Numerical solution of a non-classical parabolic problem: an integro-differential approach

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Abstract

A numerical method based on an integro-differential formulation and approximation by local interpolating functions is proposed for solving a one-dimensional parabolic partial differential equation subject to non-classical conditions. Some specific test problems are solved using the proposed method. Numerical results obtained indicate that it can give accurate solutions and that it is an interesting and viable alternative to existing numerical methods for solving the class of problems under consideration.

Keywords: Parabolic equation; non-classical conditions; local interpolating functions; integro-differential equation.

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1 Introduction

Of interest here is the numerical solution of the one-dimensional parabolic partial differential equation of the form

$$\frac{\partial \phi}{\partial t} - q(x,t) = \frac{\partial^2 \phi}{\partial x^2} \text{ for } x \in (0,1) \text{ and } t > 0$$
(1)

subject to the initial condition

$$\phi(x,0) = f(x) \text{ for } x \in (0,1)$$
 (2)

and the non-classical conditions

$$\alpha_0 \phi(0,t) + \beta_0 p(0,t) = \int_0^{\ell_0} k_0(x) \phi(x,t) dx + r_0(t)$$

$$\alpha_1 \phi(1,t) + \beta_1 p(1,t) = \int_0^{\ell_1} k_1(x) \phi(x,t) dx + r_1(t)$$
for $t > 0$, (3)

where x and t are the spatial and time coordinates respectively, $\phi(x,t)$ is the unknown function to be determined, $p(x,t) = \partial \phi / \partial x$, α_0 , α_1 , β_0 , β_1 , ℓ_0 and ℓ_1 (with ℓ_0 and ℓ_1 selected from the real interval [0, 1]) are given constants and q(x,t), f(x), $k_0(x)$, $k_1(x)$, $r_0(t)$ and $r_1(t)$ are suitably prescribed functions.

The problem defined by (1)-(3) arises in the modeling of mass and heat transfer in many modern engineering applications. Classical initial-boundary value problems for diffusion can be recovered from (1)-(3) by letting both $k_0(x) \equiv 0$ and $k_1(x) \equiv 0$. If $\alpha_0 = \beta_0 = 0$, $k_0(x) \equiv 1$ and $k_1(x) \equiv 0$, the first equation in (3) specifies the total mass or energy stored inside a given portion of the solution domain, that is, inside the region $0 < x < \ell_0$, while the second equation implies that a certain linear combination of ϕ (concentration or temperature) and its flux is known at x = 1. Certain problems in the quasistatic theory of thermoelasticity are governed by (1)-(3) with $\alpha_0 = \alpha_1 = 1$, $\beta_0 = \beta_1 = 0$ and $\ell_0 = \ell_1 = 1$ (see, e.g. Day [1] and [2]). Finite-difference methods for the numerical solution of (1)-(3) are given by various researchers for specific cases of the problem, e.g. Cannon, Lin and Wang [3] (for $q(x,t) \equiv 0$, $\alpha_0 = \alpha_1 = \beta_0 = 0$, $\beta_1 = 1$, $k_0(x) \equiv 1$ and $k_1(x) \equiv 0$), Cannon and van der Hoek [4] (for $q(x,t) \equiv 0$, $\alpha_1 = 1$, $\alpha_0 = \beta_0 = \beta_1 = 0$, $k_0(x) \equiv 1$ and $k_1(x) \equiv 0$), Dehghan [5] (for $\alpha_1 = 1$, $\alpha_0 = \beta_0 = \beta_1 = 0$, $k_0(x) \equiv 1$ and $k_1(x) \equiv 0$) and Liu [7] (for $\alpha_0 = \alpha_1 = 1$, $\beta_0 = \beta_1 = 0$ and $\ell_0 = \ell_1 = 1$). A more extensive list of references as well as a survey on progress made on this class of problems may be found in Dehghan [5] and [6].

The present paper proposes a numerical method based on an integrodifferential formulation of the parabolic equation and the use of local interpolating functions in the approximation of ϕ for solving (1)-(3). The method reduces the problem under consideration to an initial-value problem governed by a linear system of first order ordinary differential equations containing unknown functions of time t. To solve the initial-value problem numerically, the first order time derivatives of the unknown functions are approximated using quadratic functions of t. Numerical results obtained for specific test problems indicate that the proposed method can give accurate numerical solutions and it is a useful and viable alternative to existing techniques for solving the one-dimensional parabolic equation with non-classical conditions.

