Spectral Collocation Method for Parabolic Partial Differential Equations with Neumann Boundary Conditions

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Abstract
In this paper, we present a new method for solving of the parabolic partial differential equation (PPDEs) with Neumann boundary conditions by using the collocation formula for calculating spectral differentiation matrix for Chebyshev-Gauss-Lobatto point. Firstly, theory of application of spectral collocation method on parabolic partial differential equation presented. This method yields a system of ordinary differential equations (ODEs). Secondly, we use forth order Runge-Kutta formula for the numerical integration of the system of ODE. The numerical results obtained by this way have been compared with the exact solution to show the efficiency of the method.

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1 Introduction
We consider the parabolic partial differential equation (see [12]) of the form:

\[
\frac{\partial U}{\partial t}(x, t) = \frac{\partial^2 U}{\partial x^2}(x, t) + f(t, x, U(x, t)), \quad a \leq x \leq b, \quad t \geq 0, \quad (1)
\]

with the initial condition

\[
U(x, 0) = \varphi(x) \quad (2)
\]
and the Neumann boundary conditions
\[ \frac{\partial U}{\partial x}(a, t) = g_1(t), \quad \frac{\partial U}{\partial x}(b, t) = g_2(t), \quad t \geq 0, \tag{3} \]

In this paper, parabolic partial differential equation was solved by combination of pseudospectral collocation method and forth order Runge-Kutta method. The numerical results are compared with the exact solutions. It is shown that the absolute error are very small.

2 Pseudospectral Chebyshev method

One of the methods to solve partial differential equations is the spectral collocation method or the pseudospectral method (see [5, 6]). Pseudospectral methods have become increasingly popular for solving differential equations and also very useful in providing highly accurate solutions to differential equations. In this method, such an approximation of \( u_M(x) \) to \( u(x) \) is presented that \( u_M(x_i) = u(x_i) \) for some collocation point \( x_i \). After setting \( u_M \) in the differential equation, we have to use derivative(s) of \( u_M \) at the collocation point. A straightforward implementation of the spectral collocation methods involves the use of spectral differentiation matrices to compute derivatives at the collocation points, in which \( \overrightarrow{U} = \{u(x_i)\} \) is the vector consisting of values of \( u_M \) at the \( M+1 \) collocation points and \( \overrightarrow{U}' = \{u'(x_i)\} \) consists of the values of the derivatives at the collocation points, then the collocation derivative matrix \( D \) is the matrix mapping \( \overrightarrow{U} \rightarrow \overrightarrow{U}' \). The entries of derivative matrix \( D \) can be computed analytically. To obtain optimal accuracy this matrices must be computed carefully. In [4, 5, 9, 15] the authors describe the subject very well. Let \( u(x) \) be a function on \([−1, 1]\). We interpolate \( u(x) \) by the polynomial \( u_M(x) \) of degree at most \( M \) of the form:

\[ u_M(x) = \sum_{j=0}^{M} \ell_j(x)u(x_j). \tag{4} \]

In the Chebyshev-Gauss-Lobatto points: \( x_j = \cos\left(\frac{j\pi}{M}\right), \quad j = 0, 1, \ldots, M \), with \( \ell_j(x), \quad j = 0, 1, \ldots, M \) are polynomial of degree at most \( M \) such that:

\[ \ell_j(x_k) = \delta_{jk}, \quad j, k = 0, 1, \ldots, M. \]
It can be shown that \[5\]:
\[
ℓ_j(x) = \frac{(-1)^{j+1}(1 - x^2)T'_M(x)}{c_j M^2 (x - x_j)}, \quad j = 0, 1, \ldots, M, \tag{5}
\]
where \(c_0 = c_M = 2, \quad c_j = 1, \quad j = 1, 2, \ldots, M - 1\) and \(T_M(x)\) the Chebyshev polynomial, i.e.
\[T_M(x) = \cos(M \cos^{-1} x) \text{.}\]

