A DIFFUSION PROBLEM WITH NEUMANN BOUNDARY CONTROL UTILIZING TOTAL MASS

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Abstract. The author studies the diffusion problem $u_t = u_{xx}$, $0 < x < 1$, $t > 0$; $u(x,0) = 0$, and $-u_x(0,t) = u_x(1,t) = \phi(t)$, where $\phi(t)$ is a control function that ensures that the total mass $\int_0^1 u(x,t_k)dx$ stays between two predetermined values. Mathematically, $\phi(t) = 1$ for $t_{2k} < t < t_{2k+1}$ and $\phi(t) = -1$ for $t_{2k+1} < t < t_{2k+2}$, $k = 0,1,2,\ldots$ with $t_0 = 0$ and the sequence $t_k$ is determined by the equations $\int_0^1 u(x,t_k)dx = M$, for $k = 1,3,5,\ldots$, and $\int_0^1 u(x,t_k)dx = m$, for $k = 2,4,6,\ldots$ and where $0 < m < M < u_0$. Note that the switching times $t_k$ are unknowns. Determination of switching times $t_k$ and their differences $t_{k+1} - t_k$ are obtained. Numerical verifying examples are presented.

1. Introduction

As motivation for the mathematical problems considered in this work, consider a chamber in the form of a long linear transparent tube. We allow for the introduction or removal of material in a gaseous state at the ends of the tube. The material diffuses throughout the tube with or without reaction with other materials. By illuminating the tube on one side with a light source with a frequency range spanning the absorption range for the material and collecting the residual light that passes through the tube with photo-reception equipment, we can obtain a measurement of the total mass of material contained in the tube as a function of time. Using the total mass as switch points for changing the boundary conditions for introduction or removal of material. The objective is to keep the total mass of material in the tube oscillating between two set values such as $m < M$. The physical application for such a system is the control of reaction diffusion systems such as production of a chemical material in a reaction chamber via the introduction of reactants at the boundary of chamber.

Date: July 8, 2020.

Key words and phrases. Diffusion Problem, Neumann Boundary Conditions, Total Mass Control, Finite Difference.
2. Definition of the Problem

We consider the diffusion problem

\[
\begin{align*}
    u_t &= u_{xx}, & t > 0, & 0 < x < 1, \\
    u(x, 0) &= 0, & 0 < x < 1, \\
    u_x(0, t) &= -\phi(t), & t > 0, \\
    u_x(1, t) &= \phi(t), & t > 0.
\end{align*}
\]  

(2.1)

where the flux \(\phi(t)\) is set in such a way to control the level of the total mass \(\mu(t) = \int_0^1 u(x, t)dx\). Namely,

\[
\phi(t) = \begin{cases} 
1 & \text{if } t_{2n} < t < t_{2n+1} \\
-1 & \text{if } t_{2n+1} < t < t_{2n+2}
\end{cases}
\]

where the sequence

\[
0 = t_0 < t_1 < t_2 < \ldots,
\]

satisfies

\[
\begin{align*}
    \mu(t_{2n}) &= m, & n = 1, 2, 3, \ldots \\
    \mu(t_{2n+1}) &= M, & n = 0, 1, 2, \ldots
\end{align*}
\]

with \(m\) and \(M\) are certain positive threshold to ensure \(m < \mu < M\).

The total mass has a time derivative equal to

\[
\mu'(t) = \int_0^1 u_t(x, t)dx
\]

(2.2)

\[
= \int_0^1 u_{xx}(x, t)dx \\
= u_x(1, t) - u_x(0, t) \\
= 2\phi(t).
\]

where we use the fact that \(u(x, t)\) satisfies (2.1). This relationship will allow us to explicitly find the time switches \(t_n\).

Since the flux \(\phi(t)\) is initially set at 1, and \(\mu(0) = 0\) due to the initial condition on \(u\), then

\[
\mu(t) = 2t, \quad 0 \leq t \leq t_1.
\]

where \(t_1\) can be calculated as a solution of \(\mu(t_1) = M\), which implies \(t_1 = M/2\).