2 Integro-differential formulation

The partial differential equation (1) may be re-cast into an integro-differential equation of the form

$$2\phi(x,t) = \phi(0,t) + \phi(1,t) + xp(0,t) + (x-1)p(1,t) + \int_0^1 |\xi - x| (\frac{\partial}{\partial t} [\phi(\xi,t)] - q(\xi,t)) d\xi.$$
(4)

It is easy to verify that partial differentiation of the right hand side of (4) with respect to x twice yields the term on the left hand side of (1).

The problem stated in Section 1 may now be reformulated as one which requires one to determine $\phi(x,t)$ from (4) [instead of (1)] subject to (2)-(3). It is worthwhile noting that the function $p(x,t) = \partial \phi / \partial x$ (flux) in (2)-(3) appear directly in (4). Thus, an advantage in using (4) for devising a numerical method for the problem under consideration is that it is not necessary to approximate the partial derivative $\partial \phi / \partial x$ at x = 0 and x = 1 in treating the conditions in (3). A numerical method for solving (4) subject to (2)-(3) based on approximating $\phi(x,t)$ by local interpolating functions is described below. The approach adopted may be viewed as a one-dimensional version of the well known dual-reciprocity boundary element method as described in, e.g. Zhang and Zhu [8].

3 Initial-value problem

The unknown function ϕ is approximated using

$$\phi(x,t) \simeq \sum_{m=1}^{N} \phi_m(t) \sum_{n=1}^{N} c_{nm} \sigma_n(x), \qquad (5)$$

where $\phi_m(t) = \phi(\xi_m, t), \xi_1, \xi_2, \cdots, \xi_{N-1}$ and ξ_N are N distinct well-spaced points selected from the interval [0, 1] with $\xi_1 = 0$ and $\xi_N = 1, \sigma_n(x) =$ $1 + |x - \xi_n|^{3/2}$ is the local interpolating function centered about ξ_n and c_{nm} are constant coefficients defined by

$$\sum_{k=1}^{N} \sigma_n(\xi_k) c_{pk} = \begin{cases} 1 & \text{if } n = p, \\ 0 & \text{if } n \neq p. \end{cases}$$
(6)

Note that (5) implies that $[c_{pk}]$ is the inverse matrix of $[a_{ij}]$, where $a_{ij} = \sigma_j(\xi_i)$.

Substitution of (5) into (4) with $x = \xi_r$ (for $r = 1, 2, \dots, N$) yields the

system

$$2\phi_{r}(t) + S_{r}(t) = \phi_{1}(t) + \phi_{N}(t) + \xi_{r}\theta(t) + (\xi_{r} - 1)\omega(t) + \sum_{m=1}^{N} F_{rm}\frac{d}{dt}[\phi_{m}(t)]$$

for $r = 1, 2, \cdots, N$, (7)

where $\theta(t) = p(0, t), \, \omega(t) = p(1, t)$ and

$$S_{r}(t) = \int_{0}^{1} |\xi - \xi_{r}| q(\xi, t) d\xi,$$

$$F_{rm} = \sum_{n=1}^{N} c_{nm} (\frac{1}{2} [(1 - \xi_{r})^{2} + \xi_{r}^{2}] + \frac{2}{5} [(1 - \xi_{r})(1 - \xi_{n})^{5/2} + \xi_{r}\xi_{n}^{5/2}] - \frac{4}{35} [(1 - \xi_{n})^{7/2} + \xi_{n}^{7/2}] + \frac{8}{35} |\xi_{r} - \xi_{n}|^{7/2}).$$
(8)

If the function q(x,t) in (1) is such that $S_r(t)$ as defined in (8) cannot be evaluated analytically then one may approximate q(x,t) as

$$q(x,t) \simeq \sum_{m=1}^{N} q(\xi_m,t) \sum_{n=1}^{N} c_{nm} \sigma_n(x)$$
 (9)

to obtain the approximate formula

$$S_r(t) \simeq \sum_{m=1}^{N} F_{rm} q(\xi_m, t).$$
 (10)

The system (7) comprises N linear equations containing N + 2 unknown functions of t as given by $\phi_r(t)$ $(r = 1, 2, \dots, N)$, $\theta(t)$ and $\omega(t)$. Another 2 equations are needed to complete the system. These come from the nonclassical conditions (3).