The derivatives of the approximate solution \(u_M(x)\) are then estimated at the collocation points by differentiating (9) and evaluating the resulting expression [5]. This yields
\[
u^{(n)}_M(x) = \sum_{j=0}^{M} ℓ^{(n)}_j(x) u(x_j), \quad n = 1, 2, \ldots, \tag{6}
\]
or in matrix notation
\[U^{(n)} = D^{(n)} U, \quad n = 1, 2, \ldots, \]
where
\[U^{(n)} = [u^{(n)}_M(x_0), u^{(n)}_M(x_1), \ldots, u^{(n)}_M(x_M)]^T, \quad U = [u(x_0), u(x_1), \ldots, u(x_M)]^T \]
where \(D^{(n)}\) is the \((M + 1) \times (M + 1)\) matrix whose entries are given by \(d^{(n)}_{kj} = ℓ^{(n)}_j(x_k), \quad j, k = 0, 1, \ldots, M\). The first-order Chebyshev differentiation matrix \(D^{(1)} = D = (d_{kj})\) is given by (see [1, 2, 4, 6, 7]):
\[
d_{kj} = \begin{cases} 
\frac{-c_j \sin((k+j) \pi M)}{2c_j \sin((k-j) \pi M)} & \text{if } k \neq j, \\
-\frac{1}{2} \cos(k \pi M) \left(1 + \cot^2(k \pi M)\right) & \text{if } k = j, k \neq 0, M, \\
d_{00} = -d_{MM} = \frac{2M^2 + 1}{6}. 
\end{cases} \tag{7}
\]

### 3 Solution of parabolic equation

We will describe the pseudospectral Chebyshev method for (1). Let \(M\) be a nonnegative integer and denote by \(X_i = \cos(\frac{i \pi}{M}), i = 0, 1, 2, \ldots, M\), the Chebyshev-Causs-Lobatto points in the interval \([-1, 1]\) and put:
\[U(x, t) = V(X, t), \quad x = cX + d, \quad x_i = cX_i + d, \quad i = 0, 1, \ldots, M,\]
where
\[c = \frac{b - a}{2}, \quad d = \frac{b + a}{2}.\]

Then from (1), we have
\[
\frac{\partial V}{\partial t}(X, t) = \frac{1}{c^2} \frac{\partial^2 V}{\partial X^2}(X, t) + f(t, cX + d, V(X, t)), \quad -1 \leq X \leq 1, \quad t \geq 0, \tag{8}
\]
with the following initial and boundary conditions

\[ V(X,0) = \varphi(cX + d), \quad X \in [-1,1] \]  \hspace{1cm} (9)

and

\[ \frac{\partial V}{\partial X}(-1,t) = cg_1(t), \quad \frac{\partial V}{\partial X}(1,t) = cg_2(t), \quad t \geq 0. \]  \hspace{1cm} (10)

We discretize (8) in space by the method of lines replacing \( \frac{\partial V}{\partial X}(X_i,t) \) and \( \frac{\partial^2 V}{\partial X^2}(X_i,t) \) by pseudospectral approximations given by

\[ \frac{\partial V}{\partial X}(X_i,t) \approx \sum_{j=0}^{M} d^{(1)}_{ij} V(X_j,t) , \quad i = 1, \ldots, M - 1 \]  \hspace{1cm} (11)

and

\[ \frac{\partial^2 V}{\partial X^2}(X_i,t) \approx \sum_{j=0}^{N} d^{(2)}_{ij} V(X_j,t) , \quad i = 1, \ldots, M - 1. \]  \hspace{1cm} (12)

Here

\[ D^{(n)} = [d^{(n)}_{ij}]_{i,j=0}^{M} , \quad n = 1, 2, \]

are differentiation matrices of order \( n \). Put \( V_i(t) = V(X_i,t) \). By substituting (11) and (12) into (8)-(10) we obtain

\[ V'_i(t) = \frac{1}{\varphi'}(\sum_{j=0}^{M} d^{(2)}_{ij} V_j(t)) + f(t,cX+d,V_i(t)), \quad V_i(0) = \varphi(cX_i + d), \]  \hspace{1cm} (13)

\[ \sum_{j=0}^{M} d^{(1)}_{Mj} V_j(t) = cg_1(t), \quad \sum_{j=0}^{M} d^{(1)}_{0j} V_j(t) = cg_2(t). \]  \hspace{1cm} (14)

We can write the equations (14) as follows:

\[
\begin{cases}
    d_{M0} V_0(t) + d_{MM} V_M(t) = cg_1(t) - \sum_{j=1}^{M-1} d^{(1)}_{Mj} V_j(t) \\
    d_{00} V_0(t) + d_{0M} V_M(t) = cg_2(t) - \sum_{j=1}^{M-1} d^{(1)}_{0j} V_j(t)
\end{cases}
\]  \hspace{1cm} (15)

