A NUMERICAL METHOD FOR THE HEAT EQUATION WITH
A NONLOCAL BOUNDARY CONDITION

M. AKRAM AND M. A. PASHA

Abstract. In this paper an \( O(h^3+l^3) \) \( L_0 \)-stable numerical method is developed for the solution of the heat equation \( u_t = u_{xx} \), \( 0 < x < 1 \), \( 0 < t \leq T \), subject to \( u(x,0) = f(x) \), \( 0 < x < 1 \), \( u_x(1,t) = g(t) \), \( 0 < t < T \), and the nonlocal boundary condition \( \int_0^b u(x,t)dx = m(t) \), \( 0 < b < 1 \).

Key Words. Nonlocal boundary condition, rational approximation, parallel algorithm.

1. Introduction

In [3], J. R. Cannon, S. Perez Esteva, and J. van der Hoek described certain chemicals absorbing light at various frequencies. The intensity of such light on a photoelectric cell gives us an electric signal which is proportional to the total amount of chemical present in the volume through which the light passes. Let \( u(x,t) \) denote the chemical concentration which is diffusing in a straight glass tube with \( x \) measured in the direction of axis of the tube. Then the electric signal produced by a light beam passing through the tube at right angles between \( x = 0 \) and \( x = b \) is proportional to \( \int_0^b u(x,t)dx \). This integral represents the total mass of chemical in \( 0 \leq x \leq b \) at time \( t \) [17]. For such diffusion processes, the integral condition (4) arises naturally and can be used as supplementary information in the determination of unknown concentration \( u(x,t) \).

This paper considers the problem of obtaining numerical approximations to \( u(x,t) \) which satisfies the heat equation:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < 1, \quad 0 < t \leq T, \\
u(x,0) &= f(x), \quad 0 < x < 1, \\
u_x(1,t) &= g(t), \quad 0 < t < T, \\
\int_0^b u(x,t)dx &= m(t), \quad 0 < b < 1,
\end{align*}
\]

where \( f(x) \), \( g(t) \), \( b \), and \( m(t) \) are known, while the function \( u(x,t) \) is to be determined.

J. R. Cannon and J. van der Hoek [1] studied the existence and uniqueness properties of this problem. Various sequential numerical schemes have been proposed in literature for the solution of this problem [2, 3]. In [12], A. B. Gumel proposed \( O(h^2+l^2) \) \( L_0 \)-stable parallel algorithm for this problem. The algorithm is found to

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be more accurate in comparison with two existing algorithms [2, 3] for this problem. In this paper, we present \( O(h^3 + l^3) \) \( L_0 \)-stable parallel algorithm for this problem. The comparison of numerical results demonstrates the computational superiority of proposed parallel algorithm.

In this paper, the method of lines semi-discretization approach is used to transform the model of PDEs into a system of first-order ordinary differential equations (ODEs), which easily can be written in the matrix-vector form. The solution of this system satisfies a certain recurrence relation involving matrix exponential terms. A suitable rational approximant is used to approximate such exponentials leading to an \( L_0 \)-stable parallel algorithm consisting of three processors.

The paper is organized in the following way: the numerical method is described in section 2; the parallel algorithm is presented in section 3; In section 4, the numerical results produced by this method are compared with those demonstrated in [12]; the conclusion is given in section 5.

2. Derivation of the method

We divide \( X = [0, l] \) and \( T = [0, T] \) into \( M \) and \( N \) subintervals of equal lengths \( h = \frac{l}{M} \) and \( l = \frac{T}{N} \), respectively. Under the condition that \( b \) is rational, \( 0 < b < 1 \), it is always possible via the selection of \( M \) to choose \( b \) as a mesh point. Let us suppose that \( b = nh \) for some positive integer \( n \). Differentiating (4) with respect to \( t \) and then using (1), we have Neumann type condition

\[
(5) \quad u_x(0, t) = u_x(b, t) - nh(t).
\]

Thus, (5) serves as the boundary condition at zero. (1)-(3) and (5) can now be replaced by finite difference approximation:

\[
\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{12h^2} \left\{ 11u(x-h, t) - 20u(x, t) + 6u(x+h, t) \right\}
+ 4\left\{ u(x+2h, t) - u(x+3h, t) \right\}
+ \frac{h^3}{12} \frac{\partial^5 u(x, t)}{\partial x^5} + O(h^4) \quad \text{as } h \to 0.
\]

