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ORIGINAL ARTICLE

Numerical solution of time-dependent diffusion equations with nonlocal boundary conditions via a fast matrix approach

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Abstract This article contributes a matrix approach by using Taylor approximation to obtain the numerical solution of one-dimensional time-dependent parabolic partial differential equations (PDEs) subject to nonlocal boundary integral conditions. We first impose the initial and boundary conditions to the main problems and then reach to the associated integro-PDEs. By using operational matrices and also the completeness of the monomials basis, the obtained integro-PDEs will be reduced to the generalized Sylvester equations. For solving these algebraic systems, we apply a famous technique in Krylov subspace iterative methods. A numerical example is considered to show the efficiency of the proposed idea.

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1. Introduction

One dimensional parabolic partial differential equations (PDEs) have an extensive application in the study of problems in engineering and applied sciences. It should be mentioned that, such PDEs together with classical boundary conditions have received considerable attention in research works. However, these PDEs with nonlocal boundary conditions were studied by researchers in the literature, but extensions and modifications of the existing methods should be explored to obtain more accurate solutions. The usual numerical methods for PDEs subject to the nonlocal boundary conditions are finite difference methods [1–3], Galerkin techniques [4], collocation approaches [5], Tau schemes [6] and reproducing kernel space methods [7]. Moreover, some other new methods were considered in [8–11].

It should be noted that, in all of the research works that are based on the operational matrices, the basic PDEs (with classical boundary conditions) were finally transformed into the matrix–vector algebraic system $Ax = b$, which can be solved

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by robust iterative solvers such as Krylov subspace iterative methods (e.g., restarted GMRES and Bi-CGSTAB methods). For this purpose, one can use simple MATLAB commands for applying these iterative solvers. On the other hand, if the PDEs contain nonlocal boundary conditions, they may be transformed into the associated generalized Sylvester equations by using operational matrices. Since for solving such generalized Sylvester equations, there is no MATLAB commands, we should extend Krylov subspace iterative methods. Moreover, Taylor matrix approaches have had no results for solving PDEs subject to non-classical boundary conditions. These are basic motivations of the paper. In this paper, we present a new matrix method for solving one-dimensional parabolic time-dependent diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + K(x,t), \qquad 0 < x < 1, \quad 0 < t \leqslant 1, \tag{1}$$

with the initial condition

$$u(x,0) = f(x), \qquad 0 < x < 1, \tag{2}$$

and the nonlocal boundary conditions

$$\begin{aligned} u(0,t) &= \int_0^1 \rho(x)u(x,t)dx, \qquad 0 < t \leqslant 1,\\ u(1,t) &= \int_0^1 \psi(x)u(x,t)dx, \qquad 0 < t \leqslant 1, \end{aligned} \tag{3}$$

where K, f, ρ and ψ are known functions, while the function u should be determined. It should be mentioned that we develop a new matrix approach, which was previously examined in [12–15], for solving one-dimensional parabolic PDEs with nonlocal boundary conditions. Some straightforward manipulations, enable us to impose the initial and boundary conditions (2) and (3) to the main problem. Thus, completeness of monomials basis together with the operational matrices of differentiation and integration can be used to reduce the main problem to the associated generalized Sylvester equations. Actually this is the first operational matrix approach for which the final associated algebraic system (i.e., generalized Sylvester equations) will be considered with more details.

2. Method of the solution

In this section, the basic Eq. (1) subject to the initial and boundary conditions (2) and (3) will be transformed into the associated integro-PDE by some straightforward manipulations. Then, completeness of monomials basis together with the operational matrices of differentiation and integration can be used to reduce the main problem to the associated generalized Sylvester equations. For this purpose, we should recall the operational matrices as follows

$$X'(x) = \begin{bmatrix} 1 \\ x \\ \vdots \\ x^{N-1} \\ x^N \end{bmatrix}' = \overbrace{\begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 2 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & N & 0 \end{bmatrix}}^{M} \begin{bmatrix} 1 \\ x \\ \vdots \\ x^{N-1} \\ x^N \end{bmatrix}, \tag{4}$$