At the second time interval \(t_1 < t < t_2\), the flux is reversed, that is \(\phi(t) = -1\), therefore the total mass will be

\[
\mu(t) = -2t + M + 2t_1, \quad t_1 \leq t \leq t_2,
\]
where due to the continuity of $\mu(t)$ at $t_1$, The second time switch $t_2$ will be calculated as a solution of $\mu(t_2) = m$, this gives

$$t_2 = t_1 + \left(\frac{M}{2} - \frac{m}{2}\right) = M - \frac{m}{2},$$

Now, if we bring the flux back to $\phi(t) = 1$, where $t_2 \leq t \leq t_3$, we will find

$$\mu(t) = 2t + m - 2t_2, \quad t_2 \leq t \leq t_3,$$

Setting $\mu(t_3) = M$ yields

$$t_3 = t_2 + \left(\frac{M}{2} - \frac{m}{2}\right) = \frac{3M}{2} - m,$$

Following the same pattern, we will successively get

$$\mu(t) = -2t + M + 2t_3, \quad t_3 \leq t \leq t_4,$$

$$t_4 = t_3 + \left(\frac{M}{2} - \frac{m}{2}\right) = 2M - \frac{3m}{2},$$

$$\mu(t) = 2t + m - 2t_4, \quad t_4 \leq t \leq t_5,$$

$$t_5 = t_4 + \left(\frac{M}{2} - \frac{m}{2}\right) = \frac{5M}{2} - 2m,$$

$$\vdots$$

$$\mu(t) = \begin{cases} 
2t + m - 2t_{2n} \quad & \text{if } t_{2n} < t < t_{2n+1} \\
-2t + M + 2t_{2n+1} \quad & \text{if } t_{2n+1} < t < t_{2n+2}
\end{cases},$$

$$t_n = t_{n-1} + \left(\frac{M}{2} - \frac{m}{2}\right) = \frac{nM}{2} - \frac{(n-1)m}{2},$$

where $n \geq 1$. We infer from these calculations that the time switches $t_n$ are equispaced with $t_n - t_{n-1} = 0.5M - 0.5m$. 
3. Finite difference analysis

We study a finite difference discretization for the control problem (2.1). We consider the implicit backward scheme

\[
\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2}, \quad j = 1, \ldots, J-1, \quad n = 0, 1, 2, \ldots
\]

\[
U_j^0 = 0, \quad j = 0, \ldots, J
\]

\[
\frac{U_1^{n+1} - U_0^{n+1}}{\Delta x} = -\phi(\tau_{n+1}), \quad n = 0, 1, 2, \ldots
\]

\[
\frac{U_J^{n+1} - U_{J-1}^{n+1}}{\Delta x} = \phi(\tau_{n+1}), \quad n = 0, 1, 2, \ldots
\]

where \(\tau_n\) is not necessarily a uniform grid. The total mass can be computed by the following Riemann type sum

\[
\mu_n = \Delta x \sum_{j=1}^{J-1} U_j^n
\]

A discrete version of (2.2) may look like

\[
\frac{\mu_{n+1} - \mu_n}{\Delta t} = \Delta x \sum_{j=1}^{J-1} \frac{U_j^{n+1} - U_j^n}{\Delta t},
\]

\[
= \Delta x \sum_{j=1}^{J-1} \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2},
\]

\[
= \frac{U_{j-1}^{n+1} - U_j^{n+1}}{\Delta x} - \frac{U_j^{n+1} - U_{j+1}^{n+1}}{\Delta x},
\]

\[
= 2\phi(\tau_{n+1}).
\]

Next we shall explicitly find \(\mu_n\) and the time switches \(t_n\) with some restriction on the mesh size. In the first subinterval \(0 < \tau_n < t_1\), we choose \(\Delta t = \Delta t_0 = \frac{M}{2N_0}\), where \(N_0\) is a positive integer, along with the flux \(\phi(\tau_n) = 1\). We obtain

\[
\mu_n = 2n\Delta t_0 = 2\tau_n, \quad 0 \leq \tau_n \leq t_1
\]

