, t_{n-1/2}) \right] dx + \int_{0}^{1} \alpha(x)u_{t}(x, t_{n-1/2})dx - \langle \alpha, u_{t}(\cdot, t_{n-1/2}) \rangle \\ &- \langle \alpha, \left[ \partial_{t}u^{n} - u_{t}(\cdot, t_{n-1/2}) \right] \rangle + \langle \alpha, \partial_{t}\eta^{n} \rangle + \langle \alpha, \partial_{t}\nu^{n} \rangle, \\ &= \mathcal{O}(h^{4} + \tau^{2}) + \langle \alpha, \partial_{t}\nu^{n} \rangle, \quad n = 1, \cdots, M. \end{aligned}$$

$$(4.11)$$

Using (4.11), a similar relation for  $\partial_t v^n(1)$ , (2.10), the Cauchy-Schwarz inequality, and (2.7), for all *h* sufficiently small, we obtain

$$\begin{split} \left[\partial_{t}\nu^{n}(0)\right]^{2} + \left[\partial_{t}\nu^{n}(1)\right]^{2} \\ \leq \langle \alpha, \partial_{t}\nu^{n} \rangle^{2} + \langle \alpha, \partial_{t}\nu^{n} \rangle \mathcal{O}(h^{4} + \tau^{2}) + \langle \beta, \partial_{t}\nu^{n} \rangle^{2} + \langle \beta, \partial_{t}\nu^{n} \rangle \mathcal{O}(h^{4} + \tau^{2}) + C(h^{8} + \tau^{4}) \\ \leq (1 + \epsilon) \left[ \langle \alpha, \partial_{t}\nu^{n} \rangle^{2} + \langle \beta, \partial_{t}\nu^{n} \rangle^{2} \right] + C(h^{8} + \tau^{4}) \\ \leq (1 + \epsilon) \left[ \langle \alpha, \alpha \rangle + \langle \beta, \beta \rangle \right] \langle \partial_{t}\nu^{n}, \partial_{t}\nu^{n} \rangle + C(h^{8} + \tau^{4}) \\ \leq (1 + \epsilon)\rho \langle \partial_{t}\nu^{n}, \partial_{t}\nu^{n} \rangle + C(h^{8} + \tau^{4}), \quad n = 1, \cdots, M, \quad \epsilon > 0. \end{split}$$
(4.12)

It follows from (2.6) that  $0 < \rho < 2$ . Hence, for  $\epsilon = (2-\rho)/\rho$ , we have  $\epsilon > 0$  and  $(1+\epsilon)\rho = 2$ . Therefore (4.12) gives

$$\frac{1}{2}\left(\left[\partial_t \nu^n(0)\right]^2 + \left[\partial_t \nu^n(1)\right]^2\right) \le \langle \partial_t \nu^n, \partial_t \nu^n \rangle + C(h^8 + \tau^4), \quad n = 1, \cdots, M.$$
(4.13)

Using (4.8), (4.9), (4.13), we have

$$2\langle \partial_t \nu^n, \partial_t \overline{\nu}^n \rangle \ge \langle \partial_t \overline{\nu}^n, \partial_t \overline{\nu}^n \rangle - C(h^8 + \tau^4), \quad n = 1, \cdots, M.$$
(4.14)

For the right-hand side of (4.7), using the Cauchy-Schwarz inequality, (2.10), we have

$$\langle \mathcal{O}(h^4 + \tau^2), \partial_t \overline{\nu}^n \rangle \leq \langle \partial_t \overline{\nu}^n, \partial_t \overline{\nu}^n \rangle + C(h^8 + \tau^4), \quad n = 1, \cdots, M.$$
(4.15)

Using (4.7), (4.14), and (4.15), we obtain

$$-2\langle \overline{\nu}_{xx}^{n-1/2}, \partial_t \overline{\nu}^n \rangle \leq C(h^8 + \tau^4), \quad n = 1, \cdots, M,$$

which, on using  $\overline{\nu}^n \in V_h^0$  and (2.1), gives

$$\langle -\overline{\nu}_{xx}^{n},\overline{\nu}^{n}\rangle \leq \langle -\overline{\nu}_{xx}^{n-1},\overline{\nu}^{n-1}\rangle + C\tau(h^{8}+\tau^{4}), \quad n=1,\cdots,M.$$
 (4.16)