$$\int_0^x X(x')dx' = \int_0^x \begin{bmatrix} 1 \\ x' \\ \vdots \\ x'^{N-1} \\ x'^N \end{bmatrix} dx' \approx \overbrace{\begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & \frac{1}{2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{N} \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}}^{P} \begin{bmatrix} 1 \\ x \\ \vdots \\ x^{N-1} \\ x^N \end{bmatrix}, \tag{5}$$

where M and P are operational matrices of differentiation and integration, respectively. It should be recalled that $\int_0^1 X(x)X^T(x)dx = Q$, where $Q = hilb(N+1)$ is the Hilbert matrix of dimension $N+1$. Throughout of the paper, Q denotes the hilbert matrix of dimension $N+1$ and we do not show its index for clarity of presentation. Now, one can rewrite the basic Eq. (1) in the form

$$u_{xx}(x,t) = u_t(x,t) - K(x,t).$$

So direct integration from both sides of the above equation with respect to x in the interval $[0,x]$ yields

$$\begin{aligned} u_x(x,t) &= u_x(0,t) + \int_0^x u_{xx}(x',t)dx' \\ &= u_x(0,t) + \int_0^x (u_t(x',t) - K(x',t))dx'. \end{aligned} \tag{6}$$

On the other hand, by assuming $u(0,t) = A(t)$, one can write

$$u(x,t) = A(t) + \int_0^x u_x(x',t)dx'. \tag{7}$$

From (6) and (7) one can conclude that

$$u(x,t) = A(t) + xu_x(0,t) + \int_0^x \int_0^{x'} (u_t(x'',t) - K(x'',t))dx''dx'. \tag{8}$$

We suppose that $u(1,t) = B(t)$, and hence

$$\begin{aligned} B(t) &= u(1,t) \\ &= A(t) + u_x(0,t) + \int_0^1 \int_0^x (u_t(x',t) - K(x',t))dx'dx. \end{aligned}$$

The above equation can be rewritten in the form

$$\begin{aligned} u_x(0,t) &= B(t) \\ &\quad - \left(A(t) + \int_0^1 \int_0^x (u_t(x',t) - K(x',t))dx'dx \right). \end{aligned} \tag{9}$$

Replacing (9) into (8) yields

$$\begin{aligned} u(x,t) &= (1-x)A(t) + xB(t) - x\int_0^1 \int_0^x (u_t(x',t) \\ &\quad - K(x',t))dx'dx + \int_0^x \int_0^{x'} (u_t(x'',t) \\ &\quad - K(x'',t))dx''dx'. \end{aligned} \tag{10}$$

For imposing the initial condition (2), we should differentiate both sides of (10) with respect to t in the following form

$$\begin{aligned} \frac{\partial u(x,t)}{\partial t} &= \frac{\partial}{\partial t}[(1-x)A(t) + xB(t) \\ &\quad - x\int_0^1 \int_0^x (u_t(x',t) - K(x',t))dx'dx \\ &\quad + \int_0^x \int_0^{x'} (u_t(x'',t) - K(x'',t))dx''dx' \end{aligned}$$

and then integrating both sides of the above equation with respect to t in the interval $[0,t]$ as follows

$$u(x,t)-u(x,0)=\int_0^t \frac{\partial}{\partial t}((1-x)A(t)+xB(t) - x\int_0^1\int_0^x (u_t(x',t)-K(x',t))dx'dx + \int_0^x\int_0^{x'} (u_t(x'',t)-K(x'',t))dx''dx'$$

In other words

$$u(x,t)=f(x)+\int_0^t \frac{\partial}{\partial t}\Bigg((1-x)A(t)+xB(t) - x\int_0^1\int_0^x (u_t(x',t)-K(x',t))dx'dx + \int_0^x\int_0^{x'} (u_t(x',t)-K(x'',t))dx''dx'\Bigg)dt. \tag{11}$$