Now we solve the algebraic system (15) related to \( V_0(t) \) and \( V_M(t) \) as follows

\[ V_0(t) = \begin{vmatrix}
    cg_1(t) - \sum_{j=1}^{M-1} d^{(1)}_{Mj} V_j(t) & d_{MM} \\
    cg_2(t) - \sum_{j=1}^{M-1} d^{(1)}_{0j} V_j(t) & d_{0M}
\end{vmatrix} / \begin{vmatrix}
    d_{M0} & d_{MM} \\
    d_{00} & d_{0M}
\end{vmatrix} \]  \hspace{1cm} (16)

\[ = \frac{d_{0M}(cg_1(t) - \sum_{j=1}^{M-1} d^{(1)}_{Mj} V_j(t)) - d_{MM}(cg_2(t) - \sum_{j=1}^{M-1} d^{(1)}_{0j} V_j(t))}{d_{M0}d_{0M} - d_{00}d_{MM}} \]  \hspace{1cm} (17)
and

\[
V_M(t) = \begin{bmatrix} d_{M0} & cg_1(t) - \sum_{j=1}^{M-1} d_{Mj}^{(1)} V_j(t) \\ d_{00} & cg_2(t) - \sum_{j=1}^{M-1} d_{0j}^{(1)} V_j(t) \end{bmatrix} / \begin{bmatrix} d_{M0} \\ d_{00} \end{bmatrix},
\tag{18}
\]

\[
= \frac{d_{M0}(cg_2(t) - \sum_{j=1}^{M-1} d_{0j}^{(1)} V_j(t)) - d_{00}(cg_1(t) - \sum_{j=1}^{M-1} d_{Mj}^{(1)} V_j(t))}{d_{M0}d_{0M} - d_{00}d_{MM}}
\tag{19}
\]

By substituting (17) and (19) into (13) we obtain

\[
V_i'(t) = \frac{1}{c^2}(d_{i0} \times \frac{d_{M0}(cg_1(t) - \sum_{j=1}^{M-1} d_{Mj}^{(1)} V_j(t)) - d_{MM}(cg_2(t) - \sum_{j=1}^{M-1} d_{Mj}^{(1)} V_j(t))}{d_{M0}d_{0M} - d_{00}d_{MM}}
+ \sum_{j=1}^{M-1} d_{ij}^{(2)} V_j(t) 
+ d_{iM} \times \frac{d_{M0}(cg_2(t) - \sum_{j=1}^{M-1} d_{0j}^{(1)} V_j(t)) - d_{00}(cg_1(t) - \sum_{j=1}^{M-1} d_{Mj}^{(1)} V_j(t))}{d_{M0}d_{0M} - d_{00}d_{MM}}
+ f(t, cX + d, V_i(t)),
\]

\[
i = 1, 2, \ldots, M - 1.
\tag{20}
\]

Then the system (20) can be rewritten in the following form:

\[
\begin{cases}
V'(t) = F(t, V(t)), \\
V(0) = V_0,
\end{cases}
\tag{21}
\]

Where

\[
V(t) = [V_1(t), V_2(t), \ldots, V_{M-1}(t)]^T, \quad V_0 = [V_1(0), V_2(0), \ldots, V_{M-1}(0)]^T,
\]

\[
V'(t) = [V'_1(t), V'_2(t), \ldots, V'_{M-1}(t)]^T,
\]

\[
F(t, V(t)) = [F_1(t, V(t)), F_2(t, V(t)), \ldots, F_{M-1}(t, V(t))]^T
\]

and

\[
F_i(t, V(t)) = \frac{1}{c^2}(d_{i0} \times \frac{d_{M0}(cg_1(t) - \sum_{j=1}^{M-1} d_{Mj}^{(1)} V_j(t)) - d_{MM}(cg_2(t) - \sum_{j=1}^{M-1} d_{Mj}^{(1)} V_j(t))}{d_{M0}d_{0M} - d_{00}d_{MM}}
+ \sum_{j=1}^{M-1} d_{ij}^{(2)} V_j(t) 
+ d_{iM} \times \frac{d_{M0}(cg_2(t) - \sum_{j=1}^{M-1} d_{0j}^{(1)} V_j(t)) - d_{00}(cg_1(t) - \sum_{j=1}^{M-1} d_{Mj}^{(1)} V_j(t))}{d_{M0}d_{0M} - d_{00}d_{MM}}
+ f(t, cX + d, V_i(t)),
\tag{22}
\]

Equations (21) form a system of ordinary differential equations (ODEs) in time. Therefore, to advance the solution in time, we use ODE solver such as the Runge-Kutta methods of order four.
4 Numerical results

In this section we obtain numerical solutions of parabolic PDEs in the form (1) with the initial condition (2) and Neumann boundary conditions (3). To show the efficiency of the present method for our problem in comparison with the exact solution we report absolute error which is defined by

$$U_{ij} = |\hat{U}(x_i, t_j) - U(x_i, t_j)|,$$

in the point $(x_i, t_j)$, where $\hat{U}(x_i, t_j)$ is the solution obtained by equation (21) solved by forth order Runge-Kutta method and $U(x_i, t_j)$ is the exact solution. For computational work we select the following problems. In the problem 1-3 we are taken $M = 16, \Delta t = 0.0001$.