Applying (4.16) repeatedly, we obtain

$$\langle -\overline{\nu}_{xx}^{n}, \overline{\nu}^{n} \rangle \leq \langle -\overline{\nu}_{xx}^{0}, \overline{\nu}^{0} \rangle + C(h^{8} + \tau^{4}), \quad n = 0, \cdots, M.$$
(4.17)

Using  $\overline{v}_{xx}^{0} = v_{xx}^{0}$ , (4.2), (1.2), and (1.11), we see that  $\overline{v}_{xx}^{0}(\xi) = 0$ ,  $\xi \in \mathcal{G}$ , and hence (4.17) yields

$$\langle -\overline{\nu}_{xx}^n, \overline{\nu}^n \rangle^{1/2} \le C(h^4 + \tau^2), \quad n = 0, \cdots, M.$$
 (4.18)

It follows from (4.6), the triangle inequality, and (2.8), that

$$\|\nu^{n}\|_{L^{\infty}(0,1)} \leq \|\overline{\nu}^{n}\|_{L^{\infty}(0,1)} + \max\{|\nu^{n}(0)|, |\nu^{n}(1)|\}, \quad n = 0, \cdots, M.$$
(4.19)

Using (4.10), a similar relation for  $v^n(1)$ , (1.13), and the triangle inequality, we have

$$|\nu^{n}(0)| \leq Ch^{4} + \langle |\alpha|, 1 \rangle ||\nu^{n}||_{L^{\infty}(0,1)}, \quad |\nu^{n}(1)| \leq Ch^{4} + \langle |\beta|, 1 \rangle ||\nu^{n}||_{L^{\infty}(0,1)}, \quad n = 0, \cdots, M,$$

which, on using (2.7) gives, for all h sufficiently small,

$$\max\{|\nu^{n}(0)|,|\nu^{n}(1)|\} \leq Ch^{4} + \max\{\rho_{\alpha},\rho_{\beta}\} \|\nu^{n}\|_{L^{\infty}(0,1)}, \quad n = 0, \cdots, M.$$
(4.20)

Since, by (2.6),  $\max\{\rho_{\alpha}, \rho_{\beta}\} < 1$ , (4.19) and (4.20) imply

$$\|\nu^n\|_{L^{\infty}(0,1)} \le C \|\overline{\nu}^n\|_{L^{\infty}(0,1)} + Ch^4, \quad n = 0, \cdots, M.$$
 (4.21)

Using Sobolev's inequality

$$\|\overline{\nu}^n\|_{L^{\infty}(0,1)} \leq \|\overline{\nu}_x^n\|_{L^2(0,1)}$$

(since  $\overline{\nu}^n(0) = 0$ ),  $\overline{\nu}^n \in V_h^0$ , and (2.2), we have

$$\|\overline{\nu}^n\|_{L^{\infty}(0,1)} \leq \langle -\overline{\nu}^n_{xx}, \overline{\nu}^n \rangle^{1/2}, \quad n = 0, \cdots, M.$$
(4.22)

Hence (4.21), (4.22), and (4.18) give

$$\|\nu^n\|_{L^{\infty}(0,1)} \le C(h^4 + \tau^2), \quad n = 0, \cdots, M.$$
 (4.23)

Finally, it follows from (4.1), the triangle inequality, (4.4), and (4.23) that, for all h sufficiently small,

$$\|u^{n} - U^{n}\|_{L^{\infty}(0,1)} = \|\eta^{n}\|_{L^{\infty}(0,1)} + \|v^{n}\|_{L^{\infty}(0,1)} \le C(h^{4} + \tau^{2}), \quad n = 0, \cdots, M,$$
(4.24)

which shows that the scheme (1.10)-(1.12) is fourth-order accurate in x and second-order accurate in t.

This completes the proof of the following theorem.

**Theorem 4.1.** Assume that  $\alpha, \beta \in C^4[0,1]$ , (1.4) and (1.6) hold,  $u \in C^{0,3}([0,1] \times [0,T])$ ,  $u \in C^{2,2}([0,1] \times [0,T])$ ,  $u \in C([0,T]; H^6(0,1))$ ,  $u_t \in C([0,T]; H^6(0,1))$ . Then, for all h sufficiently small, we have (4.24).