In this stage, we should approximate all the existing (known and unknown) functions in terms of their truncated Taylor expansions in the form

$$\begin{aligned}
&u(x,t)\approx X^T(x)UX(t), \qquad (12)\\
&f(x)\approx X^T(x)FX(t),\\
&K(x,t)\approx X^T(x)KX(t),\\
&\rho(x)\approx \rho^T X(x),\\
&\psi(x)\approx \psi^T X(x),\\
&1-x = X^T(x)\beta,\\
&x = X^T(x)\alpha.
\end{aligned}$$

It should be noted that $F\in\Re^{(N+1)\times(N+1)}$, $K\in\Re^{(N+1)\times(N+1)}$, $\rho^T\in\Re^{1\times(N+1)}$, $\psi^T\in\Re^{1\times(N+1)}$, $\alpha\in\Re^{(N+1)\times 1}$ and $\beta\in\Re^{(N+1)\times 1}$ are known, in which $F_{i,j}=\frac{1}{i!j!}\frac{\partial^{i+j}f(0,0)}{\partial x^i\partial t^j}$, $K_{i,j}=\frac{1}{i!j!}\frac{\partial^{i+j}K(0,0)}{\partial x^i\partial t^j}$, $\rho^T_{1,j}=\frac{\rho^j(0)}{j!}$, $\psi^T_{1,j}=\frac{\psi^j(0)}{j!}$ for all $i,j=0,1,\ldots,N$, $\beta=[1\ -1\ 0\ \cdots 0]^T$ and $\alpha=[0\ 1\ 0\ \cdots 0]^T$. However, $U\in\Re^{(N+1)\times(N+1)}$ is an unknown matrix and should be determined.

By using (12), one can approximate the boundary conditions (3) as follows

$$\begin{aligned}
A(t)=u(0,t)&=\int_0^1 \rho(x)u(x,t)dx=\int_0^1 \rho^T X(x)X^T(x)UX(t)dx\\
&=\rho^T QUX(t), \qquad (13)\\
B(t)=u(1,t)&=\int_0^1 \psi(x)u(x,t)dx=\int_0^1 \psi^T X(x)X^T(x)UX(t)dx\\
&=\psi^T QUX(t).
\end{aligned}$$

By using approximation terms (12) and (13) and replacing in (11) we have

$$X^T(x)UX(t)\approx X^T(x)FX(t)+\int_0^t \frac{\partial}{\partial t}\left[X^T(x)\overbrace{\left(\beta\rho^T QU+\alpha\psi^T QU-\alpha w P^T(UM-K)+(P^T)^2(UM-K)\right)}^{Y}X(t)\right]dt, \tag{14}$$

where $w=\int_0^1 X^T(x)dx=\left[1\ \frac{1}{2}\ \cdots,\frac{1}{N+1}\right]$. Now, one can apply operational matrices of differentiation and integration (see (4) and (5)) for obtaining

$$X^T(x)UX(t)\approx X^T(x)FX(t)+X^T(x)YMPX(t).$$

In other words

$$X^T(x)\widetilde{U}X(t)=X^T(x)FX(t)+X^T(x)\widetilde{Y}MPX(t). \tag{15}$$

where $\widetilde{U}$ is an approximation of U and $\widetilde{Y}=\beta\rho^T Q\widetilde{U}+\alpha\psi^T Q\widetilde{U}-\alpha w P^T(\widetilde{U}M-K)+(P^T)^2(\widetilde{U}M-K)$. Since monomials form a complete basis, one can factorize both of the vectors $X^T(x)$ and $X(t)$ from (15) for obtaining the following equation

$$\widetilde{U}=F+\beta\rho^T Q\widetilde{U}MP+\alpha\psi^T Q\widetilde{U}MP-\alpha w P^T\left(\widetilde{U}M-K\right)MP + (P^T)^2\left(\widetilde{U}M-K\right)MP.$$

The above equation can be rewritten in the following form

$$\widetilde{U}=C+\beta\rho^T Q\widetilde{U}MP+\alpha\psi^T Q\widetilde{U}MP-\alpha w P^T\widetilde{U}M^2P + (P^T)^2\widetilde{U}M^2P, \tag{16}$$

where $C=F+\alpha wP^TKMP-(P^T)^2KMP$.