**Problem 1.** The first test problem is selected from [3]. This problem is the heat equation with Neumann boundary conditions:

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2}, \quad (x, t) \in [0, 1] \times (0, 0.25],$$

(23)

with the boundary conditions $\frac{\partial U}{\partial x}(x, t) = \pi e^{-\pi^2 t} \cos(\pi x)$ at $x = 0$ and $x = 1$. The initial condition is consistent with the analytic solution $U(x, t) = e^{-\pi^2 t} \sin(\pi x)$. In Table 1 we shows absolute error $U_{ij}$ for problem 1.

**Problem 2.** This problem was used by Hopkins and Wait [10] to provide an example of a problem with a nonlinear source term and with Neumann boundary conditions:

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} + \exp(-U) + \exp(-2U), \quad (x, t) \in [0, 1] \times (0, 50],$$

(24)

with boundary conditions $\frac{\partial U}{\partial x}(x, t) = \frac{1}{x + t + 2}$ at $x = 0$ and $x = 1$. The initial condition is consistent with the analytic solution $U(x, t) = \ln(x + t + 2)$. In Table 2 we shows absolute error $U_{ij}$ for problem 2.

**Table 1.** Absolute error for various values of $x$ and $t$

<table>
<thead>
<tr>
<th>$x_i/t_j$</th>
<th>0.05</th>
<th>0.10</th>
<th>0.15</th>
<th>0.20</th>
<th>0.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x[2]$</td>
<td>2.0327e-11</td>
<td>1.2412e-11</td>
<td>7.5695e-12</td>
<td>4.6261e-12</td>
<td>2.8301e-12</td>
</tr>
<tr>
<td>$x[16]$</td>
<td>2.0330e-11</td>
<td>1.2414e-11</td>
<td>7.5716e-12</td>
<td>4.6279e-12</td>
<td>2.8314e-12</td>
</tr>
</tbody>
</table>

**Table 2.** Absolute error for various values of $x$ and $t
Problem 3. This problem is selected from [12]. The problem is

\[
\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} + (\pi^2 - 1)U - pU + (pe^{-t} + e^{-pt})\sin \pi x, \quad (x,t) \in [0,1] \times (0,1],
\]

with boundary conditions \( \frac{\partial U}{\partial x}(x,t) = \pi(e^{-t} + e^{-pt})\cos \pi x \) at \( x = 0 \) and \( x = 1 \).

The initial condition is consistent with the analytic solution \( U(x,t) = (e^{-t} + e^{-pt})\sin \pi x \). The solution of this problem contains both a slow transient \( e^{-t} \), and a rapid transient \( e^{-pt} \) where \( p = 5000 \), characteristic of stiff problems. In Table 3 we shows absolute error \( U_{ij} \) for problem 3.

Table 3. Absolute error for various values of \( x \) and \( t \)

<table>
<thead>
<tr>
<th>( x_i/t_j )</th>
<th>0.2</th>
<th>0.4</th>
<th>0.6</th>
<th>0.8</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x[1] )</td>
<td>1.1187e-07</td>
<td>1.1187e-07</td>
<td>1.1187e-07</td>
<td>1.1187e-07</td>
<td>1.1187e-07</td>
</tr>
<tr>
<td>( x[4] )</td>
<td>6.9987e-12</td>
<td>5.7301e-12</td>
<td>4.6914e-12</td>
<td>3.8410e-12</td>
<td>3.1447e-12</td>
</tr>
<tr>
<td>( x[10] )</td>
<td>2.5856e-11</td>
<td>2.1169e-11</td>
<td>1.7332e-11</td>
<td>1.4190e-11</td>
<td>1.1618e-11</td>
</tr>
<tr>
<td>( x[16] )</td>
<td>1.4935e-12</td>
<td>1.2228e-12</td>
<td>1.0011e-12</td>
<td>8.1967e-13</td>
<td>6.7108e-13</td>
</tr>
<tr>
<td>( x[17] )</td>
<td>1.1187e-07</td>
<td>1.1187e-07</td>
<td>1.1187e-07</td>
<td>1.1187e-07</td>
<td>1.1187e-07</td>
</tr>
</tbody>
</table>

5 Conclusions

In this paper, we have proposed an efficient spectral collocation for parabolic partial differential equation with Neumann boundary conditions, with highly convergence and very small error. As seen in Table 1-3, errors are very small and they are very better than the results of another papers cited in this article.

References


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