With the approximation

$$k_i(x)\phi(x,t) \simeq \sum_{m=1}^N k_i(\xi_m)\phi_m(t) \sum_{n=1}^N c_{nm}\sigma_n(x) \text{ for } i = 0, 1,$$
 (11)

the conditions in (3) may be approximately re-written as

$$\alpha_0 \phi_1(t) + \beta_0 \theta(t) - \sum_{m=1}^N G_m(\ell_0) k_0(\xi_m) \phi_m(t) = r_0(t),$$

$$\alpha_1 \phi_N(t) + \beta_1 \omega(t) - \sum_{m=1}^N G_m(\ell_1) k_1(\xi_m) \phi_m(t) = r_1(t),$$
(12)

where

$$G_m(\ell) = \sum_{n=1}^{N} c_{nm} \left(\ell + \frac{2}{5} \operatorname{sgn}(\ell - \xi_n) \left|\ell - \xi_n\right|^{5/2} + \frac{2}{5} \xi_n^{5/2}\right).$$
(13)

Thus, the problem stated in Section 1 can now be formulated approximately as an initial-value problem which requires solving (7) and (12) subject to

$$\phi_m(0) = f(\xi_m) \text{ for } m = 1, 2, \cdots, N.$$
 (14)

Note that (14) is obtained from (2).

4 Numerical procedure

A numerical procedure for solving (7) and (12) subject to (14) is as described below.

The function $\phi_n(t)$ $(n = 1, 2, \dots, N)$ is approximated as a cubic function of time t over the interval $[\tau, \tau + 3\Delta t]$, that is,

$$\phi_n(t) \simeq \frac{1}{(\Delta t)^3} \left[-\frac{1}{6} (t - \tau - \Delta t) (t - \tau - 2\Delta t) (t - \tau - 3\Delta t) \phi_n(\tau) + \frac{1}{2} (t - \tau) (t - \tau - 2\Delta t) (t - \tau - 3\Delta t) \phi_n(\tau + \Delta t) - \frac{1}{2} (t - \tau) (t - \tau - \Delta t) (t - \tau - 3\Delta t) \phi_n(\tau + 2\Delta t) + \frac{1}{6} (t - \tau) (t - \tau - \Delta t) (t - \tau - 2\Delta t) \phi_n(\tau + 3\Delta t) \right]$$
for $t \in [\tau, \tau + 3\Delta t]$. (15)

Differentiation of (15) with respect to t gives

$$\frac{d}{dt}[\phi_n(t)] \simeq \frac{1}{(\Delta t)^3} [-(\frac{1}{2}[t-\tau]^2 - 2[t-\tau]\Delta t + \frac{11}{6}[\Delta t]^2)\phi_n(\tau) \\
+ (\frac{3}{2}[t-\tau]^2 - 5[t-\tau]\Delta t + 3[\Delta t]^2)\phi_n(\tau + \Delta t) \\
- (\frac{3}{2}[t-\tau]^2 - 4[t-\tau]\Delta t + \frac{3}{2}[\Delta t]^2)\phi_n(\tau + 2\Delta t) \\
+ (\frac{1}{2}[t-\tau]^2 - [t-\tau]\Delta t + \frac{1}{3}[\Delta t]^2)\phi_n(\tau + 3\Delta t)] \\$$
for $t \in [\tau, \tau + 3\Delta t].$
(16)