By assumptions $A_1=-\beta\rho^T Q$, $B_1=MP$, $A_2=-\alpha\psi^T Q$, $B_2=MP$, $A_3=\alpha wP^T$, $B_3=M^2P$, $A_4=-(P^T)^2$, $B_4=M^2P$, Eq. (16) can be rewritten as follows

$$\widetilde{U}+A_1\widetilde{U}B_1+A_2\widetilde{U}B_2+A_3\widetilde{U}B_3+A_4\widetilde{U}B_4=C, \tag{17}$$

which is a generalized Sylvester equation. For solving this generalized Sylvester equation, we use the global GMRES method that is selected from [17].

We note that the Sylvester Eq. (17) has a unique solution if the matrix $\left(I_{N+1}\otimes I_{N+1}+\sum_{i=1}^4 B_i^T\otimes A_i\right)$ is nonsingular. Throughout this paper, we assume that this condition is verified. As [16], we use the modified global Arnoldi algorithm to construct an F-orthonormal basis $V_1,V_2,\cdots,V_k$ of the corresponding matrix Krylov subspace. This algorithm is described as follows:

Algorithm 1. Modified Global Arnoldi algorithm for matrix equation $\widetilde{U}+\sum_{i=1}^4 A_i\widetilde{U}B_i=C$.

1. Set $V_1=V/\|V\|_F$
2. For $j=1,2,\ldots,k$, Do:
3. Compute $W=V_j+\sum_{i=1}^4 A_iV_jB_i$
4. For $i=1,2,\ldots,j$, Do
5. $h_{ij}=\langle W,V_i\rangle_F$
6. $W=W-h_{ij}V_i$
7. End Do
8. $h_{j+1,j}=\|W\|_F$. If $h_{j+1,j}=0$ then Stop
9. $V_{j+1}=W/h_{j+1,j}$
10. End Do

Let $\mathcal{V}_k=[V_1,V_2,\cdots,V_k]\in\Re^{(N+1)\times k(N+1)}$ and $\widetilde{H}_k\in\Re^{(k+1)\times k}$ denotes the upper Hessenberg matrix with nonzero entries h_{ij}, which are defined by the modified global Arnoldi algorithm, and also $H_k\in\Re^{k\times k}$ is the matrix obtained from $\widetilde{H}_k$ by deleting its last row.

As seen in [17], to save memory and CPU-time requirements, the Global GMRES method should be used in a

Table 1 Absolute values of the error $|e_N(x,t)|(=|u(x,t)-u_N(x,t)|)$ at the selected points of numerical example.

(x,t)	$N=6$	$N=10$	$N=14$	$N=18$	$N=22$	$N=26$
(0,0)	0	0	0	0	0	0
(0.1,0.1)	5.187e−002	3.499e−004	7.722e−007	6.420e−010	2.431e−013	1.110e−016
(0.2,0.2)	9.538e−002	6.652e−004	1.478e−006	1.234e−009	4.696e−013	2.220e−016
(0.3,0.3)	1.300e−001	9.398e−004	2.103e−006	1.764e−009	6.723e−013	5.551e−016
(0.4,0.4)	1.553e−001	1.168e−003	2.635e−006	2.220e−009	8.495e−013	0
(0.5,0.5)	1.705e−001	1.347e−003	3.065e−006	2.595e−009	9.965e−013	2.220e−016
(0.6,0.6)	1.741e−001	1.468e−003	3.385e−006	2.882e−009	1.110e−012	4.440e−016
(0.7,0.7)	1.639e−001	1.502e−003	3.560e−006	3.070e−009	1.190e−012	4.440e−016
(0.8 0.8)	1.369e−001	1.372e−003	3.423e−006	3.061e−009	1.214e−012	8.881e−016
(0.9,0.9)	8.971e−002	8.860e−004	2.237e−006	2.145e−009	9.225e−013	2.220e−016
(1.0,1.0)	1.900e−002	3.745e−004	2.650e−006	3.812e−009	2.076e−012	1.554e−015