This special choice for \(\Delta t_0\) leads to

\[
\mu_{N_0} = M
\]

i.e. \(N_0\) specifies the first time switch

\[
t_1 = \tau_{N_0} = \frac{M}{2}
\]
which coincides with the one computed analytically. Next, we reverse
the flux, i.e. \( \phi(\tau_n) = -1 \), for \( n > N_0 \), and define \( \Delta t = \frac{M - m}{2N} \), for
some positive integer \( N \). Then in view of (3.1), we obtain
\[
\mu_n = M - 2(n - N_0)\Delta t, \quad n \geq N_0.
\]
Notice that in the second stage, the time mesh size is not necessarily
equal to the one at the first stage. With a carefully chosen \( \Delta t \), we can
easily get
\[
\mu_{N_0+N} = m
\]
with the second time switch equal to
\[
t_2 = N_0\Delta t_0 + N\Delta t = t_1 + \left( \frac{M}{2} - \frac{N}{2} \right).
\]
This result is in agreement with the one computed analytically.

For the next upcoming stages, we keep the time mesh size as \( \Delta t = \frac{M - m}{2N} \). The following are the total mass and the time switches for the
third and the forth stages respectively
\[
\mu_n = m + 2(n - N_0 - N)\Delta t, \quad n \geq N_0 + N,
\]
\[
t_3 = N_0\Delta t_0 + 2N\Delta t = t_2 + \left( \frac{M}{2} - \frac{N}{2} \right),
\]
\[
\mu_n = M - 2(n - N_0 - 2N)\Delta t, \quad n \geq N_0 + 2N,
\]
\[
t_4 = N_0\Delta t_0 + 3N\Delta t = t_3 + \left( \frac{M}{2} - \frac{N}{2} \right),
\]
This inductively gives
\[
\mu_n = \begin{cases} 
M - 2(n - N_0 - kN)\Delta t, & \text{if } N_0 + kN \leq n \leq N_0 + (k + 1)N, \quad k \text{ is even} \\
m + 2(n - N_0 - kN)\Delta t, & \text{if } N_0 + kN \leq n \leq N_0 + (k + 1)N, \quad k \text{ is odd}
\end{cases}
\]
\[
t_k = N_0\Delta t_0 + (k - 1)N\Delta t = t_{k-1} + \left( \frac{M}{2} - \frac{N}{2} \right),
\]
The above calculations shows that if the time grid is chosen properly, the time switches computed by the above difference scheme coincides with those computed analytically.

**Remark:** The situation when the $\tau_n$ is equispaced does not, in general, generate the exact time switches $t_n$. However, if we take the switching criteria as, $\mu_n \geq M$, and $\mu_n \leq m$ instead of $\mu_n = M$ and $\mu_n = m$, respectively, where $n$ is the least integer that satisfies such inequalities, we obtain a new set of switching points, say $T_n$, with the errors

\[
0 \leq T_1 - t_1 < \Delta t, \\
0 \leq T_2 - t_2 < 2\Delta t, \\
0 \leq T_3 - t_3 < 3\Delta t, \\
\vdots \\
0 \leq T_k - t_k < k\Delta t.
\]

If the maximum time limit $T$ is specified, with $\Delta t = T/N$, for some integer $N$, then for a fixed integer $k$, we will have $T_k - t_k < k\Delta t = kT/N$ convergent to 0 as $N \to \infty$.

**4. Numerical Example**

In this section, we consider a finite difference method to discretize the problem

\[
\begin{align*}
  u_t &= \alpha u_{xx}, \quad 0 < x < 1, \quad 0 < t \leq T \\
  -u_x(0, t) &= u_x(1, t) = \phi(t), \quad 0 < t \leq T \\
  u(x, 0) &= 0, \quad 0 < x < 1
\end{align*}
\]

where the boundary control function is

\[
\phi(t) = \begin{cases} 
  1, & t_{2n} \leq t \leq t_{2n+1} \\
  -1, & \text{elsewhere}
\end{cases}
\]

and \{t_n\} depends on

\[
\mu(t) = \int_0^1 u(x, t)dx
\]

where

\[
\begin{align*}
  \mu(t_{2n}) &= 0.1, \quad n = 1, 2, \ldots \\
  \mu(t_{2n+1}) &= 0.2, \quad n = 0, 1, \ldots.
\end{align*}
\]

The time limit and the diffusivity constant are taken as $T = 10$ and $\alpha = 0.05$.