If one lets $t = \tau + j\Delta t$ (for j = 1, 2, 3) in (7), after using (16), one obtains

$$2\phi_{r}(\tau + j\Delta t) + S_{r}(\tau + j\Delta t)$$

$$= \phi_{1}(\tau + j\Delta t) + \phi_{N}(\tau + j\Delta t) + \xi_{r}\theta(\tau + j\Delta t) + (\xi_{r} - 1)\omega(\tau + j\Delta t)$$

$$+ \frac{1}{\Delta t}\sum_{m=1}^{N}F_{rm}[-(\frac{1}{2}j^{2} - 2j + \frac{11}{6})\phi_{m}(\tau) + (\frac{3}{2}j^{2} - 5j + 3)\phi_{m}(\tau + \Delta t)$$

$$- (\frac{3}{2}j^{2} - 4j + \frac{3}{2})\phi_{m}(\tau + 2\Delta t) + (\frac{1}{2}j^{2} - j + \frac{1}{3})\phi_{m}(\tau + 3\Delta t)]$$
for $r = 1, 2, \cdots, N$ and $j = 1, 2, 3$. (17)

Letting $t = \tau + j\Delta t$ (for j = 1, 2, 3) in (12) gives

$$\alpha_0 \phi_1(\tau + j\Delta t) + \beta_0 \theta(\tau + j\Delta t) - \sum_{m=1}^N G_m(\ell_0) k_0(\xi_m) \phi_m(\tau + j\Delta t)$$
$$= r_0(\tau + j\Delta t) \text{ for } j = 1, 2, 3, \quad (18)$$

and

$$\alpha_1 \phi_N(\tau + j\Delta t) + \beta_1 \omega(\tau + j\Delta t) - \sum_{m=1}^N G_m(\ell_1) k_1(\xi_m) \phi_m(\tau + j\Delta t)$$
$$= r_1(\tau + j\Delta t) \text{ for } j = 1, 2, 3.$$
(19)

If $\phi_m(\tau)$ is assumed known for $m = 1, 2, \dots, N$, then (17)-(19) may be regarded as a system of 3(N+2) linear algebraic equations with 3(N+2) unknowns given by $\theta(\tau + j\Delta t)$, $\omega(\tau + j\Delta t)$ and $\phi_m(\tau + j\Delta t)$ for j = 1, 2, 3and $m = 1, 2, \dots, N$.

A time-stepping scheme for solving (17)-(19) is as follows.

Compute $\phi_m(0)$ using (14) and solve (17)-(19) with $\tau = 0$ for $\theta(\Delta t)$, $\theta(2\Delta t)$, $\theta(3\Delta t)$, $\omega(\Delta t)$, $\omega(2\Delta t)$, $\omega(3\Delta t)$, $\phi_m(\Delta t)$, $\phi_m(2\Delta t)$ and $\phi_m(3\Delta t)$. With $\phi_m(3\Delta t)$ just determined, one may then let $\tau = 3\Delta t$ in (17)-(19) to solve for $\theta(4\Delta t)$, $\theta(5\Delta t)$, $\theta(6\Delta t)$, $\omega(4\Delta t)$, $\omega(5\Delta t)$, $\omega(6\Delta t)$, $\phi_m(4\Delta t)$, $\phi_m(5\Delta t)$ and $\phi_m(6\Delta t)$. The process may be repeated using $\tau = 6\Delta t$, $9\Delta t$, $12\Delta t$, \cdots to solve for the unknown functions $\phi_m(t)$, $\theta(t)$ and $\omega(t)$ at higher and higher time levels.

5 Specific problems

Problem 1. For an example problem from Day [1], take

$$q(x,t) = -[x(x-1) + \frac{\delta}{6\{1+\delta\}} + 2] \exp(-t),$$

$$f(x) = -[x(x-1) + \frac{\delta}{6\{1+\delta\}} + 2],$$

$$\ell_0 = \ell_1 = 1, \ \alpha_0 = 1, \ \beta_0 = 0, \ \alpha_1 = 1, \ \beta_1 = 0,$$

$$k_0(x) = -\delta, \ k_1(x) = -\delta, \ r_0(t) = 0, \ r_1(t) = 0,$$

(20)

where δ is a constant with the value 0.0144.