Equation (6) is valid only for \( m = 1, 2, \ldots, N-2 \). To attain the same accuracy at the end points \((x_{N-1}, t_n)\) and \((x_N, t_n)\), special formulae must be developed which approximate \( \partial^2 u(x, t)/\partial x^2 \) not only to third order but also with dominant error term \( \frac{1}{12} h^3 \frac{\partial^5 u(x, t)}{\partial x^5} \) for \( x = x_{N-1}, x_N \) and \( t = t_n \).

\[
\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{12h^2} \left\{ u(x-3h, t) - 6u(x-2h, t) + 26u(x-h, t) - 40u(x, t) \right\}
+ 21u(x+h, t) - 2u(x+2h, t) \right\}
+ \frac{h^3}{12} \frac{\partial^5 u(x, t)}{\partial x^5} + O(h^4) \quad \text{as } h \to 0.
\]

and

\[
\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{12h^2} \left\{ 2u(x-4h, t) - 11u(x-3h, t) + 24u(x-2h, t) \right\}
- 14u(x-h, t) - 10u(x, t) - 9u(x+h, t) \right\}
+ \frac{h^3}{12} \frac{\partial^5 u(x, t)}{\partial x^5} + O(h^4) \quad \text{as } h \to 0.
\]
Applying (1) with (6), (7) and (8) to the mesh points of the interval \([0, 1]\) at time level \(t = nl\) produces a system of ODE’s of the form

\[
\frac{dU(t)}{dt} = AU(t) + v(t), \quad t > 0
\]

with the initial condition

\[
U(0) = \mathbf{f}
\]

in which

\[
U(t) = [U_1(t), U_2(t), \ldots, U_N(t)]^T,
\]

\[
\mathbf{f} = [f(x_1), f(x_2), \ldots, f(x_N)]^T,
\]

\[
A = \frac{1}{12h^2} \begin{bmatrix}
-20 & 6 & 4 & -1 \\
11 & -20 & 6 & 4 & -1 \\
11 & -20 & 6 & 4 & -1 \\
& & & & \ddots \\
11 & -20 & 6 & 4 & -1 \\
11 & -20 & 6 & 4 & -1 \\
1 & -6 & 26 & -40 & 21 \\
2 & -11 & 24 & -14 & -10 \\
\end{bmatrix}_{N \times N}
\]

and

\[
v(t) = \frac{h^{-2}}{12} [11(g(t) - \dot{m}(t)), 0, 0, \ldots, 0, -g(t), -2g(t), 9g(t)]^T.
\]

Solving (9) subject to (10) gives

\[
U(t) = \exp(lA)f + \int_0^t \exp((t + l - s)A)v(s)ds; \quad t \geq 0
\]

which satisfies the recurrence relation

\[
U(t + l) = \exp(lA)U(t) + \int_t^{t+l} \exp((t + l - s)A)v(s)ds; \quad t = 0, l, 2l, \ldots,
\]

in which \(l\) is a constant time step in the discretization of the time variable \(t \geq 0\) at the points \(t_n = nl(n = 0, 1, 2, \ldots, N)\).

To approximate the matrix exponential function in (13), we consider the rational approximation [15] to \(\exp(lA)\) of the form

\[
\exp(lA) = \frac{b_0 + b_1lA + b_2(lA)^2}{a_0 - a_1lA + a_2(lA)^2 - a_3(lA)^3},
\]

where \(b_0 = 1, b_1 = 1 - a_1, b_2 = \frac{1}{2} - a_1 + a_2,\) and \(a_3 = \frac{1}{6} - \frac{a_1}{2} + a_2.\) Thus

\[
\exp(lA) = G^{-1} \left( I + (1 - a_1)lA + \left(\frac{1}{2} - a_1 + a_2\right)l^2A^2 \right),
\]

where

\[
G = I - a_1lA + a_2l^2A^2 - \left(\frac{1}{6} - \frac{a_1}{2} + a_2 - a_3\right)l^3A^3.
\]

The denominator of \(\exp(lA)\) has distinct real zeros provided that \(a_2^2 - 3a_1a_3 > 0\) by choosing values \(a_1 = 1.308617, a_2 = 0.570502, a_3 = 0.082856,\) and the \(L_0\)-stability
is granted in [15].