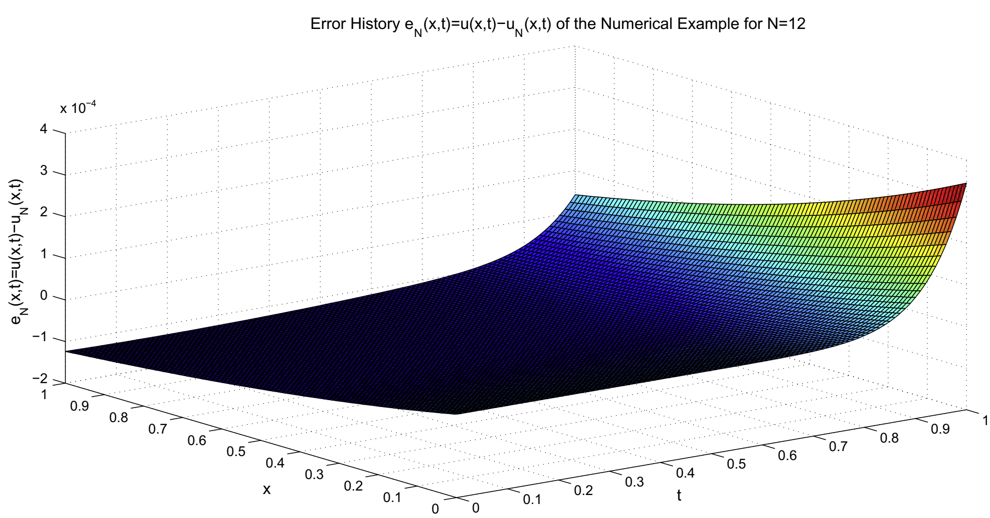

Figure 1 Error history $e_N(x,t)(=u(x,t)-u_N(x,t))$ of numerical example for $N=12$.

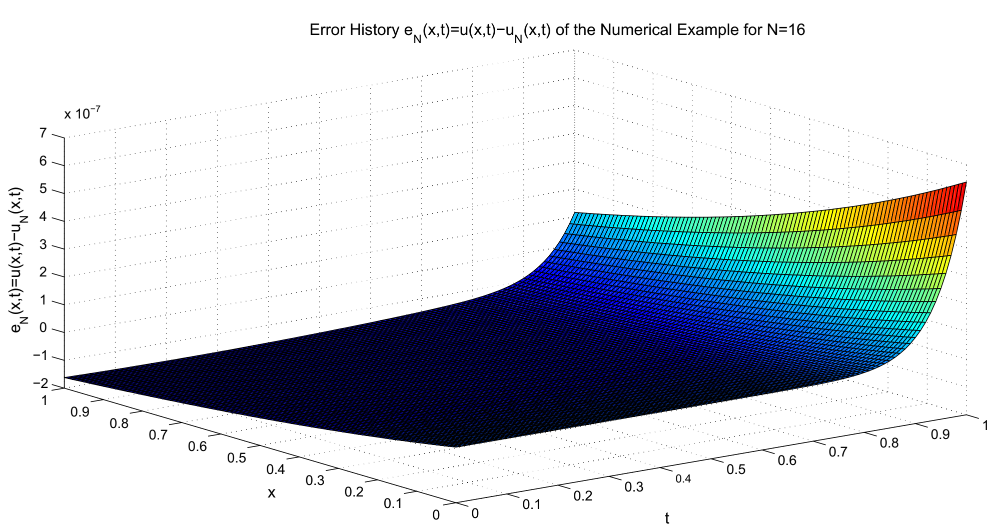

Figure 2 Error history $e_N(x,t)(=u(x,t)-u_N(x,t))$ of numerical example for $N=16$.

restarted mode. This means that we have to restart the algorithm every k inner iterations, where k is a fixed integer. The restarted Global GMRES algorithm for solving the linear matrix Eq. (17), denoted by GlGMRES(k) and summarized as follows: (we note that γ_{k+1} is the last component of the vector $g_k = \|R_0\|_F \widetilde{Q}_k e_1$).