The exact solution of this problem is

$$\phi(x,t) = [x(x-1) + \frac{\delta}{6\{1+\delta\}}] \exp(-t).$$
(21)

To apply the numerical procedure in Section 4 to solve the problem here, the collocation points $\xi_1, \xi_2, \dots, \xi_{N-1}$ and ξ_N are taken to be given by $\xi_i = (i-1)/(N-1)$ for $i = 1, 2, \dots, N$. Table 1 shows the absolute errors of the numerical values of ϕ at x = 0.50 and selected time levels. The numerical values of ϕ are obtained by using various values of N and Δt . There is a good agreement between the numerical and exact values, even for N = 5 and $\Delta t = 0.10$. It is obvious from Table 1 that the numerical values converge to the exact ones when the calculation is refined by increasing N and decreasing Δt .

		N = 5	N = 17	N = 33
t	Exact	$\Delta t = 0.10$	$\Delta t = 0.05$	$\Delta t = 0.025$
		Absolute error	Absolute error	Absolute error
0.30	-0.18345183	$2.3 imes 10^{-4}$	5.4×10^{-6}	8.2×10^{-7}
0.60	-0.13590446	1.9×10^{-4}	4.3×10^{-6}	6.5×10^{-7}
0.90	-0.10068049	1.4×10^{-4}	3.2×10^{-6}	$4.9 imes 10^{-7}$
1.20	-0.07458595	1.1×10^{-4}	2.3×10^{-6}	3.6×10^{-7}
1.50	-0.05525463	7.6×10^{-5}	1.7×10^{-6}	2.7×10^{-7}
1.80	-0.04093364	5.6×10^{-5}	1.3×10^{-6}	1.9×10^{-7}
2.10	-0.03032438	4.2×10^{-5}	9.5×10^{-7}	1.5×10^{-7}
2.30	-0.02246486	3.1×10^{-5}	7.1×10^{-7}	1.1×10^{-7}
2.70	-0.01664237	2.3×10^{-5}	8.1×10^{-7}	8.1×10^{-8}
3.00	-0.01232897	1.7×10^{-5}	3.9×10^{-7}	$5.9 imes 10^{-8}$

Table 1. Absolute errors of the numerical values of ϕ at x = 0.50 and selected time levels, as obtained by using various values of N and Δt , for Problem 1.

Problem 2. Take

$$q(x,t) = 0, \ f(x) = \cos(\frac{1}{2}\pi x) + \cos(\frac{1}{3}\pi x), \ \ell_0 = \ell_1 = 1/2,$$

$$\alpha_0 = 0, \ \beta_0 = 0, \ k_0(x) = 1, \ \alpha_1 = 1, \ \beta_1 = 0, \ k_1(x) = 0,$$

$$r_0(t) = -\frac{1}{2\pi} [2\sqrt{2}\exp(-\frac{1}{4}\pi^2 t) + 3\exp(-\frac{1}{9}\pi^2 t)],$$

$$r_1(t) = \frac{1}{2}\exp(-\frac{1}{9}\pi^2 t).$$
(22)

It is easy to verify that the exact solution for this problem is given by

$$\phi(x,t) = \exp(-\frac{1}{4}\pi^2 t)\cos(\frac{1}{2}\pi x) + \exp(-\frac{1}{9}\pi^2 t)\cos(\frac{1}{3}\pi x).$$
(23)

Table 2. Absolute errors of the numerical values of $\phi(x, t)$ at selected points and at t = 0.90, as computed using various values of N and Δt , for Problem 2.

		N = 5	N = 17	N = 33
x	Exact ϕ	$\Delta t = 0.10$	$\Delta t = 0.05$	$\Delta t = 0.025$
		Absolute error	Absolute error	Absolute error
0.00	0.481245	2.9×10^{-3}	1.2×10^{-4}	2.4×10^{-5}
0.25	0.460284	2.3×10^{-3}	9.7×10^{-5}	1.9×10^{-5}
0.50	0.399522	$1.6 imes 10^{-3}$	$6.7 imes 10^{-5}$	1.4×10^{-5}
0.75	0.305080	7.1×10^{-4}	3.3×10^{-5}	6.9×10^{-6}

Figure 1. Plots of numerical and exact $|\omega(t)|$ against t for Problem 2.