Lemma 2.1. If the integral term in (13) is approximated by a quadrature formula of the form
\[
\int_t^{t+l} \exp((t + l - s)A)v(s)ds \simeq \sum_j \frac{3}{j} W_j v(s_j)
\]
where all \(s_j(i = 1, 2, 3)\) are different and \(W_1, W_2\) and \(W_3\) are matrices. Then
\[
U(t + l) = \exp(lA)U(t) + W_1 v(t) + W_2 v(t + \frac{l}{2}) + W_3 v(t + l).
\]

Proof. Since
\[
(17) \quad \int_t^{t+l} \exp((t + l - s)A)v(s)ds \simeq W_1 v(s_1) + W_2 v(s_2) + W_3 v(s_3),
\]
it can easily be shown that when \(v(s) = [1, 1, 1, \ldots, 1]^T\)
\[
(18) \quad W_1 + W_2 + W_3 = M_1,
\]
where \(M_1 = A^{-1}(\exp(lA) - I)\); when \(v(s) = [s, s, s, \ldots, s]^T\)
\[
(19) \quad s_1 W_1 + s_2 W_2 + s_3 W_3 = M_2,
\]
where \(M_2 = A^{-1}\{t \exp(lA) - (t + l) I + A^{-1}(\exp(lA) - I)\}\}; and when \(v(s) = [s^2, s^2, \ldots, s^2]^T\)
\[
(20) \quad s_1^3 W_1 + s_2^3 W_2 + s_3^3 W_3 = M_3,
\]
where \(M_3 = A^{-1}[t^2 \exp(lA) - (t + l)^2 I + 2 A^{-1}(t \exp(lA) - (t + l) I + A^{-1}(\exp(lA) - I))]\). Taking \(s_1 = t, s_2 = t + \frac{l}{2}, s_3 = t + l,\) and then solving (18), (19) and (20) simultaneously, and replacing by \(\exp(lA)\) (using software Mathematica) gives
\[
(21) \quad W_1 = \frac{l}{6} \{(I + (4 - 9a_1 + 12a_2)lA) G^{-1},
\]
\[
(22) \quad W_2 = \frac{2l}{3} \{(I - (1 - 3a_1 + 6a_2)lA) G^{-1},
\]
and
\[
(23) \quad W_3 = \frac{l}{6} \{(I + (3 - 9a_1 + 12a_2)lA + (1 - 3a_1 + 6a_2)l^2 A^2) G^{-1}.
\]
Hence
\[
(24) \quad U(t + l) = \exp(lA)U(t) + W_1 v(t) + W_2 v(t + \frac{l}{2}) + W_3 v(t + l)
\]
in which \(W_1, W_2\) and \(W_3\) are given by (21)-(23), respectively. \(\square\)

We focused on the construction of a rational approximation with real and distinct poles. The algorithm readily admits parallelization through partial fraction expansion [11].
Lemma 2.2. If

\[ y_1 = A_1^{-1} \left\{ p_1 U(t) + \frac{l}{6} \left( p_4 v(t) + 4p_7 v(t + \frac{l}{2}) + p_{10} v(t + l) \right) \right\}, \]

\[ y_2 = A_2^{-1} \left\{ p_2 U(t) + \frac{l}{6} \left( p_5 v(t) + 4p_8 v(t + \frac{l}{2}) + p_{11} v(t + l) \right) \right\}, \]

and

\[ y_3 = A_3^{-1} \left\{ p_3 U(t) + \frac{l}{6} \left( p_6 v(t) + 4p_9 v(t + \frac{l}{2}) + p_{12} v(t + l) \right) \right\}, \]

are the solutions of the linear systems, then

\[ U(t + l) = y_1 + y_2 + y_3. \]