Let’s consider the space and time discretization
i) \( \Delta x = \frac{1}{j}, \quad x_j = j\Delta x, \quad j = 0, 1, \ldots, J \)

ii) \( \Delta t = \frac{T}{N}, \quad \tau_n = n\Delta t, \quad n = 0, \ldots, N \)

where \( J = 50 \) and \( N = 200 \). The integer \( N \) is chosen large enough so that the time step \( \Delta t \) is much smaller than an estimated differences between two consecutive values of the time switches.

We consider the backward implicit finite difference scheme

\[
\frac{U_j^{n+1} - U_j^n}{\Delta t} = \alpha \frac{U_{j-1}^{n+1} - 2U_j^{n+1} + U_{j+1}^{n+1}}{(\Delta x)^2}
\]

which can be written as

\[
-\nu U_{j-1}^{n+1} + (1 + 2\nu)U_j^{n+1} - \nu U_{j+1}^{n+1} = U_j^n
\]

where \( \nu = \frac{\alpha \Delta t}{(\Delta x)^2} \), \( j = 1, \ldots, J - 1 \) and \( n = 0, 1, \ldots, N - 1 \). The initial condition is \( U_j^0 = 0 \) for \( j = 1, \ldots, J - 1 \), and the boundary conditions are

\[
-\frac{U_1^n - U_0^n}{\Delta x} = \frac{U_J^n - U_{J-1}^n}{\Delta x} = \phi(\tau_n)
\]

for \( n = 0, 1, \ldots, N \). The total mass integral is calculated by the following trapezoidal rule

\[
\mu_n = \frac{h}{2} \sum_{j=0}^{N-1} \left( U_j^{n+1} + U_j^n \right).
\]

The numerical experiment is carried out in the following way. We start by setting the flux at \( \phi = 1 \) then we solve a tridiagonal system coming out of the difference method. We evaluate the total mass \( \mu_n \) and compare it with the upper threshold \( M = 0.2 \). We move to the next time step while keeping the flux at \( \phi = 1 \), as long as \( \mu_n < M \), otherwise, we switch the flux to \( \phi = -1 \), as long as \( \mu_n \geq M \). At the moment, say \( \tau_{n_1} \), for some integer \( n_1 \), when the total mass exceeds \( M \) for the first time, we take \( T_1 = \tau_{n_1} \) as an approximation for the first time switch. With \( \phi = 0 \), we proceed our solution along the time, as long as \( \mu_n \) does not fall below the threshold \( m = 0.1 \). By the moment, when \( \mu_{n_2} \leq m \), for some integer \( n_2 \), we set \( T_2 = \tau_{n_2} \), and we switch the flux back to \( \phi = 1 \) at the next step. We keep switching the flux between \( (\phi = 1) \) and \( (\phi = -1) \) and calculating the time switches \( T_k \) until the end of the run when \( \tau_n = 10 \).

Table (1) shows the times switches \( T_n \). As we can see there, the difference between any two consecutive time switches tend to 0.95. For the same set of data, graphs (1) through (4) show the concentration versus the space at consecutive time steps. The graphs are obtained for different stages, where at each stage the flux is kept constant at the
Table 1. The Time switches $T_n$ and the differences $T_n - T_{n-1}$. Note the differences between any two consecutive times tends to 0.95.

| n | $T_n$ | $T_n - T_{n-1}$ |
|---|---|---|
| 1 | 1.9500 | 1.9000 |
| 2 | 2.9000 | 0.9500 |
| 3 | 3.8500 | 0.9500 |
| 4 | 4.8000 | 0.9500 |
| 5 | 5.7500 | 0.9500 |
| 6 | 6.7000 | 0.9500 |
| 7 | 7.6500 | 0.9500 |
| 8 | 8.6000 | 0.9500 |
| 9 | 9.5500 | 0.9500 |

end points. A profile of the concentrations at $x = 0.5$ for various times is shown in graph (5) with the same specified data. Graph (6) shows the total mass computed analytically and numerically.

References

[1] J. R. Cannon, The one-dimensional heat equation, *Encyclopedia of Mathematics and its Applications* 23 (1984).

[2] J. R. Cannon, Yapping Lin and Shuzhan Xu, Numerical procedures for the determination of an unknown coefficient in semi-linear parabolic differential equation. *Inverse Problems* 10 (1994), 227-243.