In the remainder of this section, we re-examine the CN scheme and its convergence analysis, with  $U^0 \in V_h$  satisfying (1.12) for n = 0 and (1.11) replaced by

$$U_{xx}^{0}(\xi) = \tilde{g}^{\prime\prime}(\xi), \quad \xi \in \mathcal{G}, \tag{4.25}$$

where  $\tilde{g} \in V_h$  is defined by

$$\tilde{g}(x_i) = g(x_i), \quad \tilde{g}'(x_i) = g'(x_i), \quad i = 0, \cdots, N;$$
(4.26)

that is,  $\tilde{g}$  is the Hermite cubic spline interpolant of g. In this case  $W(\cdot, t) \in V_h$ ,  $t \in [0,T]$ , is defined as in [22,23] by

$$W(x_i,t) = u(x_i,t), \quad W_x(x_i,t) = u_x(x_i,t), \quad i = 0, \cdots, N.$$
 (4.27)

In place of (4.5), we have

$$\partial_t v^n(\xi) - v_{xx}^{n-1/2}(\xi) = \mathcal{O}(h^4 + \tau^2) + \eta_{xx}^{n-1/2}(\xi), \quad \xi \in \mathcal{G}, \quad n = 1, \cdots, M.$$

Consequently, in place of (4.16), we have

$$\langle -\overline{\nu}_{xx}^{n}, \overline{\nu}^{n} \rangle \leq \langle -\overline{\nu}_{xx}^{n-1}, \overline{\nu}^{n-1} \rangle + C\tau(h^{8} + \tau^{4}) + 2\tau \langle \eta_{xx}^{n-1/2}, \partial_{t}\overline{\nu}^{n} \rangle, \quad n = 1, \cdots, M,$$

whose repeated application yields

$$\langle -\overline{\nu}_{xx}^{n}, \overline{\nu}^{n} \rangle \leq \langle -\overline{\nu}_{xx}^{0}, \overline{\nu}^{0} \rangle + C(h^{8} + \tau^{4}) + 2\tau \sum_{k=1}^{n} \langle \eta_{xx}^{k-1/2}, \partial_{t} \overline{\nu}^{k} \rangle, \quad n = 1, \cdots, M.$$

$$(4.28)$$

We now follow closely the approach of [23]. First we verify directly that

$$\tau \sum_{k=1}^{n} \langle \eta_{xx}^{k-1/2}, \partial_t \overline{\nu}^k \rangle = \langle \eta_{xx}^{n-1/2}, \overline{\nu}^n \rangle - \langle \eta_{xx}^{1/2}, \overline{\nu}^0 \rangle - \frac{1}{2} \sum_{k=1}^{n-1} \langle \eta_{xx}^{k+1} - \eta_{xx}^{k-1}, \overline{\nu}^k \rangle, \quad n = 1, \cdots, M.$$
(4.29)

Next, the relation

$$\eta_{xx}^{k+1}(\xi) - \eta_{xx}^{k-1}(\xi) = \int_{t_{k-1}}^{t_{k+1}} \eta_{xxt}(\xi, s) ds, \quad \xi \in \mathcal{G}, \quad k = 1, \cdots, M-1,$$

yields

$$\langle \eta_{xx}^{k+1} - \eta_{xx}^{k-1}, \overline{\nu}^k \rangle = \int_{t_{k-1}}^{t_{k+1}} \langle \eta_{txx}(\cdot, s), \overline{\nu}^k \rangle ds, \quad k = 1, \cdots, M-1.$$
(4.30)

Using (2.18), we have

$$\langle \eta_{xx}^{n-1/2}, \overline{\nu}^n \rangle \leq \epsilon \langle -\overline{\nu}_{xx}^n, \overline{\nu}^n \rangle + Ch^8, \quad \langle \eta_{xx}^{1/2}, -\overline{\nu}^0 \rangle \leq \langle -\overline{\nu}_{xx}^0, \overline{\nu}^0 \rangle + Ch^8.$$
 (4.31)

Using also (2.18) but with u and W replaced with  $u_t$  and  $W_t$ , respectively, we have

$$\langle \eta_{txx}(\cdot,s), -\overline{\nu}^k \rangle \leq \langle -\overline{\nu}^k_{xx}, \overline{\nu}^k \rangle + Ch^8, \quad s \in [t_{k-1}, t_{k+1}], \quad k = 1, \cdots, M-1,$$

which along with (4.30) gives

$$\langle \eta_{xx}^{k+1} - \eta_{xx}^{k-1}, -\overline{\nu}^k \rangle \leq 2\tau \langle -\overline{\nu}_{xx}^k, \overline{\nu}^k \rangle + C\tau h^8, \quad k = 1, \cdots, M-1.$$
(4.32)