Proof. Let \( r_1, r_2 \) and \( r_3 \) be distinct real zeros of the denominator of \( \exp(lA) \). Then

\[ G = (I - \frac{l}{r_1} A)(I - \frac{l}{r_2} A)(I - \frac{l}{r_3} A), \]

and the approximation to the matrix exponential function may be written in partial-fraction form as

\[ \exp(lA) = \sum_{j=1}^{3} p_j \left( I - \frac{l}{r_j} A \right)^{-1}, \]

in which \( p_j (j = 1, 2, 3) \), the partial-fraction coefficients of \( R(lA) \), are defined by

\[ p_j = \frac{1 + (1 - a_1) r_j + (1 - a_j + a_2) r_j^2}{\prod_{i=1, i \neq j}^{3} (1 - \frac{r_i}{r_j})}, \quad j = 1, 2, 3. \]

So

\[ \exp(lA)U(t) = \left\{ p_1 (I - \frac{l}{r_1} A)^{-1} + p_2 (I - \frac{l}{r_2} A)^{-1} + p_3 (I - \frac{l}{r_3} A)^{-1} \right\} U(t). \]

The implementation of the method by using a parallel architecture with three processors is based on the partial fraction decomposition of \( \exp(lA)U(t) \), \( W_1 v(t) \), \( W_2 v(t + \frac{l}{2}) \), and \( W_3 v(t + l) \) in (24).

Hence

\[ U(t + l) = A_1^{-1} \left\{ p_1 U(t) + \frac{l}{6} (p_4 v(t) + 4p_7 v(t + \frac{l}{2}) + p_{10} v(t + l)) \right\}, \]

\[ + A_2^{-1} \left\{ p_2 U(t) + \frac{l}{6} (p_5 v(t) + 4p_8 v(t + \frac{l}{2}) + p_{11} v(t + l)) \right\}, \]

\[ + A_3^{-1} \left\{ p_3 U(t) + \frac{l}{6} (p_6 v(t) + 4p_9 v(t + \frac{l}{2}) + p_{12} v(t + l)) \right\}, \]

where

\[ A_i = I - \frac{l}{r_i} A (i = 1, 2, 3), \]

\[ p_{3+j} = \frac{1 + (4 - 9a_1 + 12a_2) r_j}{\prod_{i=1, i \neq j}^{3} (1 - \frac{r_i}{r_j})}, \quad j = 1, 2, 3, \]
\[ p_{6+j} = \frac{1 - (1 - 3a_1 + 6a_2)r_j}{\prod_{i=1}^{3} (1 - \frac{r_i}{r_j})}, \quad j = 1, 2, 3 \]
\[ p_{9+j} = \frac{1 + (3 - 9a_1 + 12a_2)r_j + (1 - 3a_1 + 6a_2)r_j^2}{\prod_{i=1}^{3} (1 - \frac{r_i}{r_j})}, \quad j = 1, 2, 3. \]

Hence
\[ U(t + l) = y_1 + y_2 + y_3 \]
in which \( y_1, y_2 \) and \( y_3 \) are the solutions of the linear systems
\[ A_1 y_1 = p_1 U(t) + \frac{l}{6} \left( p_4 v(t) + 4p_7 v(t + \frac{l}{2}) + p_{10} v(t + l) \right), \]
\[ A_2 y_2 = p_2 U(t) + \frac{l}{6} \left( p_5 v(t) + 4p_8 v(t + \frac{l}{2}) + p_{11} v(t + l) \right), \]
and
\[ A_3 y_3 = p_3 U(t) + \frac{l}{6} \left( p_6 v(t) + 4p_9 v(t + \frac{l}{2}) + p_{12} v(t + l) \right), \]
respectively. \( \square \)

**Definition 2.3.** Let \( R(lA) \) be a rational approximation. The numerical methods of the form \( U^{n+1} = R(lA)U^n, \quad n = 0, 1, 2, \ldots, \) is said to be stable, if \( \| R(lA) \|_s \leq 1 \). This is equivalent to requiring \( | R(l\lambda_s) | \leq 1 \), where \( \lambda_s \) is an eigenvalue of \( A \). If the eigenvalues are negative and real then \( \lambda_s < 0 \), and so \( z = -l\lambda_s > 0 \). Hence stability (\( A_0 \)-stability) requires \( | R(-z) | \leq 1 \). The term \( R(-z) \) is called the amplification symbol.