Algorithm 2. Global GMRES(k) algorithm for matrix equation $\widetilde{U} + \sum_{i=1}^{4} A_i \widetilde{U} B_i = C$.

1. Choose $\widetilde{U}_0$, a tolerance ε and $itr = 0$, and compute $R_0 = C - \widetilde{U}_0 - \sum_{i=1}^{4} A_i \widetilde{U}_0 B_i$
2. Compute $\theta = \|R_0\|_F$, and $V_1 = R_0/\theta$
3. Construct the F-orthonormal basis $V_1, V_2, \ldots, V_k$ by modified global Arnoldi algorithm
4. Determine y_k as solution of the least square problem: $\min_{y\in\mathbb{R}^k} \|\theta e_1 - \widetilde{H}_k y\|_2$
5. Compute $\widetilde{U}_k = \widetilde{U}_0 + \mathcal{V}_k(y_k \otimes I_{N+1})$
6. Compute $R_k = \gamma_{k+1}\mathcal{V}_{k+1}(\widetilde{Q}_k^T e_{k+1} \otimes I_{N+1})$, and $\|R_k\|_F = |\gamma_{k+1}|$
7. If $\|R_k\|_F < \varepsilon$ Stop
8. $\widetilde{U}_0 = \widetilde{U}_k, R_0 = R_k, itr = itr + 1$, go to 2.

3. Numerical experiments

In this part of paper, a numerical example is provided to show the effectiveness of the presented method. In this example, the associated Sylvester matrix equations are solved by using Global GMRES(10) algorithm. It should be noted that this algorithm is written in MATLAB 7:12:0 software with the Digits environment variable assigned to be 20 to determine the unknown matrix $\widetilde{U}$ and hence the approximated solution $X^T(x)\widetilde{U}X(t)$. All calculations are run on a Pentium 4 PC laptop with 2 GHz of CPU and 2 GB of RAM. The proposed scheme obtain high order accuracy for dealing with the mentioned PDEs which are enough smooth. The readers can see the efficiency of the proposed method from the provided figures and table in the following example.

3.1. Numerical example

We consider the PDE (1) together with the initial conditions (2) and (3) with the assumptions

$$f(x) = \sin(\pi x) + \cos(\pi x),$$
$$K(x,t) = (\pi^2 - 1)e^{-t}(\sin(\pi x) + \cos(\pi x)),$$
$$\rho(x) = 2\sin(\pi x),$$
$$\psi(x) = -\cos(\pi x),$$

which has the exact solution $u(x,t) = e^{-t}(\sin(\pi x) + \cos(\pi x))$. For solving this problem, we use different values of N such as 6, 10, 12, 14, 16, 18, 22 and 26 and obtain the numerical solution $u_N(x,t) = X^T(x)\widetilde{U}X(t)$. It should be mentioned that, the tolerance in all of these values of N for solving the associated generalized Sylvester equation via GMRES(10) is chosen to be 10^{-16}. Moreover, the initial matrix is taken to be the zero matrix. The numerical results are provided in Table 1 and Figs. 1 and 2. These results confirm the efficiency of the proposed idea.

4. Conclusions and future works

Operational matrices of differentiation and integration together with the completeness of monomials basis have been utilized to numerically solve a class of one-dimensional parabolic partial differential equations (PDEs) by a new framework. The proposed approach reduces the main problem to the generalized linear Sylvester matrix equations. By using the idea of global GMRES(10) method, an iterative algorithm is proposed to solve the obtained Sylvester matrix equations. A numerical example has illustrated to show the efficiency and applicably of the presented method. In our future research works, we will solve two-dimensional equations with nonlocal boundary conditions.

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