Combining (4.29), (4.31), and (4.32), we have

$$\tau \sum_{k=1}^{n} \langle \eta_{xx}^{k-1/2}, \partial_t \overline{\nu}^k \rangle \leq \epsilon \langle -\overline{\nu}_{xx}^n, \overline{\nu}^n \rangle + \langle -\overline{\nu}_{xx}^0, \overline{\nu}^0 \rangle + \tau \sum_{k=1}^{n-1} \langle -\overline{\nu}_{xx}^k, \overline{\nu}^k \rangle + Ch^8, \quad n = 1, \cdots, M.$$
(4.33)

Using (4.28) and (4.33) with  $\epsilon$  sufficiently small, we obtain

$$\langle -\overline{\nu}_{xx}^{n}, \overline{\nu}^{n} \rangle \leq C \langle -\overline{\nu}_{xx}^{0}, \overline{\nu}^{0} \rangle + C(h^{8} + \tau^{4}) + C\tau \sum_{k=0}^{n-1} \langle -\overline{\nu}_{xx}^{k}, \overline{\nu}^{k} \rangle, \quad n = 0, \cdots, M.$$

$$(4.34)$$

The discrete Gronwall inequality states that if  $\alpha_n \ge 0$  and  $\beta_n \ge 0$  for  $n = 0, \dots, M$ ,  $\beta_n \le \beta_{n+1}$  for  $n = 0, \dots, M-1$ , and

$$\alpha_n \leq \beta_n + C\tau \sum_{k=0}^{n-1} \alpha_k, \quad n = 0, \cdots, M,$$

then

$$\alpha_n \leq e^{C\tau n}\beta_n, \quad n=0,\cdots,M.$$

Applying the discrete Gronwall inequality to (4.34), we get (cf. (4.17))

$$\langle -\overline{\nu}_{xx}^{n}, \overline{\nu}^{n} \rangle \leq C \langle -\overline{\nu}_{xx}^{0}, \overline{\nu}^{0} \rangle + C(h^{8} + \tau^{4}), \quad n = 0, \cdots, M.$$
 (4.35)

Using  $\overline{v}_{xx}^0 = v_{xx}^0$ , (4.27), (1.2), (4.25), and (4.26), we see that  $\overline{v}_{xx}^0(\xi) = 0$ ,  $\xi \in \mathcal{G}$ ; hence (4.35) yields (4.18). Proceeding now as in the first convergence analysis we arrive at (4.24), which shows that the scheme consisting of (1.10), (4.25), (4.26), and (1.12) is fourth-order accurate in *x* and second order-accurate in *t*.

Note that  $U^0$  of (1.11) requires knowledge of g'' while  $U^0$  of (4.25) and (4.26) requires knowledge of g and g'. Hence the second choice of  $U^0$  seems more advantageous.

### 5 Algebraic problem

For  $n = 0, \dots, M, U^n \in V_h$  and hence

$$U^{n}(x) = \sum_{i=0}^{N} [c_{2i}v_{i}(x) + c_{2i+1}s_{i}(x)], \quad x \in [0,1],$$

where, with  $\delta_{ij}$  denoting the Kronecker delta, the value and scaled slope basis functions  $v_i$  and  $s_i$  for  $V_h$  are defined by

$$v_i(x_j) = \delta_{ij}, \quad v'_i(x_j) = 0, \quad s_i(x_j) = 0, \quad s'_i(x_j) = h^{-1}\delta_{ij}, \quad i, j = 0, \cdots, N.$$

Finding  $U^n$ ,  $n = 1, \dots, M$ , which satisfy (1.10) and (1.12), is equivalent to solving a linear system

$$A\mathbf{c} = \mathbf{d},\tag{5.1}$$

where

$$\mathbf{c} = [c_0, \cdots, c_{2N+1}]^T$$
,  $\mathbf{d} = [d_0, \cdots, d_{2N+1}]^T$ ,

and the  $(2N+2) \times (2N+2)$  nonsingular matrix *A* has the following form, displayed here for N = 4:

The first and last rows of *A* correspond to (1.12). Hence all matrix entries in these rows are nonzero. The remaining rows of *A* form  $2 \times 4$  nonzero blocks overlapping in two columns. Assume that *B* is the matrix whose rows are the same as the corresponding rows in *A*, except that the first and last rows of *B* are

$$[1,0,\cdots,0,0,0,0], [0,0,\cdots,0,0,1,0],$$

respectively. These two rows correspond to Dirichlet boundary conditions; that is,  $\alpha = \beta = 0$  in (1.12). Then *B* is almost block diagonal (ABD) [26] and nonsingular [23]. A linear system with coefficient matrix *B* can be solved at a cost O(N) using the package COLROW of [19, 20] for solving ABD linear systems. Since *A* and *B* differ only in the first and last rows, the system (5.1) can be solved using the capacitance matrix approach of [10] as follows. We look for the solution **c** of (5.1) in the form

$$\mathbf{c} = \mathbf{r} + \gamma_1 \mathbf{p} + \gamma_2 \mathbf{q}, \tag{5.2}$$

where the numbers  $\gamma_1$  and  $\gamma_2$  are to be determined and the vectors **r**, **p**, **q** satisfy

$$B\mathbf{r} = [0, d_1, \cdots, d_{2N}, 0]^T, \quad B\mathbf{p} = [1, 0, \cdots, 0, 0]^T, \quad B\mathbf{q} = [0, 0, \cdots, 0, 1]^T.$$
(5.3)

It follows from

$$A(i,:) = B(i,:), \quad i = 1, \cdots, 2N,$$

and (5.3) that

$$A(i,:)(\mathbf{r}+\gamma_1\mathbf{p}+\gamma_2\mathbf{q})=d_i, \quad i=1,\cdots,2N,$$

for any  $\gamma_1$  and  $\gamma_2$ . Moreover,

$$A(i,:)(\mathbf{r}+\gamma_1\mathbf{p}+\gamma_2\mathbf{q}) = A(i,:)\mathbf{r}+\gamma_1A(i,:)\mathbf{p}+\gamma_2A(i,:)\mathbf{q}, \quad i=0,2N+1.$$

Hence **c** given by the right-hand side of (5.2) satisfies (5.1) if and only if  $\gamma_1$  and  $\gamma_2$  satisfy the linear system

$$\begin{bmatrix} A(0,:)\mathbf{p} & A(0,:)\mathbf{q} \\ A(2N+1,:)\mathbf{p} & A(2N+1,:)\mathbf{q} \end{bmatrix} \begin{bmatrix} \gamma_1 \\ \gamma_2 \end{bmatrix} = \begin{bmatrix} d_0 \\ d_{2N+1} \end{bmatrix} - \begin{bmatrix} A(0,:)\mathbf{r} \\ A(2N+1,:)\mathbf{r} \end{bmatrix}.$$
 (5.4)

Since *A* and *B* are nonsingular, it follows from Theorem 1 in [10] that the 2×2 matrix in (5.4) is nonsingular also. Hence we obtain the solution **c** of the system (5.1) by first computing, with the help of COLROW, **r**, **p**, and **q** of (5.3). Then we set up and solve the system (5.4), and finally we form **c** using (5.2). The cost of the entire computation is O(N).

### 6 Numerical results

Since, according to (4.24), the scheme (1.10)-(1.12) is fourth-order accurate in *x* and second-order accurate in *t* with T = 1, we set  $M = N^2$  so that  $\tau^2 = h^4$  and solved a test problem in which

$$u(x,t) = e^{-t}[\sin(\pi x) + \cos(\pi x)], \quad \alpha(x) = 2\sin(\pi x), \quad \beta(x) = -2\cos(\pi x),$$

for which

$$f(x,t) = (\pi^2 - 1)e^{-t}[\sin(\pi x) + (\cos \pi x)], \quad g(x) = \sin(\pi x) + \cos(\pi x), \quad g_0(t) = g_1(t) = 0,$$

cf. [38,48,49]. At the final time level  $t_M = 1$ , we computed the nodal and global errors for u, defined by

$$E_N^n(u) = \max_{\substack{i=0,\dots,N\\j=0,\dots,N-1\\j=0,\dots,10}} |u(x_i,1) - U^M(x_i)|,$$
  
$$E_N^g(u) = \max_{\substack{i=0,\dots,N-1\\j=0,\dots,10}} |u(x_i+jh/10,1) - U^M(x_i+jh/10)| \approx ||u(\cdot,1) - U^M||_{L^{\infty}(0,1)},$$

and the nodal and global errors for  $u_x$  defined by the same formulas but with  $u_x$  and  $U_x^M$  replacing u and  $U^M$ , respectively. We also computed the corresponding convergence rates using the formula