**Definition 2.4.** An \( A_0 \)-stable method is said to be \( L_0 \)-stable, if \( \lim_{z \to \infty} R(-z) = 0 \).

**Remark 2.5.** In (11), the matrix \( h^2A \) has distinct eigenvalues with negative real parts for different values of \( N \), which guarantees that the parallel algorithm is \( L_0 \)-stable.

### 3. The parallel algorithm

Equations (30)-(32) have great importance in the parallel environment since they can be used to solve the corresponding linear algebraic systems on processors operating concurrently. \( U(t + l) \) in (24), the solution vector at time \( t = (n + 1)l \), may now be obtained via the parallel algorithm using three different processors in the following form:

**Processor 1**
(a) Input \( l, r_1, U(0), A; \)
(b) Compute \( p_1, p_4, p_7, p_{10} \) and \( I - \frac{l}{r_1} A; \)
(c) Decompose \( I - \frac{l}{r_1} A = L_1 U_1; \)
(d) Evaluate \( v(t), v(t + \frac{l}{2}), v(t + l); \)
(e) Use \( z_1(t) = \frac{l}{2} (p_4 v(t) + 4p_7 v(t + \frac{l}{2}) + p_{10} v(t + l)); \)
(f) Solve \( L_1 U_1 y_1(t) = p_1 U(t) + z_1(t). \)

**Processor 2**
(a) Input \( l, r_2, U(0), A; \)
(b) Compute \( p_2, p_5, p_8, p_{11}, \) and \( I - \frac{l}{r_2} A; \)
(c) Decompose \( I - \frac{l}{r_1} A = L_2 U_2 \);
(d) Evaluate \( v(t), v(t + \frac{l}{2}), v(t + l) \);
(e) Use \( z_2(t) = \frac{1}{6} (p_5 v(t) + 4p_6 v(t + \frac{l}{2}) + p_{11} v(t + l)) \);
(f) Solve \( L_2 U_2 y_2(t) = p_2 U(t) + z_2(t) \).

**Processor 3**
(a) Input \( l, r_3, U(0), A \);
(b) Compute \( p_3, p_6, p_9, p_{12}, I - \frac{l}{r_2} A \);
(c) Decompose \( I - \frac{l}{r_2} A = L_3 U_3 \);
(d) Evaluate \( v(t), v(t + \frac{l}{2}), v(t + l) \);
(e) Use \( z_3(t) = \frac{1}{6} (p_6 v(t) + 4p_9 v(t + \frac{l}{2}) + p_{12} v(t + l)) \);
(f) Solve \( L_3 U_3 y_3(t) = p_3 U(t) + z_3(t) \).

Hence \( U(t + l) = y_1(t) + y_2(t) + y_3(t) \).

Implementing the algorithm, Processor 1 generates the decomposition of \( I - \frac{l}{r_1} A \), while Processor 2 generates the decomposition of \( I - \frac{l}{r_2} A \) and Processor 3 generates the decomposition of \( I - \frac{l}{r_3} A \) simultaneously.

### 4. Numerical Experiments

In this section, four examples from the literature are considered to test the accuracy of the method.

**Example 4.1.** Consider the heat equation with

\[
\begin{align*}
    f(x) &= 0.5x^2, \\
    g(t) &= 1.0, \\
    m(t) &= 0.75t + \frac{1}{6}(0.75)^3.
\end{align*}
\]

The analytical solution is \( u(x, t) = 0.5x^2 + t \). The absolute relative error \( |(u-U)/u| \) computed at various time lengths with \( h = l = 0.0025 \) are shown in Table 1.