As in the first problem above, the collocation points $\xi_1, \xi_2, \dots, \xi_{N-1}$ and ξ_N are given by $\xi_i = (i-1)/(N-1)$ for $i = 1, 2, \dots, N$. For various values of N and Δt , the absolute errors of the numerically obtained ϕ at selected points and at time t = 0.90 are given in Table 2. The numerical and exact values of ϕ agree well with each other. Convergence is also observed when the calculation is repeated using larger N and smaller Δt .

The flux function at x = 1, that is, $\omega(t)$ as defined by $\partial \phi / \partial x$ at x = 1, is directly obtained after (17)-(19) is solved. Figure 1 compares graphically the numerical magnitude of $\omega(t)$ as obtained by using N = 21 and $\Delta t = 0.025$ with the exact value over the time interval [0.15, 2.0]. The graphs for the numerical and exact $|\omega(t)|$ are visually indistinguishable, as the two sets of results agree to at least 4 significant figures.

Problem 3. Take

$$q(x,t) = \left[1 + \left(\frac{\pi^2}{4} - 1\right)t\right] \exp(-t) \cos\left(\frac{1}{2}\pi x\right),$$

$$f(x) = 0, \ \ell_0 = \ell_1 = 1, \ \alpha_0 = 0, \ \beta_0 = 0,$$

$$k_0(x) = \sin\left(\frac{1}{2}\pi x\right), \ \alpha_1 = 0, \ \beta_1 = 1, \ k_1(x) = 0,$$

$$r_0(t) = -\frac{1}{\pi}t \exp(-t), \ r_1(t) = -\frac{\pi}{2}t \exp(-t).$$
(24)

The exact solution of this problem is

$$\phi(x,t) = t \exp(-t) \cos(\frac{1}{2}\pi x). \tag{25}$$

The collocation points are chosen as in the first two problems above. In Figure 2, the numerical solution ϕ at t = 1, as obtained using N = 21 and $\Delta t = 1/15$, is compared graphically with the exact solution for $x \in [0, 1]$. The numerical values of ϕ agree well with the exact ones.



Figure 2. Plots of numerical and exact $\phi(x, 1)$ against x for Problem 3.

6 Conclusion

A numerical method for solving a one-dimensional parabolic partial differential equation subject to non-classical conditions has been successfully developed and implemented on the computer.

It (the method) uses an integro-differential formulation of the parabolic equation and approximation by local interpolating functions to reduce the problem under consideration into a linear system of first order ordinary differential equations and may be viewed as a one-dimensional version of the well known dual-reciprocity boundary element method. The unknown functions of time in the ordinary differential equations are approximated using cubic functions over a time interval consisting of 4 consecutive time levels. This gives rise to a system of linear algebraic equations $\mathbf{AX} = \mathbf{B}$, where \mathbf{A} and \mathbf{B} are known matrices of order $N \times N$ and $N \times 1$ respectively and \mathbf{X} is an unknown $N \times 1$ matrix, over the time interval. An approximate solution to the problem under consideration can then be obtained at higher and higher time levels by using a time-stepping scheme which requires solving the linear algebraic equations over consecutive time intervals. If the size of each of the time intervals is the same, the matrix \mathbf{A} has to be evaluated and processed only once in order to solve the linear algebraic equations. For example, if the *LU* decomposition technique together with backward substitutions is used to solve the linear algebraic equations, then the square matrix has to be decomposed only once.

To check the numerical method, it is applied to solve several different test problems with known exact solutions. The numerical solutions obtained agree well with the exact ones. Convergence is also observed in the numerical solutions when the calculation is refined by increasing the number of collocation points used or by reducing the size of the time interval over which the unknown functions are approximated by cubic functions of time. The numerical results confirm the validity of the numerical method and suggest that it is an interesting and viable alternative to existing numerical methods for solving the problem under consideration.

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Captions for Figures and Tables

Figure 1. Plots of numerical and exact $|\omega(t)|$ against t for Problem 2.

Figure 2. Plots of numerical and exact $\phi(x, 1)$ against x for Problem 3.

Table 1. Absolute errors of the numerical values of ϕ at x = 0.50 and selected time levels, as obtained by using various values of N and Δt , for Problem 1.

Table 2. Absolute errors of the numerical values of $\phi(x, t)$ at selected points and at t = 0.90, as computed using various values of N and Δt , for Problem 2.