$$\operatorname{Rate} = \frac{\log(E_{N/2}/E_N)}{\log 2},$$

	$E_N^n(u)$		$E_N^g(u)$		$E_N^n(u_x)$		$E_N^g(u_x)$	
Ν	Error	Rate	Error	Rate	Error	Rate	Error	Rate
10	8.93-06		1.61-05		3.07-05		4.13-04	
20	5.59-07	3.998	1.08-06	3.904	1.92-06	3.998	5.10-05	3.019
30	1.10-07	3.999	2.17-07	3.950	3.80-07	3.996	1.51-05	3.002
40	3.49-08	4.000	6.94-08	3.966	1.20-07	4.000	6.36–06	3.007
50	1.43-08	4.000	2.86-08	3.974	4.92-08	4.001	3.25-06	3.001

Table 1: Nodal and global errors and convergence rates.

where  $E_{N/2}$  and  $E_N$  represent either the nodal or global errors for either u or  $u_x$ . The results presented in Table 1 show the fourth-order convergence rates for  $E_N^n(u)$ ,  $E_N^g(u)$ ,  $E_N^n(u_x)$ , and the third-order convergence rate for  $E_N^g(u_x)$ . The fourth-order convergence rate for  $E_N^n(u_x)$  demonstrates superconvergence. We obtained essentially the same results as in Table 1 for  $U^0 \in V_h$  defined by (1.11) and (1.12) replaced, for n = 0, by

$$U^{0}(0) = g(0), \quad U^{0}(1) = g(1).$$
 (6.1)

For this choice of  $U^0$ , our theoretical convergence analysis is not applicable, since, for example, (4.10) and (4.11) were obtained assuming (1.12) for all *n*, including n = 0. In some papers on the finite difference solution of (1.1)-(1.3), the initial finite difference approximation  $U^0 = \{U_i^0\}_{i=0}^N$  corresponding to t = 0 is defined by

$$U_i^0 = g(x_i), \quad i = 0, \cdots, N.$$
 (6.2)

However, for such finite difference choice of the initial approximation, it is claimed incorrectly, for example, by Ekolin [24] and Liu [36], that their theoretical convergence analyses give the optimal error bounds. These convergence analyses do yield the optimal error bounds but for the finite difference initial approximation  $U^0$  defined by (6.2) with  $i=1, \dots, N-1$ , and the two equations

$$U_0^0 = \frac{h}{2}\alpha(0)U_0^0 + h\sum_{i=1}^{N-1}\alpha(x_i)U_i^0 + \frac{h}{2}\alpha(1)U_N^0 + g_0(0),$$
  
$$U_N^0 = \frac{h}{2}\beta(0)U_0^0 + h\sum_{i=1}^{N-1}\beta(x_i)U_i^0 + \frac{h}{2}\beta(1)U_N^0 + g_1(0),$$

the composite trapezoidal rule discretizations of (1.3).

We obtained essentially the same results as in Table 1 for  $U^0 \in V_h$  defined by (1.12) with n = 0, (4.25) and (4.26), for  $U^0$  defined by  $U^0 = \tilde{g}$ , where  $\tilde{g} \in V_h$  is given by (4.26), as well as for  $U^0 \in V_h$  defined by

$$U^0(\xi) = g(\xi), \quad \xi \in \mathcal{G}, \quad U^0(0) = g(0), \quad U^0(1) = g(1).$$

Note that the last choice of  $U^0$  requires knowledge of g only.

#### 7 Concluding remarks

We have formulated and analyzed a CN method for the approximation of the heat equation with nonlocal boundary conditions. Two choices of the approximation to the initial condition were analyzed and it was found that both gave the predicted accuracy. This was confirmed by a numerical example from which it was also found that other choices produced similar results.

Future work will involve the extension of the analysis to nonlocal boundary conditions of the form

$$\int_0^1 u(x,t)dx = g_0(t),$$

corresponding to the specification of mass or energy (see [17] and references therein), and to splines of degree r > 3 which are expected to produce superconvergent approximations of order  $h^{2r-2}$  to both u and  $u_x$  at the nodes; cf. [23]. Nonlinear reaction-diffusion equations of the form

$$c(x,t,u)u_t - u_{xx} + b(x,t,u)u_x = f(x,t,u),$$

(cf. [35, 37, 39, 44]) and problems in higher dimensions (see [34], and [46] and references therein) will also be considered.

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