<table>
<thead>
<tr>
<th>Time length</th>
<th>( O(h^2 + l^2) )</th>
<th>( O(h^3 + l^3) )</th>
<th>Analytical Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t=0.1 )</td>
<td>8.07E - 4</td>
<td>4.32E - 5</td>
<td>0.13125</td>
</tr>
<tr>
<td>( t=0.025 )</td>
<td>8.81E - 5</td>
<td>5.75E - 6</td>
<td>5.625E - 2</td>
</tr>
<tr>
<td>( t=0.010 )</td>
<td>1.61E - 6</td>
<td>1.02E - 7</td>
<td>4.125E - 2</td>
</tr>
</tbody>
</table>
Example 4.2. Consider the heat equation with
\[ f(x) = \sin(x), \]
\[ g(t) = -\pi e^{-\pi^2 t}, \]
\[ m(t) = \frac{1}{\pi} \left( \frac{1}{\sqrt{2}} + 1 \right) e^{-\pi^2 t}, \]
\[ u(x, t) = e^{-\pi^2 t} \sin(\pi x). \]
This example has an analytical solution \( u(x, t) = e^{-t} \cos(x) \). The computed results at various time lengths with \( h = l = 0.0025 \) are shown in Table 2.

<table>
<thead>
<tr>
<th>Time length</th>
<th>( O(h^2 + l^2) )</th>
<th>( O(h^3 + l^3) )</th>
<th>Analytical Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t = 0.1 )</td>
<td>6.29E - 5</td>
<td>2.30E - 6</td>
<td>0.8767</td>
</tr>
<tr>
<td>( t = 0.025 )</td>
<td>2.82E - 6</td>
<td>2.13E - 7</td>
<td>0.9450</td>
</tr>
<tr>
<td>( t = 0.010 )</td>
<td>3.73E - 8</td>
<td>2.31E - 9</td>
<td>0.9593</td>
</tr>
</tbody>
</table>

Example 4.3. Consider the heat equation with
\[ f(x) = \sin(x), \]
\[ g(t) = -\pi e^{-\pi^2 t}, \]
\[ m(t) = \frac{1}{\pi} \left( \frac{1}{\sqrt{2}} + 1 \right) e^{-\pi^2 t}. \]
This example has an analytical solution \( u(x, t) = e^{-\pi^2 t} \sin(\pi x) \). The computed results at various time lengths with \( h = l = 0.0025 \) are shown in Table 3.

<table>
<thead>
<tr>
<th>Time length</th>
<th>( O(h^2 + l^2) )</th>
<th>( O(h^3 + l^3) )</th>
<th>Analytical Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t = 0.1 )</td>
<td>3.55E - 5</td>
<td>6.35E - 7</td>
<td>0.2635</td>
</tr>
<tr>
<td>( t = 0.025 )</td>
<td>2.81E - 7</td>
<td>8.65E - 9</td>
<td>0.5525</td>
</tr>
<tr>
<td>( t = 0.010 )</td>
<td>2.95E - 6</td>
<td>1.43E - 8</td>
<td>0.6407</td>
</tr>
</tbody>
</table>
Example 4.4. Example 4.3 is solved with three different time-steps, namely $l = 0.01$, $l = 0.05$ and $l = 0.025$. The relative errors at $t = 0.1$ are given in Table 4.

Table 4. Relative errors at $t = 0.1$ with $h = 0.0025$ using various time-steps

<table>
<thead>
<tr>
<th>Time step</th>
<th>$O(h^2 + l^2)$ [12]</th>
<th>$O(h^3 + l^3)$</th>
<th>Analytical Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l = 0.01$</td>
<td>$3.99E-4$</td>
<td>$3.23E-5$</td>
<td>0.2635</td>
</tr>
<tr>
<td>$l = 0.05$</td>
<td>$1.28E-2$</td>
<td>$7.65E-4$</td>
<td>0.2635</td>
</tr>
<tr>
<td>$l = 0.025$</td>
<td>$3.355E-5$</td>
<td>$2.43E-6$</td>
<td>0.2635</td>
</tr>
</tbody>
</table>

Clearly, discontinuities between initial conditions and boundary conditions exist in all four examples. Tables 1 to 4 confirm that our $L_0$-stable method is very accurate.

5. Conclusion

An $O(h^3 + l^3)$ $L_0$-stable parallel algorithm is tested on model problems presented in previous literature related to the heat equations with Neumann time-dependent boundary condition. It works efficiently for such problems. The comparison of the results demonstrates the computational superiority of our $L_0$-stable method. The explicit use of real arithmetic especially in multispace dimensions can yield large saving in CPU time. This parallel algorithm is suitable for parallel computing.

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HEAT EQUATION WITH NONLOCAL BOUNDARY CONDITION


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