[3] J.R. Cannon and J. Van der Hoek, The existence and a continuous dependance result for the solution of the heat equation subject to the specification of energy. *Boll. Uni. Math. Ital. Suppl.* bf 1(1981), 253-282.

[4] J.R. Cannon and J. Van der Hoek, An implicit finite difference scheme for the diffusion of mass in a portion of a domain. *Numerical Solutions of Partial Differential Equations.* (J. Noye, ed), 527-539, *North-Holland, Amsterdam*, 1982.

[5] J.R. Cannon and J. Van der Hoek, Diffusion subject to a specification of mass. *J. Math. Anal. Appl.* 115 (1986), No.2, 517-529.

[6] J.R. Cannon & M. Salman, The Utilization of Total Mass to Determine the Switching Points in the Symmetric Boundary Control Problem with a Linear Reaction Term. *Journal of Mathematical Analysis and Applications* 311 (2005), No. 1, 147–161.

[7] J.R. Cannon & M. Salman, A Boundary Control Problem with a Nonlinear Reaction Term. *Electron. J. Diff. Eqns.*, Conf 17 (2009), pp. 39-49.

[8] W. A. Day, Existence of a property of solutions of the heat equation to linear thermoelasticity and other theories. *Quart. Appl. Math.*, 40, (1982) 319-330.

[9] W. A. Day, A decreasing property of solutions of a parabolic equation with applications to thermoelasticity. *Quart. Appl. Math.*, 41, (1983) 468-4475.
[10] J. Kevorkian, Partial differential equations, analytical solution techniques. 2nd edition. *Texts in Applied Mathematics* 35 (2000).

[11] Pao, C. V. Blowing-up of solution for a nonlocal reaction-diffusion problem in combustion theory. *J. Math. Anal. Appl.* 166 (1992), no. 2, 591-600.

[12] Pao, C. V. Dynamics of reaction-diffusion equations with nonlocal boundary conditions. *Quart. Appl. Math.* 53 (1995), no. 1, 173-186.

[13] Pao, C. V. Reaction diffusion equations with nonlocal boundary and nonlocal initial conditions. *J. Math. Anal. Appl.* 195 (1995), no. 3, 702-718.

[14] Pao, C. V. Dynamics of weakly coupled parabolic systems with nonlocal boundary conditions. *Advances in nonlinear dynamics*, 319-327, Stability Control Theory Methods Appl., 5, *Gordon and Breach, Amsterdam*, 1997.

[15] Pao, C. V. Asymptotic behavior of solutions of reaction-diffusion equations with nonlocal boundary conditions. Positive solutions of nonlinear problems. *J. Comput. Appl. Math.* 88 (1998), no. 1, 225-238.

[16] Pao, C. V. Numerical solutions of reaction-diffusion equations with nonlocal boundary conditions. *J. Comput. Appl. Math.* 136 (2001), no. 1-2, 227-243.

[17] Protter, Murray H.; Weinberger, Hans F. Maximum principles in differential equations. *Prentice-Hall, Inc., Englewood Cliffs, N.J.* 1967 x+261 pp.

[18] M. Salman, The utilization of total mass to determine the switching points in the symmetric boundary control of a diffusion problem. (Manuscript)

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Figure 1. The first stage where the flux $\phi$ is held at 1 at the end points. Each curve shows the concentration profile at various discrete time steps $\tau_n = n\Delta t$. As the time goes on, the level of concentrations gets higher.
Figure 2. The second stage where the flux $\phi$ is held at -1 at the end points. As the time goes on, the level of concentrations decreases. Notice the fluctuations when the concentration is dropped suddenly to 0 at the beginning of the stage.
Figure 3. The third stage where the flux $\phi$ is switched to 1 at the end points. Each curve shows the concentration profile at various discrete time steps. Notice the fluctuations due to the sudden change on the concentrations. After a little while, the concentrations levels increase monotonically.
Figure 4. The fourth stage where the flux $\phi$ is switched to -1 at the end points. Notice the similarity with the second stage.
Figure 5. The concentration profile $U$ at $x = 0.5$ versus the time shows periodic behavior due to the periodic change of the boundary conditions.
Figure 6. The total mass computed analytically and numerically. Note how the error in calculating the time switches accumulates as the time gets large.